

Transport theory / James J. Duderstadt, William R. Martin.

Duderstadt, James J., 1942-

New York : Wiley, c1979.

<http://hdl.handle.net/2027/mdp.39015040316401>

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□ Transport Theory □

JAMES J. DUDERSTADT

WILLIAM R. MARTIN

**Department of Nuclear Engineering
The University of Michigan, Ann Arbor**

A WILEY-INTERSCIENCE PUBLICATION

JOHN WILEY & SONS, New York • Chichester • Brisbane • London

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Library of Congress Cataloging in Publication Data:

Duderstadt, James J 1942–

Transport Theory

“A Wiley-Interscience publication.”

Includes index.

1. Transport Theory. I. Martin, William Russell,
1945- joint author. II. Title.

QC175.2.D83 530.1'3 78-13672

ISBN 0-471-04492-X

Printed in the United States of America

10 9 8 7 6 5 4 3 2 1

61-1113

To

SUSAN, KATHY, and AMY

□ Preface □

The mathematical description of the transport of microscopic particles such as neutrons, photons, electrons, and molecules through matter is commonly called transport theory. These processes are important in a wide variety of physical phenomena, and a thorough understanding of particle transport is frequently necessary in science and engineering. This book presents a general theory of particle transport processes. In particular, we have drawn together and presented in a unified manner the array of methods used to analyze transport phenomena in many fields ranging from nuclear reactor physics and astrophysics to gas and plasma dynamics to statistical mechanics.

This material has been developed over the past decade in a graduate level course on transport theory at the University of Michigan. The course was taught to students from disciplines including physics and chemistry; nuclear, mechanical, electrical, and aerospace engineering; and applied mathematics. The interests and demands presented by such a varied audience quickly made it apparent how similar the applications of transport theory are from field to field and how useful a unified treatment of the subject might prove to be.

The treatment of transport theory presented here assumes a background level of mathematics typical of most graduate students in the physical sciences or engineering (some rudimentary knowledge of boundary value problems, integral transforms, complex variable theory, and numerical analysis). More specialized mathematical topics such as integral equations, the spectral theory of operators, and generalized functions are developed in a self-contained fashion as needed.

Although this book is intended to survey the methods used in analyzing particle transport processes in a wide variety of fields, the overwhelming breadth of applications makes it almost impossible to furnish a comprehensive bibliography. Fortunately a number of excellent review articles that have appeared in the technical literature summarize many of these applications and contain comprehensive reference compilations. These articles are referenced quite frequently throughout.

Certainly very little of the material presented in such a broad treatment can claim originality, and our effort has benefited enormously from the knowledge, experience, and endurance of a great number of former students, teachers, and colleagues. But a particular acknowledgment and note of gratitude must be expressed to Noel Corngold of Caltech who provided the first author with most of his understanding of the physics of transport theory, to Anthony Leonard of NASA-Ames who supplied a comparable understanding of the mathematics used to analyze transport problems, and

to colleagues at Michigan including Ziya Akcasu and Richard Osborn, who have refined rather considerably our understanding of the statistical mechanics foundation of the subject. This work also clearly displays the influence of a number of other scientists whose contributions to the modern theory of particle transport processes have been most profound: Ivan Kuščer, K. M. Case, Paul F. Zweifel, M. M. R. Williams, Carlo Cercignani, Kaye D. Lathrop, Sidney Yip, Robert Zwanzig, and Hazime Mori. Without the inspiration and insight provided by the work of these individuals, such an undertaking would have been quite impossible.

JAMES J. DUDERSTADT
WILLIAM R. MARTIN

Ann Arbor, Michigan
November 1978

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Transport Equations

The term “transport theory” is commonly used to refer to the mathematical description of the transport of particles through a host medium. For example, such a theory might be used to describe the diffusion of neutrons through the uranium fuel elements of a nuclear reactor, or the diffusion of light photons through the atmosphere, or perhaps the motion of gas molecules as they stream about, colliding with one another. (Note that in the last example, one cannot really distinguish the “transported” particles from the “host medium.”) Transport theory has become an extremely important topic in physics and engineering, since particle transport processes arise in a wide variety of physical phenomena. Much of the early development of this theory was stimulated by astrophysical studies of radiant energy transfer in stellar or planetary atmospheres.^{1,2} More recently, the subject of transport theory has been refined to a very high degree for the description of neutron and gamma transport in nuclear systems.³⁻⁶ The mathematical tools used to analyze transport processes also have been applied with some success to problems in rarefied gas dynamics and plasma physics.⁷⁻¹² And the list of such applications continues to expand rapidly (as the examples listed in Table 1.1 and Figure 1.1 make apparent).

The transport processes we wish to study can involve a variety of different types of particles such as neutrons, gas molecules, ions, electrons, quanta (photons, phonons), or waves (provided the wavelength is much less than a mean free path), moving through various background media such as the components of a nuclear reactor core, stellar or planetary atmospheres, gases, or plasmas. Transport phenomena range from random walk processes, in which particles stream freely between random interaction events, to highly ordered collective phenomena, in which large numbers of particles interact in a correlated fashion to give rise to wave motion. And yet all these processes can be described by a single unifying theory—indeed, all are governed by the same type of equation. Hence the mathematical tools needed to study these processes are quite similar, although the information desired and the physical interpretation of the solutions differ quite markedly from field to field.

We are concerned with the mathematical description of the transport of particles in matter. Transport theory differs from the usual approaches encountered in classical physics because it is a particle, not a continuum

Table 1.1 □ Applications of Transport Theory

Nuclear reactors
Determination of neutron distributions in reactor cores
Shielding against intense neutron and gamma radiation
Astrophysics
Diffusion of light through stellar atmospheres (radiative transfer)
Penetration of light through planetary atmospheres
Rarefied gas dynamics
Upper atmosphere physics
Sound propagation
Diffusion of molecules in gases
Charged particle transport
Multiple scattering of electrons
Gas discharge physics
Diffusion of holes and electrons in semiconductors
Development of cosmic ray showers
Transport of electromagnetic radiation
Multiple scattering of radar waves in a turbulent atmosphere
Penetration of X-rays through matter
Plasma physics
Microscopic plasma dynamics, microinstabilities
Plasma kinetic theory
Other
Traffic flow (transport of vehicles along highways)
Molecular orientations of macromolecules
The random walk of undergraduates during registration

theory of matter as, for instance, electromagnetism or fluid dynamics. The concept of a continuous field still plays a significant role in transport studies, but it now appears as a probability field, much as one encounters in quantum mechanics.

To be more specific, the usual macroscopic fields encountered in physics involve continuum descriptions. For example, in electromagnetic theory one introduces the electric and magnetic fields $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$ and the charge and current densities $\rho(\mathbf{r}, t)$ and $\mathbf{j}(\mathbf{r}, t)$. In hydrodynamics the field variables are the mass density $\rho(\mathbf{r}, t)$, local flow velocity $\mathbf{u}(\mathbf{r}, t)$, and local temperature $T(\mathbf{r}, t)$. However in the study of particle transport, the random nature of particle interaction events obliges us to introduce instead a field of probability densities or distribution functions. That is, we cannot predict with certainty the exact number of particles in a certain region at a

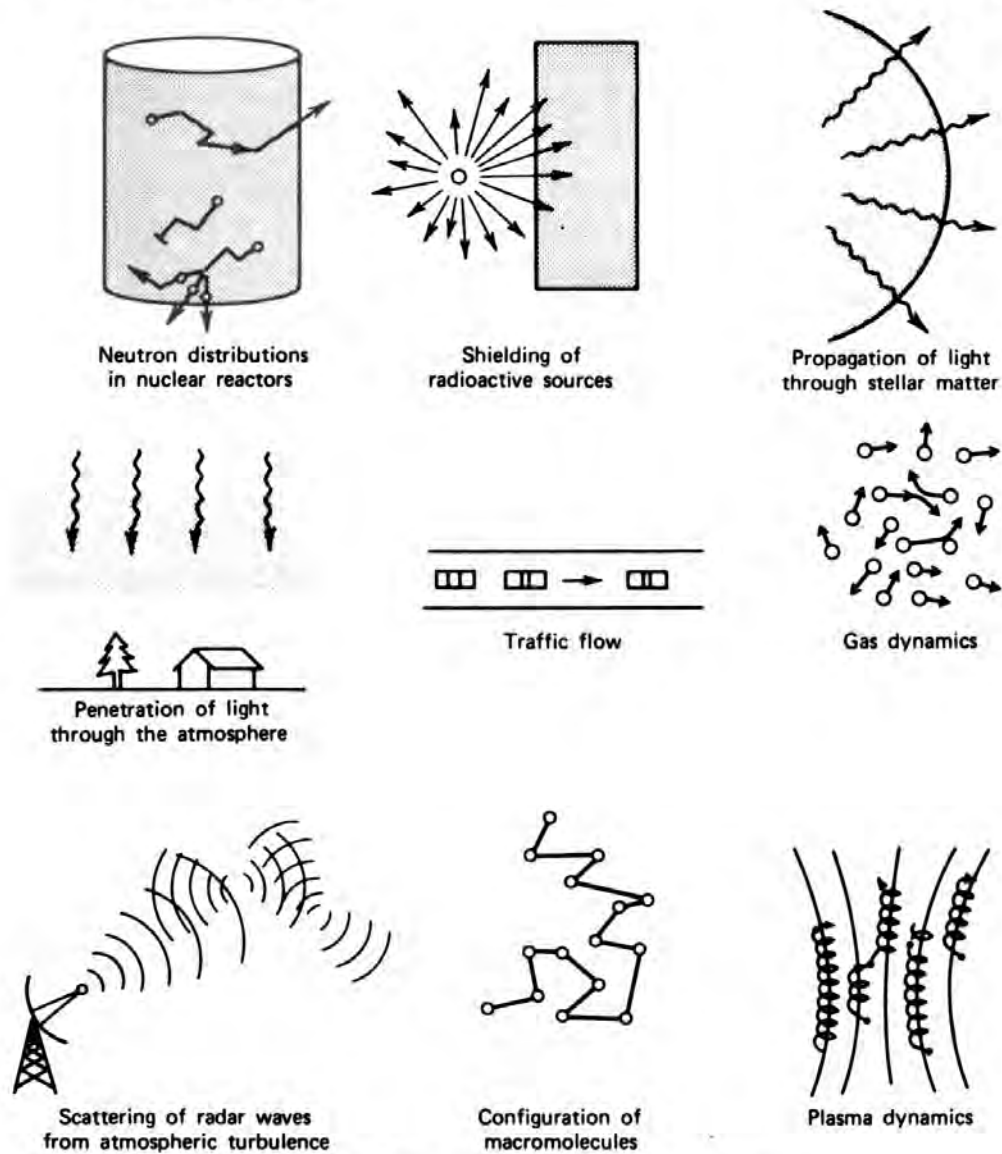


Fig. 1.1 □ Examples of transport processes.

given time, but only the expected particle density $N(\mathbf{r}, t)$ defined by

$$N(\mathbf{r}, t)d^3r = \text{expected number of particles in } d^3r \text{ about } \mathbf{r} \text{ at time } t$$

This density would then be described by an appropriate partial differential

equation such as the diffusion equation:

$$\frac{\partial N}{\partial t} - \nabla \cdot D \nabla N(\mathbf{r}, t) = S(\mathbf{r}, t)$$

It is important to stress here that $N(\mathbf{r}, t)$ characterizes only the expected or average particle density at $\mathbf{r}$ and t . Our mathematical description of particle transport processes involves such a statistical approach. We return to consider this feature and provide a more precise definition of this statistical average in the last section of this chapter.

One can distinguish between two classes of problems that arise in transport theory. First are the *direct problems* in which one is given the composition and geometry of the host medium and the location and magnitude of any sources of particles and asked to determine the distribution of particles in the medium. This is the most common class of transport problems. It arises in a host of applications, including nuclear reactor theory, radiation transport, plasma physics, and gas dynamics. The second and far more difficult class involves *inverse problems* in which one is given the distribution and asked to determine characteristics of the medium through which the particles have propagated or the sources that have generated the particles. Such problems are encountered in fields such as astrophysics in which one measures the intensity and spectral distribution of light in order to infer properties of stars, and in nuclear medicine where radioisotopes are injected into patients, and the radiation emitted by such sources is used in diagnosis—for example, to determine whether a tumor is present.

Although transport theory arises in a wide variety of disciplines, within each field it has become a very specialized subject, almost an art, dealing with the solution of a very particular type of equation. Furthermore, most of the applications of transport theory have developed almost totally independent of one another. For example, the essential physics of transport processes was already highly developed in the kinetic theory of gases developed by Boltzmann more than a century ago. The mathematical methods used to solve transport equations were developed to analyze problems in radiative transfer during the 1930s. Despite this heritage, the field of neutron transport theory has developed almost independently of kinetic theory or radiative transfer, partly because of the highly specialized nature of neutron transport problems in nuclear systems, but also partly because of the enormous emphasis placed on this discipline in the atomic energy program. Particular emphasis was directed toward the development of accurate computational (computer-based) methods, most of which are quite unfamiliar to physicists in other fields.

Hence there is a very strong incentive to unify the various approaches used to analyze and solve transport problems in different fields. The task of drawing together these applications and presenting a general, unified theory of particle transport processes is one of the primary motivations for writing this book.

1.1 □ PARTICLE DISTRIBUTION FUNCTIONS □ The ultimate goal of transport theory is to determine the distribution of particles in a medium, taking account of the motion of the particles and their interactions with the host medium. Although knowledge of the particle density $N(\mathbf{r}, t)$ would be sufficient for most applications, unfortunately there is no equation that adequately describes this quantity in most physical situations. Therefore we must generalize the concept of the particle density somewhat to account for more of the independent variables that characterize particle motion.

The state of a classical point particle can be characterized by specifying the particle position $\mathbf{r}$ and velocity $\mathbf{v}$. This level of description is usually sufficient for describing the transport of more complicated particles (neutrons, photons, molecules, automobiles), since internal variables such as spin, polarization, or structure usually do not influence the motion of the particles as they stream freely between interactions—although such internal variables certainly influence the interactions between the particles and the host medium. (Exceptions to this include the transport of polarized light through an atmosphere¹³ and the transport of a polarized neutron beam through a magnetic field.¹⁴ We indicate later how the theory can be generalized to account for spin or polarization effects.) Therefore it suffices to define a particle *phase space density* function $n(\mathbf{r}, \mathbf{v}, t)$ that depends only on the particle position and velocity:

$$n(\mathbf{r}, \mathbf{v}, t) d^3r d^3v = \text{expected number of particles in } d^3r \text{ about } \mathbf{r} \text{ with velocity in } d^3v \text{ about } \mathbf{v} \text{ at time } t$$

This function contains all the information that is usually required for the description of transport processes. For example, we can integrate $n(\mathbf{r}, \mathbf{v}, t)$ over velocity to obtain the particle density

$$N(\mathbf{r}, t) = \int d^3v n(\mathbf{r}, \mathbf{v}, t)$$

In certain special cases $n(\mathbf{r}, \mathbf{v}, t)$ may be rather easy to calculate. For example, if the particles are in thermal equilibrium at a temperature T ,

then $n(\mathbf{r}, \mathbf{v}, t)$ becomes just the familiar Maxwell-Boltzmann distribution function

$$n(\mathbf{r}, \mathbf{v}, t) \rightarrow n_0 M(\mathbf{v}) = n_0 \left(\frac{m}{2\pi kT} \right)^{3/2} \exp \left(\frac{-mv^2}{2kT} \right)$$

where n_0 is the average number density of the particles. More generally we are faced with solving a special type of equation for $n(\mathbf{r}, \mathbf{v}, t)$ known as a “transport” or “kinetic” equation. However it is usually possible to derive such an equation to describe $n(\mathbf{r}, \mathbf{v}, t)$ to a rather high degree of accuracy.

In kinetic theory⁹ it is common to normalize $n(\mathbf{r}, \mathbf{v}, t)$ by dividing through by the particle density $N(\mathbf{r}, t)$

$$f(\mathbf{r}, \mathbf{v}, t) = \frac{n(\mathbf{r}, \mathbf{v}, t)}{N(\mathbf{r}, t)}$$

This terminology is useful because $f(\mathbf{r}, \mathbf{v}, t)$ can then be identified as a probability distribution or density function with a unit normalization:

$$\int d^3v f(\mathbf{r}, \mathbf{v}, t) = 1$$

Both $n(\mathbf{r}, \mathbf{v}, t)$ and $f(\mathbf{r}, \mathbf{v}, t)$ contain information only about the expected number of particles in a differential volume element of phase space, $d^3r d^3v$. Neither function provides any information about higher order statistical correlations such as the “doublet” distribution $f(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_2, \mathbf{v}_2; t)$ characterizing the probability that two particles will be found simultaneously with coordinates in $d^3r_1 d^3v_1 d^3r_2 d^3v_2$. Actually there is little interest in such higher order correlations or fluctuations from $n(\mathbf{r}, \mathbf{v}, t)$ for random walk processes in which the particles of interest do not interact and therefore can be correlated only by special types of source conditions (e.g., the simultaneous emission of two or more neutrons in a fission reaction⁶). However such higher order phase space densities or distribution functions are of major interest in collective processes that are dominated by interactions (hence correlations) among particles.

It is sometimes convenient to decompose the particle velocity vector $\mathbf{v}$ into two components, one variable characterizing the particle speed, and a second corresponding to the direction of motion. The particle kinetic energy, $E = \frac{1}{2} mv^2$ is used frequently instead of the speed v . To specify the direction of particle motion, we introduce a unit vector $\hat{\Omega}$ in the direction of the velocity vector $\mathbf{v}$ (see Figure 1.2)

$$\hat{\Omega} = \frac{\mathbf{v}}{|\mathbf{v}|} = \hat{\mathbf{e}}_x \sin \theta \cos \phi + \hat{\mathbf{e}}_y \sin \theta \sin \phi + \hat{\mathbf{e}}_z \cos \theta$$

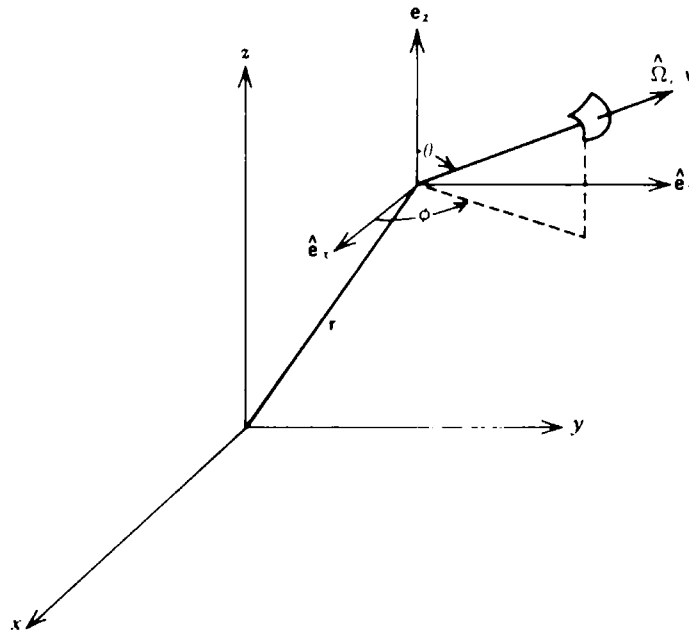


Fig. 1.2 □ The position and direction variables characterizing the state of a particle.

where we have chosen to represent this direction unit vector in spherical velocity-space coordinates (θ, ϕ) . The particle phase space density can then be defined in terms of these new variables as

$$n(\mathbf{r}, E, \hat{\Omega}, t) d^3r dE d\hat{\Omega} = \text{expected number of particles in } d^3r \text{ about } \mathbf{r} \text{ with kinetic energy } E \text{ in } dE \text{ moving in direction } \hat{\Omega} \text{ in solid angle } d\hat{\Omega}$$

Integration over these velocity space variables would then take the form

$$\begin{aligned} \int d^3v n(\mathbf{r}, \mathbf{v}, t) &= \int_0^\infty dv v^2 \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin\theta n(\mathbf{r}, v, \hat{\Omega}, t) \\ &= \int_0^\infty dE \int d\hat{\Omega} n(\mathbf{r}, E, \hat{\Omega}, t) \end{aligned}$$

where we have identified the differential solid angle $d\hat{\Omega} = \sin\theta d\theta d\phi$. One can easily transform back and forth between various sets of variables by

noting:

$$n(\mathbf{r}, E, \hat{\Omega}, t) = \left(\frac{v}{m} \right) n(\mathbf{r}, \mathbf{v}, t)$$

$$n(\mathbf{r}, v, \hat{\Omega}, t) = v^2 n(\mathbf{r}, \mathbf{v}, t)$$

$$n(\mathbf{r}, E, \hat{\Omega}, t) = \left(\frac{1}{mv} \right) n(\mathbf{r}, v, \hat{\Omega}, t)$$

where $E = \frac{1}{2} mv^2$ and $\hat{\Omega} = \mathbf{v}/|\mathbf{v}|$.

When the particle phase space density is written in terms of the variables $(\mathbf{r}, E, \hat{\Omega}, t)$, it is sometimes referred to as the *angular* density (since it depends on the angles θ and ϕ characterizing the direction of particle motion) to distinguish it from the *total* particle density $N(\mathbf{r}, t)$.

A closely related concept is the *phase space current density* function or *angular current density* $\mathbf{j}(\mathbf{r}, \mathbf{v}, t)$, which is defined by

$$\mathbf{j}(\mathbf{r}, \mathbf{v}, t) \cdot d\mathbf{S} d^3v = \mathbf{v} n(\mathbf{r}, \mathbf{v}, t) \cdot d\mathbf{S} d^3v = \text{expected number of particles that cross an area } d\mathbf{S} \text{ per second with velocity } \mathbf{v} \text{ in } d^3v \text{ at time } t \text{ (see Figure 1.3)}$$

If this quantity is integrated over particle velocities, one arrives at a definition of the particle *current density* $\mathbf{J}(\mathbf{r}, t)$

$$\mathbf{J}(\mathbf{r}, t) = \int d^3v \mathbf{j}(\mathbf{r}, \mathbf{v}, t)$$

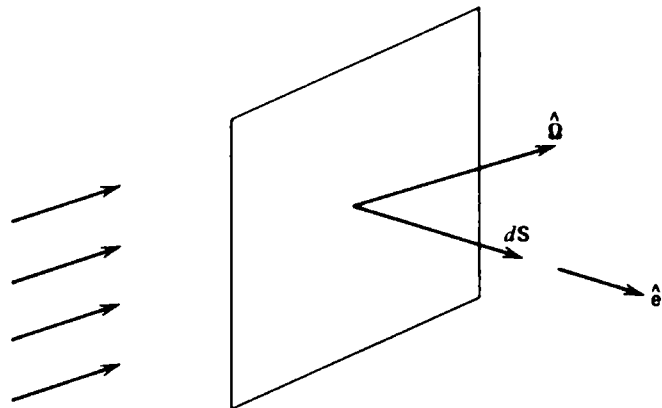


Fig. 1.3 □ Particles incident on a surface element $d\mathbf{S}$.

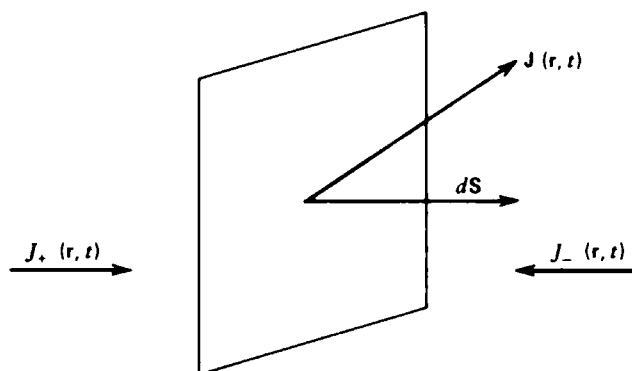


Fig. 1.4 □ Partial and total current densities.

Here, of course, $\mathbf{J}(\mathbf{r}, t) \cdot d\mathbf{S}$ would be interpreted as the rate at which particles pass through a differential surface area dS .

A similar concept is the *partial current density* $J_{\pm}(\mathbf{r}, t)$, which characterizes the rate at which particles flow through an area in a given direction. That is, we define

$$J_{\pm}(\mathbf{r}, t) = \pm \int_{\pm} d^3v \hat{\mathbf{e}}_s \cdot \mathbf{j}(\mathbf{r}, \mathbf{v}, t)$$

where $\hat{\mathbf{e}}_s$ is the unit normal to the surface, and the velocity space integration is taken over only those particle directions in the positive or negative direction (see Figure 1.4). From this definition it is apparent that

$$\hat{\mathbf{e}}_s \cdot \mathbf{J}(\mathbf{r}, t) = J_+(\mathbf{r}, t) - J_-(\mathbf{r}, t)$$

In this sense, $\mathbf{J}(\mathbf{r}, t)$ might be referred to as the “net” current density.

We have employed a consistent notation in which quantities that are dependent on phase space or angle are denoted by lowercase symbols (e.g., n or $\mathbf{j}$) and configuration space- or angle-integrated quantities are denoted by uppercase symbols (N or $\mathbf{J}$).

1.2 □ DERIVATION OF A GENERIC FORM OF THE TRANSPORT EQUATION □

We now derive an exact (albeit formal) equation for the phase space density $n(\mathbf{r}, \mathbf{v}, t)$ characterizing a transport process by simply balancing the various mechanisms by which particles can be gained or lost from a volume of material. That is, we begin by considering an arbitrary volume V and attempt to calculate the time rate of change of the number of particles in this volume that have velocities $\mathbf{v}$ in d^3v (see Figure 1.5). If

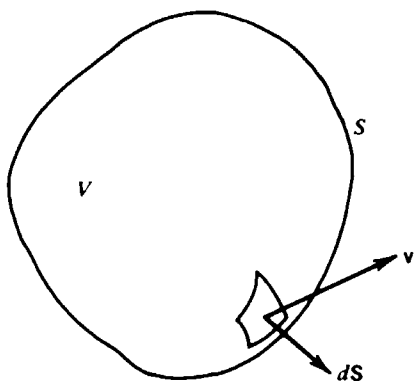


Fig. 1.5 □ An arbitrary volume V with surface area S .

we ignore for the moment macroscopic forces that might change the trajectories of the particles in V , it is apparent that the only mechanisms that can change the particle number are leakage through the surface of V , collision events that change the particle velocities, or sources in V :

$$\left[\begin{array}{c} \text{time rate} \\ \text{of change} \\ \text{of } n \end{array} \right] = \left[\begin{array}{c} \text{change due} \\ \text{to leakage} \\ \text{through } S \end{array} \right] + \left[\begin{array}{c} \text{change due} \\ \text{to} \\ \text{collisions} \end{array} \right] + \left[\begin{array}{c} \text{sources} \end{array} \right]$$

We can express this balance condition mathematically as follows:

$$\begin{aligned} \frac{\partial}{\partial t} \int_V d^3r n(\mathbf{r}, \mathbf{v}, t) d^3v = & - \int_S d\mathbf{S} \cdot \mathbf{j}(\mathbf{r}, \mathbf{v}, t) d^3v + \int_V d^3r \left(\frac{\partial n}{\partial t} \right)_{\text{coll}} d^3v \\ & + \int_V d^3r s(\mathbf{r}, \mathbf{v}, t) d^3v \end{aligned}$$

where we have defined the source density function $s(\mathbf{r}, \mathbf{v}, t)$ and the time rate of change due to collisions $(\partial n / \partial t)_{\text{coll}}$. If our choice of the arbitrary volume does not depend on time, we can bring $\partial / \partial t$ inside the integral over V . Furthermore we can use Gauss's law to rewrite the surface integral for the leakage contribution as a volume integral

$$\int_S d\mathbf{S} \cdot \mathbf{j}(\mathbf{r}, \mathbf{v}, t) = \int_V d^3r \nabla \cdot \mathbf{j}(\mathbf{r}, \mathbf{v}, t) = \int_V d^3r \nabla \cdot \mathbf{v} n(\mathbf{r}, \mathbf{v}, t) = \int_V d^3r \mathbf{v} \cdot \nabla n(\mathbf{r}, \mathbf{v}, t)$$

where we have noted that $\nabla \cdot \mathbf{v} n(\mathbf{r}, \mathbf{v}, t) = \mathbf{v} \cdot \nabla n(\mathbf{r}, \mathbf{v}, t)$, since $\mathbf{r}$ and $\mathbf{v}$ are independent variables. Thus our balance condition can be rewritten as follows:

$$\int d^3r d^3v \left\{ \frac{\partial n}{\partial t} + \mathbf{v} \cdot \nabla n - \left(\frac{\partial n}{\partial t} \right)_{\text{coll}} - s \right\} = 0 \quad (1.1)$$

But since V is arbitrary, Eq. 1.1 can be satisfied for all V only if the integrand itself is identically zero:

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \nabla n(\mathbf{r}, \mathbf{v}, t) = \left(\frac{\partial n}{\partial t} \right)_{\text{coll}} + s(\mathbf{r}, \mathbf{v}, t) \quad (1.2)$$

Hence we have arrived at an equation for the phase space density $n(\mathbf{r}, \mathbf{v}, t)$. This is the general form taken by the *transport equations* that characterize particle transport processes in an enormous variety of applications.

We can give a somewhat shorter derivation of this equation (and relax the assumption concerning macroscopic forces on the particles) by simply equating the substantial derivative¹⁵ describing the time rate of change of the local particle density along the particle trajectory to the change in the local density due to collisions and sources

$$\frac{Dn}{Dt} = \left(\frac{\partial n}{\partial t} \right)_{\text{coll}} + s$$

We can calculate Dn/Dt explicitly as

$$\frac{Dn}{Dt} = \frac{\partial n}{\partial t} + \frac{\partial \mathbf{r}}{\partial t} \cdot \frac{\partial n}{\partial \mathbf{r}} + \frac{\partial \mathbf{v}}{\partial t} \cdot \frac{\partial n}{\partial \mathbf{v}} = \frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial n}{\partial \mathbf{v}}$$

where we have introduced the obvious notation for the vector differentiation operations: $\partial/\partial \mathbf{r} \equiv \nabla$ (e.g., $\text{grad } n = \nabla n = \partial n/\partial \mathbf{r}$). Therefore we find that the transport equation takes the form

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial n}{\partial \mathbf{v}} = \left(\frac{\partial n}{\partial t} \right)_{\text{coll}} + s$$

The source term $s(\mathbf{r}, \mathbf{v}, t)$ in this equation is usually assumed to be specified in advance; therefore it is independent of the solution $n(\mathbf{r}, \mathbf{v}, t)$. However in certain situations (e.g., neutrons generated in a fission reaction) it may be convenient to allow the source to contain an “intrinsic” component dependent on the phase space density $n(\mathbf{r}, \mathbf{v}, t)$ itself.

To proceed further, we must be a bit more specific about the collision term $(\partial n/\partial t)_{\text{coll}}$, and this calls for a few more definitions, to enable us to adequately describe collision processes. For the present we assume that such collisions or interactions with the background medium occur instantaneously at a point in space. That is, we assume that particles stream along until they suffer a collision, at which point they are instantaneously absorbed or scattered to a new velocity. It should be apparent that such an assumption would not be valid for processes in which the ranges of the interaction forces are large, or in which the particle is absorbed, then reemitted some time later. We patch up these deficiencies later.

We now introduce the concept of a *mean free path* (mfp) to characterize such “local” interaction events:

$$(mfp)^{-1} \equiv \Sigma(\mathbf{r}, \mathbf{v}) \equiv \begin{array}{l} \text{probability of particle interaction per} \\ \text{unit distance traveled by particle of} \\ \text{velocity } \mathbf{v} \text{ at position } \mathbf{r} \end{array}$$

We follow the customary terminology of radiation transport by referring to the inverse *mfp* $\Sigma(\mathbf{r}, \mathbf{v})$ as the *macroscopic cross section* characterizing the interaction. This latter quantity can be related to the more familiar concept of a microscopic interaction cross section σ by noting

$$\Sigma(\mathbf{r}, \mathbf{v}) = N_B(\mathbf{r})\sigma(\mathbf{v})$$

where $N_B(\mathbf{r})$ is the number density of the background medium.

We must generalize this concept a bit to describe scattering processes or interaction processes in which the incident particle is absorbed in the collision event and several secondary particles are then emitted (e.g., nuclear fission events or the stimulated emission of light). Indeed, since transport theory is essentially just a mathematical description of “multiple scattering” processes in which the particles of interest wander through a medium, making numerous collisions as they go,⁶ it is important to introduce the concept of a *scattering probability function* $f(\mathbf{v}' \rightarrow \mathbf{v})$ defined by

$$f(\mathbf{v}' \rightarrow \mathbf{v})d^3v \equiv \begin{array}{l} \text{probability that any secondary particles} \\ \text{induced by an incident particle with} \\ \text{velocity } \mathbf{v}' \text{ will be emitted with velocity } \mathbf{v} \\ \text{in } d^3v \end{array}$$

Note that $f(\mathbf{v}' \rightarrow \mathbf{v})$ is essentially just a transition probability characterizing a change of state of the particle from $\mathbf{v}'$ to $\mathbf{v}$.

As a further characterization of such processes, we define the mean number of secondary particles emitted per collision event, $c(\mathbf{r}, \mathbf{v})$, by

$$c(\mathbf{r}, \mathbf{v}) \equiv \begin{array}{l} \text{mean number of secondary particles} \\ \text{emitted in a collision event experienced} \\ \text{by an incident particle with velocity } \mathbf{v} \text{ at} \\ \text{position } \mathbf{r} \end{array}$$

It is also useful to define the *collision kernel* $\Sigma(\mathbf{v}' \rightarrow \mathbf{v})$ characterizing such processes by

$$\Sigma(\mathbf{r}, \mathbf{v}' \rightarrow \mathbf{v}) = \Sigma(\mathbf{r}, \mathbf{v}')c(\mathbf{r}, \mathbf{v}')f(\mathbf{r}, \mathbf{v}' \rightarrow \mathbf{v})$$

This describes the probability per unit distance traveled that an incident particle of velocity $\mathbf{v}'$ will suffer a collision in which a secondary particle of velocity $\mathbf{v}$ is produced (which may be the original particle but with a new velocity in a simple scattering event). Note that by definition

$$\Sigma(\mathbf{r}, \mathbf{v}) = \int d^3v' \Sigma(\mathbf{r}, \mathbf{v} \rightarrow \mathbf{v}')$$

Again we stress that these definitions are useful only if the collision events are localized and uncorrelated. For example, if the particles are wavelike (e.g., photons or quantum mechanical particles), the interaction events would have to be sufficiently well separated to ensure the loss of phase information from one event to another—that is, mean free paths must be much larger than the particle wavelengths. In a similar sense, the mean free path must be much larger than the range of the interaction forces characterizing the collision events.

These concepts can now be used to obtain an explicit form for the collision term $(\partial n / \partial t)_{\text{coll}}$ appearing in the transport equation. First we note that the frequency of collision events experienced by a particle of velocity $\mathbf{v}$ is given by

$$v \Sigma(\mathbf{r}, \mathbf{v}) \equiv \text{collision frequency}$$

Hence the rate at which such reactions will occur in a unit volume can be written as

$$v \Sigma(\mathbf{r}, \mathbf{v}) n(\mathbf{r}, \mathbf{v}, t) \equiv \text{reaction rate density}$$

If we now note that the rate at which particles of velocity $\mathbf{v}$ suffer interactions that change their velocity or perhaps destroy the particle is $v \Sigma(\mathbf{r}, \mathbf{v}) n(\mathbf{r}, \mathbf{v}, t)$, while the rate at which particles of different velocities $\mathbf{v}'$ induce the production of secondary particles of velocity $\mathbf{v}$ is $\mathbf{v}' \Sigma(\mathbf{r}, \mathbf{v}' \rightarrow \mathbf{v}) n(\mathbf{r}, \mathbf{v}', t) d^3v'$, we can immediately identify the collision term in the transport equation as

$$\left(\frac{\partial n}{\partial t} \right)_{\text{coll}} = \int d^3v' \mathbf{v}' \Sigma(\mathbf{r}, \mathbf{v}' \rightarrow \mathbf{v}) n(\mathbf{r}, \mathbf{v}', t) - v \Sigma(\mathbf{r}, \mathbf{v}) n(\mathbf{r}, \mathbf{v}, t)$$

(If we recall the identification of $\Sigma(\mathbf{r}, \mathbf{v}' \rightarrow \mathbf{v})$ as essentially a transition kernel, it is apparent that the collision term assumes a form reminiscent of the master equation characterizing Markov stochastic processes.) We can now write the general form of the transport equation as

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial n}{\partial \mathbf{v}} + v \Sigma n = \int d^3v' \mathbf{v}' \Sigma(\mathbf{v}' \rightarrow \mathbf{v}) n(\mathbf{r}, \mathbf{v}', t) + s \quad (1.3)$$

The product $vn(\mathbf{r}, \mathbf{v}, t)$ in Eq. 1.3 arises so frequently in the calculation of reaction rate densities in transport theory that it has become customary to introduce a special notation:

$$\varphi(\mathbf{r}, \mathbf{v}, t) = vn(\mathbf{r}, \mathbf{v}, t) = \text{angular flux or phase space flux}$$

In a similar sense we can introduce the velocity-integrated flux:

$$\phi(\mathbf{r}, t) = \int d^3v \varphi(\mathbf{r}, \mathbf{v}, t) = \int d^3v vn(\mathbf{r}, \mathbf{v}, t)$$

Although it certainly proves convenient on occasion to work with $\varphi(\mathbf{r}, \mathbf{v}, t)$ rather than $n(\mathbf{r}, \mathbf{v}, t)$, since then one does not have to worry about including the particle speed v in the reaction rate densities, the tradition in some fields (notably nuclear engineering) of referring to this quantity as a “flux” is very misleading. For $\varphi(\mathbf{r}, \mathbf{v}, t)$ is not at all like the fluxes encountered in electromagnetic theory or heat conduction, since the latter fluxes are vector quantities, whereas $\varphi(\mathbf{r}, \mathbf{v}, t)$ is a scalar quantity. Actually the current density $\mathbf{J}(\mathbf{r}, t)$ corresponds more closely to the conventional interpretation of a “flux.”

The units of both $\mathbf{J}(\mathbf{r}, t)$ and $\phi(\mathbf{r}, t)$ are identical ($\text{cm}^{-2}\text{s}^{-1}$). However $\mathbf{J}(\mathbf{r}, t)$ is a vector quantity that characterizes the *net* rate at which particles pass through a surface oriented in a given direction, whereas $\phi(\mathbf{r}, t)$ simply characterizes the *total* rate at which particles pass through a unit area, regardless of orientation. Such an interpretation would suggest that $\mathbf{J}(\mathbf{r}, t)$ is a more convenient quantity for describing particle *leakage* or *flow* (e.g., through a surface), and $\phi(\mathbf{r}, t)$ is more suitable for characterizing particle *reaction rates* in which the total number of particle interactions in a sample is of interest. Although the angular flux $\varphi(\mathbf{r}, \mathbf{v}, t)$ and angular current density $\mathbf{j}(\mathbf{r}, \mathbf{v}, t)$ are very simply related,

$$\mathbf{j}(\mathbf{r}, \mathbf{v}, t) = \hat{\Omega} \varphi(\mathbf{r}, \mathbf{v}, t)$$

it should be apparent that in general there will be no simple relationship between $\phi(\mathbf{r}, t)$ and $\mathbf{J}(\mathbf{r}, t)$, since these are quite different moments of the particle distribution function:

$$\phi(\mathbf{r}, t) \equiv \int d^3v vn(\mathbf{r}, \mathbf{v}, t), \quad \mathbf{J}(\mathbf{r}, t) \equiv \int d^3v \mathbf{v} n(\mathbf{r}, \mathbf{v}, t)$$

We can rewrite the transport equation in terms of the angular flux $\varphi(\mathbf{r}, E, \hat{\Omega}, t)$ as

$$\frac{1}{v} \frac{\partial \varphi}{\partial t} + \hat{\Omega} \cdot \nabla \varphi + \Sigma \varphi = \int_0^\infty dE' \int_{4\pi} d\hat{\Omega}' \Sigma(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \varphi(\mathbf{r}, E', \hat{\Omega}', t) + s \quad (1.4)$$

The transport equation (1.3) or (1.4) is an integrodifferential equation for the unknown dependent variable $n(\mathbf{r}, \mathbf{v}, t)$ with seven independent variables, $(\mathbf{r}, \mathbf{v}, t) = (x, y, z, v_x, v_y, v_z, t) = (x, y, z, E, \theta, \phi, t)$. If the interaction cross sections $\Sigma(\mathbf{r}, \mathbf{v})$ and $\Sigma(\mathbf{r}, \mathbf{v}' \rightarrow \mathbf{v})$ are regarded as known [independent of $n(\mathbf{r}, \mathbf{v}, t)$], this equation is linear. But in many cases, (e.g., in gas dynamics or radiative transfer) these parameters depend on the particle distribution function and lead to a nonlinear transport equation.

To make this equation somewhat less abstract, let us apply it to the special case in which there is plane symmetry, that is, where the density $n(\mathbf{r}, \mathbf{v}, t)$ depends only on a single spatial coordinate, say x . It is most convenient to work with the form of the transport equation involving $\varphi(\mathbf{r}, E, \hat{\Omega}, t)$, since then we note that in Cartesian coordinates

$$\hat{\Omega} \cdot \nabla \varphi(x) = \left(\Omega_x \frac{\partial}{\partial x} + \Omega_y \frac{\partial}{\partial y} + \Omega_z \frac{\partial}{\partial z} \right) \varphi(x) = \Omega_x \frac{\partial}{\partial x} \varphi(x)$$

For convenience, we choose our angular coordinate system with its polar coordinate axis in the x -direction such that $\Omega_x = \cos \theta$. The assumption of plane symmetry also implies that there is no dependence on the azimuthal angle ϕ . If we furthermore introduce a new variable

$$\mu \equiv \cos \theta = \Omega_x$$

and note that as θ ranges between 0 and π , μ ranges from 1 to -1 , we can write the one-dimensional form of the transport equation as

$$\frac{1}{v} \frac{\partial \varphi}{\partial t} + \mu \frac{\partial \varphi}{\partial x} + \Sigma \varphi = \int_0^\infty dE' \int_{-1}^{+1} d\mu' \Sigma(E' \rightarrow E, \mu' \rightarrow \mu) \varphi(x, E', \mu', t) + s$$

Table 1.2 gives the form of the transport equation in other coordinate systems.

To complete our mathematical description of particle transport, we must specify initial and boundary conditions that accompany the transport equation. Since only a single time derivative appears in the equation, we can simply choose the initial condition to be the specification of the initial value of the phase space density for all positions and velocities:

$$\text{initial condition: } n(\mathbf{r}, \mathbf{v}, 0) = n_0(\mathbf{r}, \mathbf{v}), \quad \text{all } \mathbf{r} \text{ and } \mathbf{v}$$

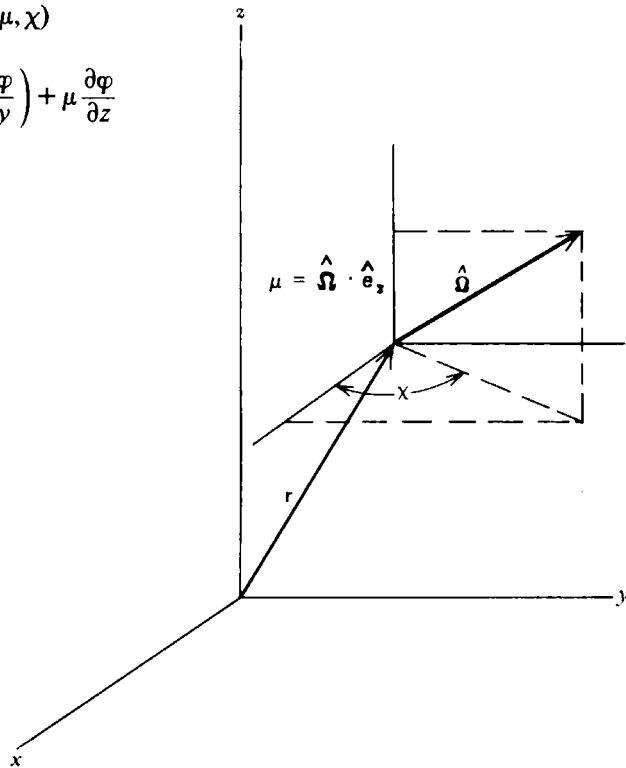
The boundary conditions are more complicated and depend on the problem of interest. Several of the more common boundary conditions include the following:

i *Free surface.* A free surface is defined such that particles can only escape a body through the surface; they cannot reenter it. Hence we would

Table 1.2 □ The Form of the Streaming Term $\hat{\Omega} \cdot \nabla \varphi$ in Common Orthogonal Geometries

Rectangular (x, y, z) : $\varphi(x, y, z, \mu, \chi)$

$$(1 - \mu^2)^{1/2} \left(\cos \chi \frac{\partial \varphi}{\partial x} + \sin \chi \frac{\partial \varphi}{\partial y} \right) + \mu \frac{\partial \varphi}{\partial z}$$



Cylindrical (r, θ, z) : $\varphi(r, \theta, z, \mu, \chi)$

$$(1 - \mu^2)^{1/2} \cos \chi \frac{\partial \varphi}{\partial r} + \frac{(1 - \mu^2)^{1/2}}{r} \sin \chi \left(\frac{\partial \varphi}{\partial \theta} - \frac{\partial \varphi}{\partial \chi} \right) + \mu \frac{\partial \varphi}{\partial z}$$

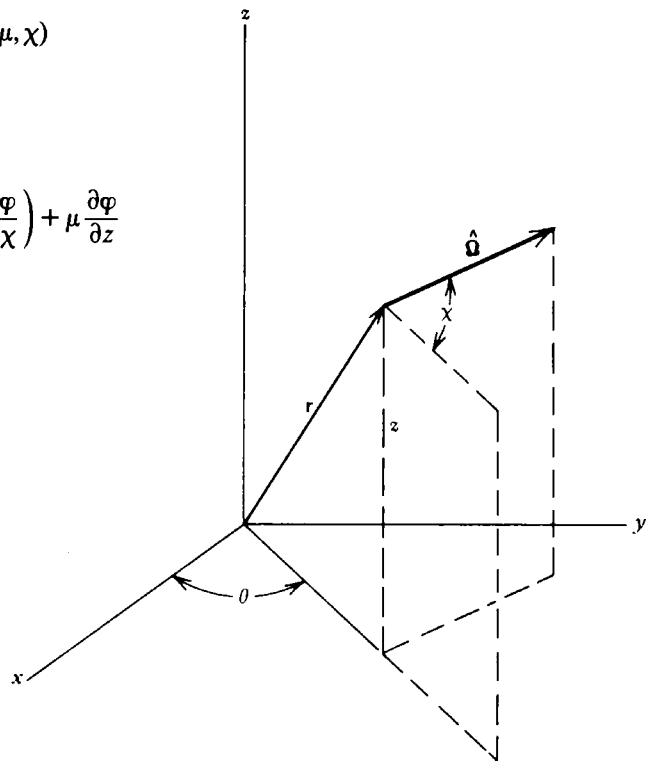
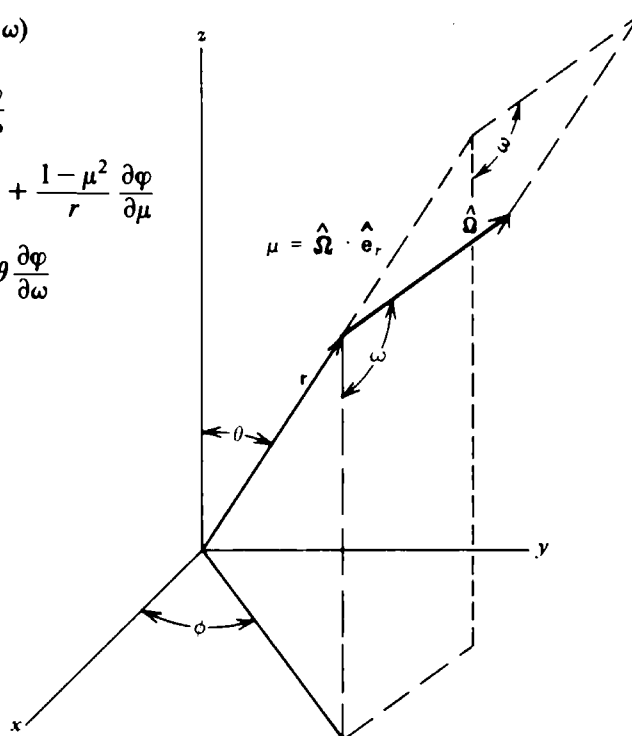


Table 1.2 □ Continued

Spherical (r, θ, ϕ) : $\varphi(r, \theta, \phi, \mu, \omega)$

$$\begin{aligned} & \mu \frac{\partial \varphi}{\partial r} + \frac{(1-\mu^2)^{1/2}}{r} \frac{\sin \omega}{\sin \theta} \frac{\partial \varphi}{\partial \phi} \\ & + \frac{(1-\mu^2)^{1/2}}{r} \cos \omega \frac{\partial \varphi}{\partial \theta} + \frac{1-\mu^2}{r} \frac{\partial \varphi}{\partial \mu} \\ & - \frac{(1-\mu^2)^{1/2}}{r} \sin \omega \cot \theta \frac{\partial \varphi}{\partial \omega} \end{aligned}$$



demand that the density vanish on the surface for all inward directions (see Figure 1.6):

$$n(\mathbf{R}_s, \mathbf{v}, t) = 0 \quad \text{for all } \mathbf{v} \text{ such that } \mathbf{v} \cdot \hat{\mathbf{e}}_s < 0$$

Of course we must be careful here to avoid “reentrant geometries” in which the escaping particle can reenter the body at a different point. These can usually be “patched up” by incorporating parts of the surrounding into the specification of the system of interest. One can also impose inhomogeneous boundary conditions at the surface by specifying the incoming density

$$n(\mathbf{R}_s, \mathbf{v}, t) = f(\mathbf{R}_s, \mathbf{v}, t) \quad \text{for all } \mathbf{v} \text{ such that } \mathbf{v} \cdot \hat{\mathbf{e}}_s < 0$$

We can always replace such inhomogeneous boundary conditions by equivalent fictitious surface sources on the boundary and return to homogeneous boundary conditions however.

ii *Reflecting boundary.* One sometimes wishes to impose a reflecting boundary condition that essentially assumes that particles are reflected at

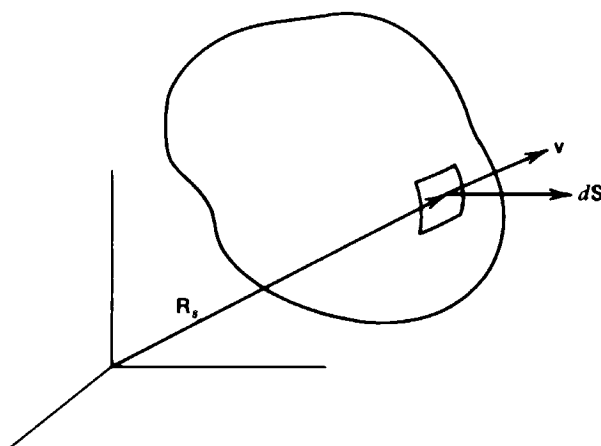


Fig. 1.6 □ A free surface boundary.

the boundary in a billiard ball fashion (i.e., angles of incidence and reflection are equal). Then one would require

$$n(\mathbf{R}_s, \mathbf{v}, t) = n(\mathbf{R}_s, \mathbf{v}_r, t) \quad \text{for } \mathbf{v} \cdot \hat{\mathbf{e}}_s < 0$$

where $\mathbf{v}_r$ is defined such that $\mathbf{v} \cdot \hat{\mathbf{e}}_s = \mathbf{v}_r \cdot \hat{\mathbf{e}}_s$ and $\mathbf{v} \times \mathbf{v}_r \cdot \hat{\mathbf{e}}_s = 0$. Such reflecting boundary conditions are occasionally used to express a symmetry property of the solution. It should be noted that unlike the case of a free surface, the reflecting boundary condition is *implicit*, since the outgoing density is expressed in terms of the incoming density at the boundary.

A variation on this theme is the albedo boundary condition in which the incoming density is reduced by a specified factor α (the “albedo”):

$$n(\mathbf{R}_s, \mathbf{v}, t) = \alpha n(\mathbf{R}_s, \mathbf{v}_r, t) \quad \text{for } \mathbf{v} \cdot \hat{\mathbf{e}}_s < 0$$

iii *Periodic boundary conditions.* In systems with periodic symmetry it occasionally becomes desirable to impose periodic boundary conditions in which the outgoing density on certain boundaries is equated with the incoming density on other boundaries that are related by symmetry conditions. Such periodic boundary conditions are particularly useful in curvilinear coordinates to treat the periodicity in the angle variables.

iv *Interfaces.* We can simply demand continuity of $n(\mathbf{r}, \mathbf{v}, t)$ across interfaces, since nothing that is of infinitesimal thickness can create or destroy particles (aside from mathematical constructs such as surface absorbers or sources)

$$n(\mathbf{R}_1, \mathbf{v}, t) = n(\mathbf{R}_2, \mathbf{v}, t) \quad \text{for all } \mathbf{v}$$

v Infinity. We usually demand that the density be well behaved at infinity, for example,

$$\lim_{|\mathbf{r}| \rightarrow \infty} n(\mathbf{r}, \mathbf{v}, t) < \infty$$

(although it may prove convenient to relax this condition and allow sources at infinity).

vi Other. A variety of more complicated boundary conditions are utilized to characterize particle surface interactions (such as occur in gas or plasma dynamics). We introduce these conditions later when we consider specific applications in these fields.

Boundary conditions (in a sense) are also required in the velocity variable. These are usually imposed implicitly by demanding a suitable behavior of $n(\mathbf{r}, \mathbf{v}, t)$ for large $\mathbf{v}$ (e.g., square integrability in velocity). We return to discuss this feature when we consider the classes (or “spaces”) of allowable solutions to the transport equation.

At this point a mathematician would ask what choices of initial and boundary conditions will guarantee a “well-posed” problem in transport theory. By “well-posed” he has something quite specific in mind: the solution to the problem must exist and it must be unique; furthermore, the solution must be stable in the sense that it is continuously dependent on the initial and boundary data.¹⁶ Such features have been rigorously demonstrated for a variety of problems in transport theory (although the mathematical detail is inappropriate for presentation at this point).^{4,17} As a general rule of thumb, time-dependent transport problems are well-posed if one specifies: (i) the initial value of the phase space density $n(\mathbf{r}, \mathbf{v}, 0)$ in the region of interest, (ii) the sources within this region, and (iii) the phase space current density incident on the surface of this region. One can furthermore demonstrate that this solution will be nonnegative if the sources in the region and on the surface are nonnegative.

The situation becomes more complicated for time-independent solutions to the transport equation (e.g., determining the density arising from a steady-state source or analyzing neutron transport in a critical fission chain reacting system). It may happen in these cases that there is no solution, or that the solution is not unique. The key role here is played by the number of secondaries per collision $c(\mathbf{r}, \mathbf{v})$. In general, if $c < 1$, it can be demonstrated that the stationary distribution in the region is determined by the sources in the region and the incident distribution on the bounding surface. For $c > 1$, solutions to the time-independent transport equation may not be unique (if they exist at all). (These statements will not be surprising to readers familiar with the theory of fission chain reactions.)

1.3 □ A BRIEF COMPARISON OF VARIOUS PARTICLE TRANSPORT THEORIES □

To illustrate the manner in which the concepts we have introduced arise in various fields, we very briefly present the form taken by the transport equation in several of the more popular applications. We also list several examples of typical transport problems that are encountered in each of these fields. A far more thorough discussion is given in later chapters.

1.3.1 □ Neutron Transport □ To describe the diffusion of neutrons through a medium, we define $n(\mathbf{r}, \mathbf{v}, t)$ to be the neutron phase space density and interpret $\Sigma(\mathbf{r}, \mathbf{v})$ as the macroscopic cross section characterizing neutron-nuclear interactions.³⁻⁶ Since neutron transport theory is essentially just a specialized form of the kinetic theory of gases in which the neutron gas diffuses through the background “gas” of nuclei, we might expect that the concepts and notation of gas kinetic theory could be adapted directly. However because of the rather specialized nature of the problems and the approximations utilized in neutron transport, it is customary to adopt a somewhat different notation:

$$\frac{1}{v} \frac{\partial \varphi}{\partial t} + \hat{\Omega} \cdot \nabla \varphi + \Sigma_r \varphi = \int_0^\infty dE' \int d\hat{\Omega}' \Sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \varphi(\mathbf{r}, E', \hat{\Omega}', t) + s \quad (1.5)$$

with initial and boundary conditions

$$\varphi(\mathbf{r}, E, \hat{\Omega}, 0) = \varphi_0(\mathbf{r}, E, \hat{\Omega})$$

$$\varphi(\mathbf{R}_s, E, \hat{\Omega}, t) = 0, \quad \hat{\Omega} \cdot \hat{\mathbf{e}}_s < 0 \quad (\text{free surface})$$

In fission chain reacting systems, the source contribution from fission neutrons is explicitly extracted and written as

$$s_f(\mathbf{r}, E, \hat{\Omega}, t) = \frac{\chi(E)}{4\pi} \int_0^\infty dE' \int d\hat{\Omega}' \nu(E') \Sigma_f(E') \varphi(\mathbf{r}, E', \hat{\Omega}', t)$$

where $\nu(E')$ is the average number of neutrons released per fission event, and $\chi(E)$ is the energy distribution or spectrum of the fission neutrons.

Sample problems:

- i *Determine the neutron flux resulting from a source (subcritical media).*
 - (a) Sources in infinite media (plane or point).
 - (b) Behavior of flux near a free surface (Milne problem).

- (c) Reflection of neutrons from a surface or interface (albedo problem).
- (d) Finite geometry problems (slabs or spheres).
- ii *Criticality problems.* Determine the system composition and geometry such that fission neutron production just balances neutron absorption and leakage to yield a time-independent solution to the transport equation (in the absence of sources).
- iii *Time-dependent problems.*
 - (a) Initial value problems (pulsed neutron problem).
 - (b) Response to time-modulated sources (neutron wave problem).

1.3.2 □ Photon Transport and Radiative Transfer □ To describe the transport of low energy photons (light) through matter (e.g., a stellar or planetary atmosphere), we define the photon energy intensity as the product of the photon energy $h\nu$ and photon flux $cn(\mathbf{r}, E, \hat{\Omega}, t)$:^{18, 19}

$$I_\nu(\mathbf{r}, \hat{\Omega}, t) = (h\nu)cn(\mathbf{r}, E, \hat{\Omega}, t)$$

The corresponding form of the transport equation (now referred to as the radiative transfer equation) is

$$\frac{1}{c} \frac{\partial I_\nu}{\partial t} + \hat{\Omega} \cdot \nabla I_\nu = \rho(\mathbf{r}, t) [-\kappa'_\nu(\mathbf{r}, \hat{\Omega}, t) I_\nu(\mathbf{r}, \hat{\Omega}, t) + \epsilon_\nu(\mathbf{r}, \hat{\Omega}, t)] \quad (1.6)$$

where $\rho(\mathbf{r}, t)$ = local matter density
 $\kappa'_\nu(\mathbf{r}, \hat{\Omega}, t)$ = absorption coefficient
 $\epsilon_\nu(\mathbf{r}, \hat{\Omega}, t)$ = emission coefficient

In local thermodynamic equilibrium, one can simplify this to write

$$\frac{1}{c} \frac{\partial I_\nu}{\partial t} + \hat{\Omega} \cdot \nabla I_\nu = \rho \kappa'_\nu [-I_\nu + S_\nu]$$

where the emission term is given by

$$S_\nu = \frac{2h\nu^3}{c^2} \left[\exp\left(\frac{h\nu}{kT}\right) - 1 \right]^{-1} \equiv B_\nu$$

If we wish to include the process of photon elastic scattering, we can generalize Eq. 1.6 to

$$\frac{1}{c} \frac{\partial I_\nu}{\partial t} + \hat{\Omega} \cdot \nabla I_\nu = \rho \kappa'_\nu \left[-I_\nu + \gamma_\nu B_\nu + (1 - \gamma_\nu) \int \frac{d\hat{\Omega}}{4\pi} I_\nu \right]$$

where γ_ν is the ratio of capture cross section to total cross section. It is customary to average this equation over frequency (which yields the analogue to the one-speed neutron transport equation). The frequency averaged interaction parameters $\langle \kappa \rangle$ are referred to as opacities. However, even in thermodynamic equilibrium, these opacities depend on temperature T , hence on the intensity I_ν , and lead to a nonlinear transport problem.

Sample problems:

- i High energy gamma transport, deep penetration and shielding.
- ii Classical stellar atmosphere (Milne problem).
- iii Radiation penetration into planetary atmospheres (albedo).
- iv Radiative transfer in plasmas.

1.3.3 □ Gas Dynamics □ We now picture the transport process as the motion of gas molecules as they move about, colliding with one another. To this end, we regard $n(\mathbf{r}, \mathbf{v}, t)$ as the phase space density of gas molecules.⁷⁻¹⁰ If the gas is sufficiently dilute that we need only consider binary interaction events, the appropriate transport equation for $n(\mathbf{r}, \mathbf{v}, t)$ takes a rather famous form known as the Boltzmann equation:

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \nabla n = \int d^3v_1 \int d\hat{\Omega} |\mathbf{v}_1 - \mathbf{v}| \sigma(\hat{\Omega}, |\mathbf{v}_1 - \mathbf{v}|) [n(\mathbf{v}')n(\mathbf{v}') - n(\mathbf{v}_1)n(\mathbf{v})] \quad (1.7)$$

Here the primes indicate the molecular velocities prior to the collision event, and $n(\mathbf{v})$ is just a shorthand notation for $n(\mathbf{r}, \mathbf{v}, t)$. It is important to note that this equation contains a quadratic nonlinearity.

We can linearize the Boltzmann equation for small disturbances about the equilibrium distribution $n_0(\mathbf{v}) = n_0 M(\mathbf{v})$ by defining

$$n(\mathbf{r}, \mathbf{v}, t) = n_0(\mathbf{v}) + n_1(\mathbf{r}, \mathbf{v}, t), \quad \|n_1\| \ll \|n_0\|$$

Then if we substitute this into the Boltzmann equation and retain only first-order terms in the perturbation $n_1(\mathbf{r}, \mathbf{v}, t)$, we arrive at the linearized Boltzmann equation:

$$\frac{\partial n_1}{\partial t} + \mathbf{v} \cdot \nabla n_1 = \int d^3v_1 \int d\hat{\Omega} |\mathbf{v}_1 - \mathbf{v}| \sigma n_0(\mathbf{v}) [n_1(\mathbf{v}') + n_1(\mathbf{v}') - n_1(\mathbf{v}_1) - n_1(\mathbf{v})]$$

If we identify $n_0(\mathbf{v})\sigma(\hat{\Omega}, |\mathbf{v}_1 - \mathbf{v}|)$ as just the collision or scattering kernel

$\Sigma_s(\mathbf{v}' \rightarrow \mathbf{v})$, this equation takes a form that is very similar to that of the transport equation characterizing neutron and photon transport (for finite range intermolecular potentials, at least). But the physics represented by this equation is considerably different, since it characterizes the collective motions of a gas rather than the diffusion of particles through a background medium.

Sample problems:

- i Steady flow (Couette flow, gas-surface interactions, heat transfer).
- ii Free and forced sound wave propagation.
- iii Shock wave propagation.

1.3.4 □ High Energy, Charged Particle Transport □ One might be tempted to apply a transport equation similar to that used to describe neutron or photon transport to processes involving high energy charged particles (e.g., electrons or light ions). However two quite different physical phenomena characterize the transport of light charged particles, and they lead to a somewhat different mathematical approach:

- i The strong, but infrequent collisions of the particles with heavy ions in which little energy transfer occurs.
- ii Frequent weak collisions with atomic electrons, which give rise to very irregular particle trajectories.

Hence one usually begins the study of charged particle transport by using an energy-independent description to account for elastic collisions with heavy ions¹⁹⁻²¹

$$\frac{1}{v} \frac{\partial \varphi}{\partial t} + \hat{\Omega} \cdot \nabla \varphi + \Sigma_s \varphi = \int d\hat{\Omega}' \Sigma_s(\hat{\Omega}' \rightarrow \hat{\Omega}) \varphi(\mathbf{r}, v, \hat{\Omega}', t) + s \quad (1.8)$$

and then introduces the frequent, weak collisions, which give rise to energy loss by using a continuous slowing down theory in which it is assumed that the energy loss over a given path length ξ is known and specified in terms of $dE/d\xi$. Then using $d\xi = v dt$, one can transform the independent variable in Eq. 1.8 to rewrite the equation characterizing charged particle transport as

$$\frac{\partial \varphi}{\partial \xi} + \hat{\Omega} \cdot \nabla \varphi + \Sigma_s \varphi = \int d\hat{\Omega}' \Sigma_s(\hat{\Omega}' \rightarrow \hat{\Omega}) \varphi(\hat{\Omega}') + s$$

Sample problems:

- i Shielding against charged particle radiation.
- ii Electron plasma production using high energy electron beams.

1.3.5 □ Transport in Ionized Gases and Plasmas □ The dynamics of an ionized gas or plasma is influenced enormously by the long-range nature of the Coulomb interaction. This produces a variety of complex phenomena including the interaction of the particle transport with collective (wavelike) modes. If we apply the general form of the transport equation (1.3) to a given species, say the electrons, we would write

$$\frac{\partial n_e}{\partial t} + \mathbf{v} \cdot \frac{\partial n_e}{\partial \mathbf{r}} - \frac{e}{m} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial n_e}{\partial \mathbf{v}} = \left(\frac{\partial n_e}{\partial t} \right)_{\text{coll}} \quad (1.9)$$

In the study of transport in ionized gases that are characterized by rather large Debye lengths so that collective effects need not be considered, we are usually given the electric and magnetic fields $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$. Then we can merely solve Eq. 1.9 as we would the equation characterizing high energy charged particle transport.^{22,23}

In a plasma, which by definition is an ionized gas with a Debye length small compared to system size, collective motions are very important, and $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$ must be determined self-consistently using Maxwell's equations.^{11,12} For example, a common problem involves the study of electrostatic oscillations in the electron density which are typically modeled by ignoring the collision term in Eq. 1.9 and writing it as

$$\frac{\partial n_e}{\partial t} + \mathbf{v} \cdot \frac{\partial n_e}{\partial \mathbf{r}} - \frac{e}{m} \mathbf{E} \cdot \frac{\partial n_e}{\partial \mathbf{v}} = 0 \quad (1.10)$$

where the electric field $\mathbf{E}(\mathbf{r}, t)$ is then determined by Poisson's equation

$$\frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{E} = -4\pi e \int d^3v [n_e(\mathbf{v}) - n_i(\mathbf{v})]$$

(A similar equation would be needed for the ion density.) This equation in which collisions have been neglected but in which the self-consistent nature of the electric field has been treated explicitly is known as the Vlasov equation. It forms the basis for 99.9% of modern plasma physics. Like the Boltzmann equation, it is nonlinear. But also like the Boltzmann equation, it can be linearized about a stationary homogeneous distribution $n_{e0}(\mathbf{v})$ by substituting

$$n_e(\mathbf{r}, \mathbf{v}, t) = n_{e0}(\mathbf{v}) + n_{e1}(\mathbf{r}, \mathbf{v}, t), \quad \|n_{e1}\| \ll \|n_{e0}\|$$

into the Vlasov equation (1.10) and neglecting second order terms in $n_{e1}(\mathbf{r}, \mathbf{v}, t)$ to find the linearized Vlasov equation

$$\frac{\partial n_{e1}}{\partial t} + \mathbf{v} \cdot \frac{\partial n_{e1}}{\partial \mathbf{r}} - \frac{e\mathbf{E}_1}{m} \cdot \frac{\partial n_{e0}}{\partial \mathbf{v}} = 0$$

$$\frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{E}_1 = -4\pi e \int d^3v n_{e1}(\mathbf{v})$$

If it is necessary to consider collisions as well, then one can choose from several possible forms of the collision term $(\partial n / \partial t)_{\text{coll}}$:

i Boltzmann collision term:

$$\left(\frac{\partial n_i}{\partial t} \right)_{\text{coll}} = \sum_j \int d^3v_1 \int d\hat{\Omega} |\mathbf{v}_1 - \mathbf{v}| \sigma_{ij}(\hat{\Omega}, |\mathbf{v}_1 - \mathbf{v}|) [n_j(\mathbf{v}_1) n_i(\mathbf{v}) - n_j(\mathbf{v}) n_i(\mathbf{v}_1)]$$

where a “Debye-shielded” Coulomb potential is used to calculate the scattering cross section σ_{ij} .

ii Fokker-Planck collision term:

$$\left(\frac{\partial n}{\partial t} \right)_{\text{coll}} = \frac{\partial}{\partial \mathbf{v}} \cdot \int d^3v' \mathbf{Q}^{\text{FP}}(\mathbf{v}, \mathbf{v}') \cdot \left[\frac{\partial n}{\partial \mathbf{v}} n(\mathbf{v}') - n(\mathbf{v}) \frac{\partial n}{\partial \mathbf{v}'} \right]$$

where

$$\mathbf{Q}^{\text{FP}} \equiv \frac{A(\mathbf{g}^2 \mathbf{I} - \mathbf{g}\mathbf{g})}{g^3}, \quad \mathbf{g} \equiv \mathbf{v} - \mathbf{v}'$$

$$A \equiv -\frac{n_0 \pi e^4}{m^2} \ln \left[\frac{(kT)^3}{4\pi n_0 e^6} \right]$$

iii Balescu-Lenard collision term:

$$\left(\frac{\partial n}{\partial t} \right)_{\text{coll}} = \frac{\partial}{\partial \mathbf{v}} \cdot \int d^3v' \mathbf{Q}^{\text{BL}}(\mathbf{v}, \mathbf{v}') \cdot \left[\frac{\partial n}{\partial \mathbf{v}} n(\mathbf{v}') - n(\mathbf{v}) \frac{\partial n}{\partial \mathbf{v}'} \right]$$

where

$$\mathbf{Q}^{\text{BL}} \equiv - \int d^3k \frac{\mathbf{k}\mathbf{k}}{k} \delta[\hat{\mathbf{k}} \cdot \mathbf{v} - \hat{\mathbf{k}} \cdot \mathbf{v}'] \frac{(2\pi)^3 n_0 V^2(k) (\pi/m)^2}{|D^+(-k, i\mathbf{k} \cdot \mathbf{v})|}$$

while $D(k, z)$ is the plasma dielectric function (see Section 3.3).

Sample problems:

- i Wave propagation in plasmas.
- ii Microinstabilities [i.e., instabilities in $n(\mathbf{r}, \mathbf{v}, t)$].
- iii Plasma turbulence.
- iv Propagation of shock waves in plasmas.

1.3.6 □ Some Generalizations of the Transport Equation □ Thus far our discussion of transport theory has been confined to processes in which the collision or interaction events could be described as essentially localized in time and space. But, of course, there are a variety of transport processes in which one can no longer assume that the particle mean free path is much larger than the range of the interaction forces (e.g., a plasma or a dense gas). For such processes one must generalize the form of the transport equation to allow for collision events that are not necessarily instantaneous or localized in space. It is possible to demonstrate (using techniques from statistical mechanics, discussed in the next section) that the most general form of the transport equation can be written as

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial n}{\partial \mathbf{v}} = \int_0^t d\tau \int d^3r' \int d^3v' \Sigma(\mathbf{v}' \rightarrow \mathbf{v}, \mathbf{r}' \rightarrow \mathbf{r}, t - \tau) n(\mathbf{r}', \mathbf{v}', \tau) + \mathcal{D}(\mathbf{r}, \mathbf{v}, t) \quad (1.11)$$

where the collision term has been generalized to account for nonlocalized processes. The term $\mathcal{D}(\mathbf{r}, \mathbf{v}, t)$ which appears in this equation depends on the initial value of the density and frequently vanishes in time rapidly enough that it can be ignored.

It should be noted that the essential transport character of the equation that appears in the streaming terms $\partial n / \partial t + \mathbf{v} \cdot \partial n / \partial \mathbf{r} + \mathbf{F} / m \cdot (\partial n / \partial \mathbf{v})$ is maintained even in this far more general formulation. Of course Eq. 1.11 is of only formal interest until one can determine the generalized collision kernels $\Sigma(\mathbf{v}' \rightarrow \mathbf{v}, \mathbf{r}' \rightarrow \mathbf{r}, t - \tau)$. Although explicit expressions for these kernels can be written down in terms of the microscopic behavior of the host material, the specific determination of these quantities remains a formidable task, and they are usually approximated using modeled calculations or experimental measurements. In many cases the collision kernels will depend in a nonlinear fashion on the particle distribution function $n(\mathbf{r}, \mathbf{v}, t)$.

1.4 □ THE RELATIONSHIP BETWEEN TRANSPORT THEORY AND KINETIC THEORY □

Transport theory is actually a very restricted subset of the more general topic of kinetic theory. One can distinguish between the two subjects by noting that *kinetic theory* is usually regarded as the aspect of statistical mechanics that is concerned with the *derivation* and study of equations for the particle phase space density $n(\mathbf{r}, \mathbf{v}, t)$ or distribution function $f(\mathbf{r}, \mathbf{v}, t)$. Such “kinetic equations”^{*} or “transport equations” are typified by the Boltzmann equation for a dilute gas, the neutron transport equation, or the Vlasov equation for a plasma. We regard *transport theory* as the more restricted mathematical discipline concerned with the *solution* of such kinetic equations and the application of such solutions to the study of particle transport processes.

Traditionally, transport theorists have concerned themselves with transport processes such as neutron diffusion, radiative transfer, or rarefied gas dynamics—all of which are characterized by particle mean free paths that are many times greater than the range over which a collision event takes place. That is, the particle transport process is dominated by particle streaming between collisions. The transport equation describing such processes in “dilute” systems is just the Boltzmann equation—either in its linear form for neutron or photon transport, or in its nonlinear form for the transport of molecules in a dilute gas.

However one can also consider transport processes in very dense systems in which the mean free path is comparable to the collision length. Such phenomena arise, for example, when we study the motions of molecules in a liquid or electrons in a plasma. Of course the physics of such transport processes is radically different, since now collision events dominate streaming behavior. Furthermore, the task of constructing a kinetic theory of such dense systems is far from trivial, and it has only recently begun to yield to the powerful tools of nonequilibrium statistical mechanics. Surprisingly enough, however, the mathematical features of the kinetic or transport equations that have been obtained for dense systems are remarkably similar to features more familiar from transport theories based on the Boltzmann or Boltzmannlike equations.

To indicate this more clearly, we briefly review the subject of kinetic theory (and transport theory) from the more general perspective of nonequilibrium statistical mechanics. To this end, we discuss several of the

^{*}Occasionally one encounters a more precise definition of a kinetic equation as an equation for $n(\mathbf{r}, \mathbf{v}, t)$ of the form $\partial n / \partial t = A[\mathbf{r}, \mathbf{v}; n(\mathbf{r}, \mathbf{v}, t)]$, where A is a time-independent functional of $n(\mathbf{r}, \mathbf{v}, t)$. We relax this definition somewhat by referring to any equation for $n(\mathbf{r}, \mathbf{v}, t)$ or similar phase space quantities as a kinetic equation (including time-dependent functionals $A[n; t]$ in this definition).

more successful methods for deriving kinetic theory descriptions of many particle systems.²⁴⁻²⁶

1.4.1 □ Nonequilibrium Statistical Mechanics □ The primary goal of any theory of a many particle system is to explain the macroscopic behavior of such a system in terms of the microscopic dynamics of the particles involved. For example, in the study of neutron transport, the primary goal is usually the calculation of various neutron-nuclear interaction rates—that is, weighted integrals of the neutron density. Frequently it suffices to determine the neutron density using a simple diffusion equation description. More frequently, however, one must go to a slightly more detailed description in the form of the angular density $n(\mathbf{r}, \mathbf{v}, t)$ and the associated neutron transport equation. Of course, even the neutron transport equation is only an approximate representation (albeit a very accurate approximation) to the true motions of the neutron-nuclei many body system that are actually described by quantum statistical mechanics.²⁷

In a similar manner one can analyze a gas either on a hydrodynamical level (e.g., the Navier-Stokes equations), by way of kinetic theory (the Boltzmann equation), or by studying the actual equations of motion for the gas molecules. The level of description one chooses depends on the type of behavior to be investigated. For example, a hydrodynamic description is usually sufficient to describe flow processes, whereas a kinetic description is necessary to analyze high frequency sound propagation or light scattering from gases. For very short wavelength, high frequency behavior, such as is encountered in inelastic neutron scattering or laser light scattering from plasmas, one may have to revert to the actual equations of motion themselves.

The mechanisms by which one passes from the microscopic equations of motion to kinetic theory and eventually to a hydrodynamical description make up the discipline of *nonequilibrium statistical mechanics* (NESM). In principle the macroscopic properties of a many body system can be defined as various averages over the possible microscopic motions of particles in the system. In this sense, then, statistical mechanics seeks to determine the relation between these macroscopic quantities directly from a knowledge of the equations of motion on a microscopic level.

On this microscopic level, particles undergo complicated motions under the influence of their mutual interactions, and these motions are governed by well-known laws of mechanics (either classical or quantum):

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i(t), \quad \frac{d\mathbf{v}_i}{dt} = \frac{1}{m} \mathbf{F}(\mathbf{x}_i(t), t), \quad i = 1, \dots, N \quad (1.12)$$

Hence given an initial value of the coordinates and momenta of all the N particles $(\mathbf{x}_1, \mathbf{v}_1, \dots, \mathbf{x}_N, \mathbf{v}_N) \equiv \Gamma_N(0)$, we can in principle solve these equations to determine the trajectories of all N particles $[\mathbf{x}_1(t), \mathbf{v}_1(t), \dots, \mathbf{x}_N(t), \mathbf{v}_N(t)] = \Gamma_N(t)$. That is, the time evolution of the system takes the form of the trajectory of the phase point $\Gamma_N(t)$ as it wanders about in a $6N$ -dimensional phase space (see Figure 1.7). The location of this phase point at any given instant t completely specifies the state of the system, since it gives $\mathbf{x}_i(t), \mathbf{v}_i(t)$ for each of the N particles. From the first order equations of motion, we can see that a given initial value for $\Gamma_N(0)$ will uniquely determine the state of the system at any later time t . Any physical measurement will presumably be a time average over this motion. That is, if A is a function of the state of the system, $A = A(\Gamma_N)$ (A is referred to as a *dynamical variable*), we associate a physical measurement with the time average of A defined as

$$\langle A \rangle_T \equiv \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt A(\Gamma_N(t))$$

It is clearly hopeless to attempt to solve directly the equations of motion for a system of N interacting particles. Furthermore, a particular solution of these equations requires a knowledge of the initial coordinates and momenta of each of the N particles. Such detailed information is impossible to obtain in practice. In fact we can hope to know only a few gross properties of the system of particles, such as its total energy or momentum. There are a very great number of points Γ_N in phase space—that is, a very great number of configurations of our system—that are compatible with the values of the limited number of variables we are at liberty to specify. These considerations led Gibbs to propose that instead of considering a single dynamical system as the object of interest, one should study the average properties of a collection or “ensemble” of systems, each identical with respect to the gross macroscopic variables that can be specified, but whose distribution in phase space is otherwise unspecified.²⁸ This ensemble

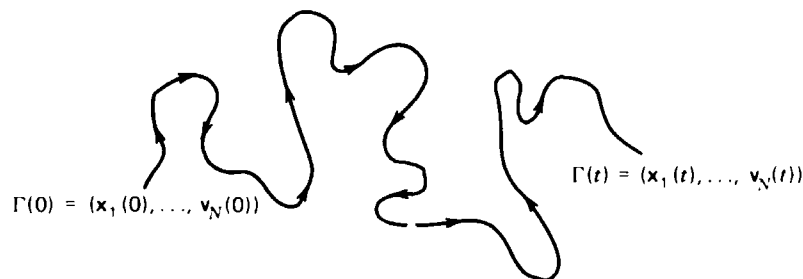


Fig. 1.7 □ The Γ -space trajectory of a many body system.

is to be specified by a function giving the probability density of a system in the ensemble having its representative phase point at a point Γ_N of phase space. This probability density function is called the ensemble distribution function or *ensemble density* and is denoted by $\rho(\Gamma_N, t)$.

Actually we are not interested in the ensemble density $\rho(\Gamma_N, t)$ itself. Rather, our interest arises because a knowledge of $\rho(\Gamma_N, t)$ permits us, in principle, to compute ensemble averages of dynamical variables. That is, if $A(\Gamma_N)$ is the dynamical variable of interest, the *ensemble average* of A is defined to be

$$\langle A \rangle \equiv \int d\Gamma_N \rho(\Gamma_N, t) A(\Gamma_N)$$

The fundamental postulate of statistical mechanics is that such ensemble averages can be identified as the measured macroscopic properties of the system. But we have also said that such measurements correspond to time averages. Hence this postulate assumes that we can equate ensemble averages with time averages:

$$\int d\Gamma_N \rho(\Gamma_N, t) A(\Gamma_N) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt A(\Gamma_N(t))$$

The study of the conditions under which this equality is valid comprises the famous “ergodic problem” of mechanics, and the rigorous justification of statistical mechanics rests on this result.²⁶ We can bypass the modern theory of mechanics and ergodicity entirely by simply assuming that the results of experimental measurements performed on many body systems can always be expressed in terms of ensemble averages.

Hence “all” we have to do is calculate $\rho(\Gamma_N, t)$ for a given system, then use this quantity to calculate all observed macroscopic properties as ensemble averages. Using Hamilton’s equations, we can derive a first order partial differential equation, the *Liouville equation*,^{26,28} which describes the time evolution of the ensemble distribution function $\rho(\Gamma_N, t)$ from a given initial value $\rho(\Gamma_N, 0)$:

$$\frac{\partial \rho}{\partial t} = \{H, \rho\} = - \sum_{i=1}^N \left(\mathbf{v}_i \cdot \frac{\partial}{\partial \mathbf{x}_i} + \frac{1}{m} F_i \cdot \frac{\partial}{\partial \mathbf{v}_i} \right) \rho(\Gamma_N, t) \equiv -iL\rho \quad (1.13)$$

where $\{ \}$ is the Poisson bracket, and we have defined the *Liouville operator* $L = i\{H, \circ\}$.

This equation is actually just a compact notation for the full set of the equations of motion for the N particles, subject to a statistical distribution of initial values given by $\rho(\Gamma_N, 0)$. Hence the solution of the Liouville

equation is equivalent to the solution of the equations of motion themselves. Nevertheless, it is possible to obtain general information concerning the time behavior of macroscopic properties (ensemble averages) from the Liouville equation by formal manipulations and suitable approximations.

It should be mentioned here that an analogous development applies for quantum mechanical systems. Now $\rho(t)$ is interpreted as the density operator or density matrix that satisfies

$$\frac{d\rho}{dt} = [H, \rho] \equiv -iL\rho$$

and the ensemble average of an observable corresponding to an operator A is given by

$$\langle A(t) \rangle = \text{Tr}\{A\rho(t)\}$$

Since we deal primarily with classical systems, we use the notation of classical mechanics in this book. Because of the formal similarities between the classical and quantum descriptions, however, most of our discussion can be carried over rather directly to quantum mechanical systems.

Therefore our primary goal is the calculation of ensemble averages of various dynamical variables of interest. That is, if $A(\Gamma_N)$ denotes a dynamical variable dependent on the state Γ_N of the system, then the ensemble average $\langle A(t) \rangle$ is calculated as

$$\langle A(t) \rangle = \int d\Gamma_N \rho(\Gamma_N, t) A(\Gamma_N) = \int d\Gamma_N \rho(\Gamma_N, 0) A(\Gamma_N(t)) \quad (1.14)$$

It has been explicitly noted here that one can include the time dependence of this average either in $\rho(\Gamma_N, t)$ or in the dynamical variable $A(\Gamma_N)$ itself. In the latter formalism, $A(t)$ is given as the solution of

$$\frac{dA}{dt} = iLA(t)$$

Usually the dynamical variables of interest depend only on the coordinates of one or two particles, or perhaps they involve a sum of such terms [e.g., $A(\Gamma_N) = A(\mathbf{x}_1, \mathbf{v}_1)$ or $A(\Gamma_N) = \sum_j A(\mathbf{x}_j, \mathbf{v}_j)$]. Hence it is useful to seek a reduced or contracted description of the system by defining quantities such as the single-particle distribution function

$$f(\mathbf{x}_1, \mathbf{v}_1, t) \equiv \int d\Gamma_{N-1} \rho(\Gamma_N, t)$$

Then $f(\mathbf{x}_1, \mathbf{v}_1, t)$ can be used to calculate ensemble averages such as

$$\langle A(t) \rangle = \int d^3x_1 \int d^3v_1 f(\mathbf{x}_1, \mathbf{v}_1, t) A(\mathbf{x}_1, \mathbf{v}_1)$$

Of course it is necessary to obtain an equation describing the time evolution of $f(\mathbf{x}_1, \mathbf{v}_1, t) = (1/n_0)n(\mathbf{x}_1, \mathbf{v}_1, t)$, and this is the objective of kinetic theory.

It is possible to go even further and obtain equations directly for the ensemble averaged quantities $\langle A(t) \rangle$ themselves. It is customary to refer to such systems of equations as a “hydrodynamic-like” description. For example, in neutron transport, the hydrodynamic level of description is just the neutron diffusion equation

$$\frac{\partial N}{\partial t} - vD \nabla^2 N(\mathbf{r}, t) = -v\Sigma_a N(\mathbf{r}, t) + S(\mathbf{r}, t)$$

where we define the ensemble averaged dynamical variable corresponding to density as

$$N(\mathbf{r}, t) \equiv \left\langle \sum_{j=1}^N \delta(\mathbf{r} - \mathbf{x}_j(t)) \right\rangle \equiv \langle \hat{N}(\mathbf{r}, t) \rangle$$

Frequently the goal of NESM is to derive such hydrodynamic equations for such a system. These equations contain various parameters known as transport coefficients (diffusion coefficients, viscosities, conductivities, etc.), which must be evaluated in terms of a more detailed description such as kinetic theory or the equations of motion themselves.²⁹

Our attention is directed instead toward the kinetic theory level of description (i.e., transport theory) in this “mechanics–kinetic theory–hydrodynamics” hierarchy (see Figure 1.8). This level concerns itself with the particle phase space density, which can also be written as the ensemble average of a microscopic dynamical variable:

$$n(\mathbf{r}, \mathbf{v}, t) = \left\langle \sum_{j=1}^N \delta(\mathbf{r} - \mathbf{x}_j(t)) \delta(\mathbf{v} - \mathbf{v}_j(t)) \right\rangle \equiv \langle \hat{n}(\mathbf{r}, \mathbf{v}, t) \rangle \quad (1.15)$$

Yet another major concern in NESM is the calculation of various equilibrium time correlation functions among dynamical variables,³⁰ $\langle A(0)A(t) \rangle_{\text{eq}}$ or $\langle A(0)B(t) \rangle_{\text{eq}}$, since the dynamical behavior of a many body system can frequently be characterized rather completely by such functions. In particular, transport coefficients can be expressed formally in

Microscopic level: equations of motion

Liouville equation

$$\frac{\partial \rho}{\partial t} = \{H, \rho\} = -iL\rho(\Gamma_N, t) \qquad \langle A(t) \rangle \equiv \int d\Gamma_N \rho(\Gamma_N, t) A(\Gamma_N)$$

(Newton's laws or Heisenberg equations)

(a)

Kinetic level

Kinetic equation

$$\frac{\partial n}{\partial t} = A[\mathbf{r}, \mathbf{v}; n(\mathbf{r}, \mathbf{v}, t)] \qquad \langle A(t) \rangle = \int d^3r \int d^3v \left[\frac{n(\mathbf{r}, \mathbf{v}, t)}{N} \right] A(\mathbf{r}, \mathbf{v})$$

(Boltzmann equation, neutron transport equation, Vlasov equation)

(b)

Hydrodynamic level

Conservation equations

$$\frac{\partial N}{\partial t} + \nabla \cdot \mathbf{J}(\mathbf{r}, t) = 0 \qquad N(\mathbf{r}, t) = \left\langle \sum_{j=1}^N \delta(\mathbf{r} - \mathbf{x}_j(t)) \right\rangle$$

Transport equations

$$\mathbf{J}(\mathbf{r}, t) = -D(\mathbf{r}) \nabla N(\mathbf{r}, t)$$

(Navier-Stokes equations, neutron diffusion equation)

(c)

Fig. 1.8 □ A flow chart of the various levels of description in NESM. (a) Microscopic level: Liouville equation in $6N$ Γ -space. (b) Kinetic level: contracted description in six-dimensional phase space. (c) Hydrodynamic level: contracted still further to three-dimensional configuration space.

terms of time correlation functions. Moreover, most experimental techniques for investigating dense systems (neutron or light scattering) measure such time correlation functions directly (usually the density-density correlation function).^{31,32} Hence a very considerable effort has been directed at determining these quantities. Once again one can proceed either by a kinetic or a hydrodynamic description. For example, to study density-density correlations, we can develop hydrodynamic-like equations for $\langle \hat{N}(\mathbf{r}, 0) \hat{N}(\mathbf{r}', t) \rangle$ or we can study a kinetic equation description of the generalization of this time correlation function to phase space $\langle \hat{n}(\mathbf{r}, \mathbf{v}, 0) \hat{n}(\mathbf{r}', \mathbf{v}', t) \rangle$.

1.4.2 □ Recent Developments in Kinetic Theory □ The development of the kinetic theory of gases can be traced back to the work of Maxwell, Rayleigh, Boltzmann, and others more than a century ago.³³ Prior to 1940, kinetic theory descriptions of many particle systems rested primarily on various phenomenological transport equations such as the Boltzmann³⁴ or Fokker-Planck³⁵ equations, which are reviewed in some detail in Chapter 3.

The modern development of kinetic theory for classical systems originated with the attempts of Kirkwood³⁶ and Bogoliubov³⁷ in 1945 to derive in a rigorous fashion kinetic equations such as the Boltzmann equation directly from the microscopic equations of motion for a many body system. Subsequent developments in kinetic theory have been varied and voluminous. Figure 1.9 summarizes the more significant methods for deriving kinetic equations. Among the more popular approaches have been the following.

Methods Based on the BBGKY Hierarchy □ Bogoliubov (and Born, Green, Kirkwood, and Yvon) demonstrated that it is possible to derive a hierarchy of equations (the BBGKY equations) for the s -particle distribution functions $f_s(\mathbf{x}_1, \mathbf{v}_1, \dots, \mathbf{x}_s, \mathbf{v}_s; t)$ characterizing a many body system. He then took advantage of the different characteristic time scales involved in gas dynamics (i.e., the time of a collision compared to the time between collisions) to postulate an ansatz in which all higher order distribution functions f_s appearing in the BBGKY hierarchy were expressed as time-independent functionals of the single particle distribution function $f_1(\mathbf{x}_1, \mathbf{v}_1, t)$. By introducing a density expansion of the BBGKY system subject to this ansatz or guess, Bogoliubov was then able to obtain an equation for f_1 to various orders in density. When carried out to the first order in density, this theory yields the Boltzmann equation. Choh and Uhlenbeck³⁸ formally calculated the next order term in this density expansion (which involves

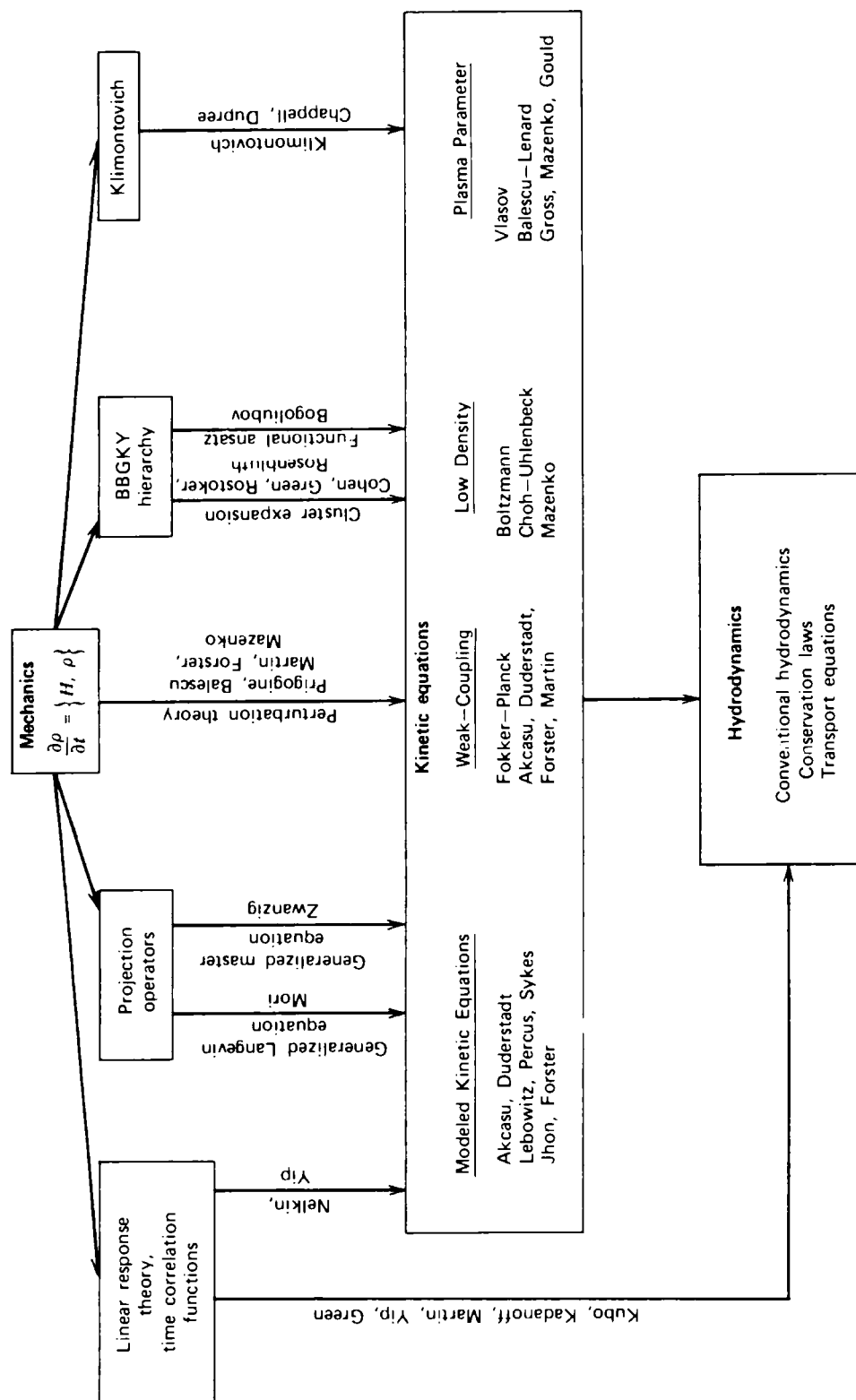


Fig. 1.9 □ A map of nonequilibrium statistical mechanics.

three-body collisions). Subsequent work by Cohen,³⁹ Green⁴⁰, and others has demonstrated that Bogoliubov's method is equivalent to a cluster expansion (similar to the Mayer expansion, familiar from equilibrium statistical mechanics). Rostoker and Rosenbluth⁴¹ used similar cluster expansions to derive the Vlasov and generalized Fokker-Planck equations for a plasma. Frieman and Sandri⁴² have used time scaling perturbation theory to truncate the BBGKY hierarchy and derive kinetic equations for gases and plasmas.

However during the mid-1960s it was demonstrated that such cluster (density) expansions lead to divergent corrections to the Boltzmann equation.⁴³ Such divergences cast considerable doubt on the validity of the standard methods for truncating the BBGKY hierarchy and furthermore have raised speculations concerning whether a kinetic equation even exists for dense systems (i.e., whether Bogoliubov's functional ansatz is valid). Such questions have been answered to some degree by the development of "renormalized" kinetic theories by Mazenko, Dorfman, and others.

Modern Perturbation Theory □ The powerful techniques of diagrammatic perturbation theory familiar from quantum field theory have been applied directly to the classical Liouville equation by Prigogine,⁴⁴ Balescu,⁴⁵ Severne,⁴⁶ and others to derive kinetic equations (e.g., the Boltzmann, Fokker-Planck, Vlasov, and Balescu-Lenard equations). More recently, Green's function techniques⁴⁷ have been applied to the kinetic theory of weakly coupled classical systems by Forster and Martin⁴⁸ and to low density systems by Mazenko.⁴⁹

Klimontovich Formalism □ Klimontovich⁵⁰ has developed a powerful formalism that has been applied with considerable success in plasma physics.⁵¹ This scheme proceeds from an equation of motion for the microscopic phase space density $\hat{n}(\mathbf{r}, \mathbf{v}, t)$ (defined in Eq. 1.15), which takes the form

$$\frac{\partial \hat{n}}{\partial t} + \mathbf{v} \cdot \frac{\partial \hat{n}}{\partial \mathbf{r}} - \frac{1}{m} \int d^3 r' \int d^3 v' \frac{\partial}{\partial \mathbf{r}} V(|\mathbf{r} - \mathbf{r}'|) \hat{n}(\mathbf{r}', \mathbf{v}', t) \cdot \frac{\partial}{\partial \mathbf{v}} \hat{n}(\mathbf{r}, \mathbf{v}, t) = 0 \quad (1.16)$$

and essentially involves the development of a hierarchy for the time correlation functions of $\hat{n}(\mathbf{r}, \mathbf{v}, t)$.

Time Correlation Functions and Linear Response Theory □ A number of schemes have been developed specifically for calculating equilibrium time correlation functions among dynamical variables. These include the sum

rule–dispersion relation methods of Kadanoff, Martin, and Yip^{52,53} and the direct perturbation techniques of Cohen and Dorfman,⁵⁴ Resibois,⁵⁵ and others.⁵⁶ Several theories have been based on kinetic or transport equations for the phase space generalizations of the time correlation functions of interest.

Projection Operator Techniques □ A very powerful and elegant procedure for deriving kinetic equations that has only recently received detailed attention is based on the projection operator techniques developed by Zwanzig⁵⁷ and Mori.⁵⁸ This scheme uses projection operator algebra to transform the Liouville equation into an alternative representation—either a “generalized master equation” or a “generalized Langevin equation”—and one proceeds to develop kinetic equations from this point. These generalized kinetic equations are formal identities with the equations of motion; therefore they are quite exact and contain all the information (and complexity) of the microscopic particle dynamics. However such equations have proved to be a very useful framework on which to base approximate theories of many body systems. For example, Akcasu and Duderstadt⁵⁹ have used this method to develop a kinetic equation that is rigorously correct to first order in the interaction potential for all frequencies and wavelengths. Mazenko,⁶⁰ Gould,⁶¹ and Baus⁶² have applied similar methods to develop the analogous kinetic equation generalizations of the Boltzmann and Balescu-Lenard equations. More recently, Mazenko^{63, 64} and others have developed renormalized kinetic theories in which the usual low density form of the kinetic equation for $f_1(\mathbf{x}, \mathbf{v}, t)$ is renormalized to include higher order correlation effects.

It should be stressed that although these elaborate approaches may appear quite different and abstract, they are in reality nothing more than schemes for introducing approximations into the equations of motion, to derive simpler descriptions of many particle dynamics (e.g., kinetic equations or hydrodynamic equations). Frequently, the approximations introduced are based on some type of perturbation theory, for example,⁶⁵

density expansions ($n r_0^3 \ll 1$) → Boltzmann equation

weak-coupling expansions ($V/kT \ll 1$) → Fokker-Planck equation

plasma parameter ($1/n r_D^3 \ll 1$) → Vlasov or Balescu-Lenard equation

It is possible as well to introduce modeled approximations into the derivation of kinetic equations (similar to the Bhatnager-Gross-Krook⁶⁶ model familiar from gas dynamics), and indeed we consider several such modeled kinetic equations in Chapter 3.

1.5 □ SCOPE OF TREATISE □ We have chosen to define transport theory as the mathematical description of particle transport, and in an even more restricted sense as the mathematical discipline concerned with the solution of transport or kinetic equations. In our treatment of this subject we develop a variety of mathematical tools that have been useful for the solution of such equations. We are most concerned with the study of general techniques that are suitable for a wide class of applications.

We first examine transport problems in which scattering or secondary particle emission is ignored entirely, for example, particle streaming in a vacuum or in a purely absorbing medium. Although this is a trivial mathematical problem (essentially requiring only a modest smattering of solid geometry), it does provide an essential foundation for more complicated problems. For example, it yields an alternative form of the transport equation (as an integral equation). The Green's functions for these simple streaming problems play a very important role in both the theoretical and numerical analysis of more complex transport processes.

We next develop a simple model of transport processes in which scattering events occur. This model assumes that the particle kinetic energy remains unchanged in the collision event. Hence the energy dependence in the transport equation can be neglected (or averaged out) to arrive at the "one-speed transport model" (referred to as the "grey atmosphere" model in radiative transfer). This model is amenable to most of the classical techniques used in the mathematical treatment of boundary value problems in partial differential equations—most notably, integral transforms and separation of variables (eigenfunction) methods. However the boundary conditions used in transport problems are unique, and thus require the introduction of several more specialized methods (the Wiener-Hopf method and singular eigenfunction expansions).

Chapter 3 develops in detail the basic collision models used in describing various transport processes. We begin by considering linear transport processes in which one can safely assume that the particles do not perturb the host medium (e.g., neutron, electron, or photon transport) and derive the general form of the appropriate transport equation (the Lorentz-Boltzmann equation). Then we treat the more general nonlinear collision models such as the Boltzmann, Landau-Fokker-Planck, and Balescu-Lenard collision terms, which characterize collective processes such as gas and plasma dynamics. We consider as well various approximate or modeled collision terms used to simplify these studies.

One of the fundamental problems in transport (or kinetic) theory concerns the derivation of "continuum" or macroscopic descriptions of the transport process such as are exemplified by diffusion or hydrodynamics equations. These are obtained by contracting the more detailed description given by the transport equation to obtain approximate equations for the

moments of the distribution function. Chapter 4 reviews the traditional schemes for accomplishing this (the Chapman-Enskog method and expansions in orthogonal polynomials). Then we introduce a more sophisticated method based on projection operator algebra.

Chapter 5 illustrates several of the applications of transport theory by examining an assortment of problems that arise in various fields, always with an eye toward stressing the underlying similarity of problems encountered in different applications. First we study the class of asymptotic relaxation problems in which the particle distribution function is allowed to relax to equilibrium in time or space. Since this problem is intimately related to the eigenvalue spectrum of the appropriate transport operator, it plays a very fundamental role in the theory of particle transport. We then examine a variety of initial value and boundary value problems in transport theory and conclude with a discussion of the rather specialized but extremely important topic of superthermal particle transport in which very energetic particles slow down by way of scattering events in the host medium.

Chapter 6 addresses the important although extremely difficult problem of nonlinear transport phenomena. This discussion is admittedly cursory, since the mathematical theory of such processes is still in a very primitive state. We develop the method of moments, which can be used to attack such problems, and we illustrate these methods by applying them to the analysis of highly nonequilibrium flows such as shock wave propagation. We also discuss methods based on the integral transport equation, concluding with a discussion of the quasilinear method used in plasma physics.

Chapter 7 develops the principal approximation methods used in transport theory. First we apply standard methods of perturbation theory to estimate integral quantities (eigenvalues or weighted integrals of the solution to the transport equation). Then we discuss the ways in which the calculus of variations can be used to approximate either the solution or the form of the transport equation. Finally, we investigate several more specialized approximation methods that are used to simplify the energy (or speed) variable in the transport equation.

Chapter 8 is concerned with numerical methods that have proved to be useful for the solution of transport problems. Of particular interest here are the powerful methods of discrete ordinates and finite elements that have been applied with considerable success to radiation transport problems. We also examine more specialized methods such as integral transport and collision probability techniques.

Chapter 9 covers methods that can be used in the direct simulation of particle transport processes. Of major interest are statistical methods (Monte Carlo), which represent the most versatile and powerful (and

usually the most expensive) approach to studying transport processes. We also consider deterministic methods for simulating particle transport, such as the molecular dynamics method, which directly solves the equations of motion for the many body system of interest.

□ PROBLEMS □

1.1 Determine the units for the following quantities: $n(\mathbf{r}, \mathbf{v}, t)$, $\varphi(\mathbf{r}, \mathbf{v}, t)$, $\varphi(\mathbf{r}, E, \hat{\Omega}, t)$, $\mathbf{j}(\mathbf{r}, E, \hat{\Omega}, t)$, and $I_\nu(\mathbf{r}, \hat{\Omega}, t)$.

1.2 Suppose that the angular density is given by $n(\mathbf{r}, \hat{\Omega}) = (n_0/4\pi)(1 - \cos\theta)$, where θ is the angle between $\hat{\Omega}$ and the z -axis. If A is the area perpendicular to the z -axis, find the rate at which particles pass through A : (i) per unit solid angle at an angle of 45° with the z -axis, (ii) from the negative z - to the positive z -direction, (iii) net rate of flow through A , and (iv) total rate at which particles pass through A .

1.3 Demonstrate that in an isotropic flux, the partial current density in any direction is given by $J_+ = \phi/4$.

1.4 Explain briefly whether the transport equation as we have derived it adequately describes: (i) an extremely dilute gas of average density less than 1 molecule cm^{-3} , (ii) neutron transport through a single crystal, (iii) light passing from the atmosphere into the ocean, (iv) the flow of automobiles down the Hollywood freeway at 5 P.M. on a Friday.

1.5 Derive the form of the transport equation that includes the effects of external forces by using the particle balance approach.

1.6 Integrate the transport equation over velocity (or angle) to obtain an equation for particle density (or flux). Then discuss qualitatively how one might expect to obtain a diffusion equation for $N(\mathbf{r}, t)$ from this exact relation. That is, discuss the approximations necessary and the conditions under which these approximations might be expected to be valid.

1.7 Consider particle transport in a one-dimensional rod of length L . Assume that the particles can move only to the left [say, as described by a distribution function $n_-(x, v, t)$] or to the right [$n_+(x, v, t)$]. Furthermore, consider only forward scattering and backward scattering processes described by $\Sigma_s^+(v', v)$ and $\Sigma_s^-(v', v)$.

- i Derive the transport equations for n_+ and n_- .
- ii Simplify these equations by introducing the one-speed approximation [e.g., $\Sigma_s(v) = \text{constant} = \Sigma_a + \Sigma_s^+ + \Sigma_s^-$, $\Sigma_s^\pm(v', v) = \Sigma_s^\pm \delta(v' - v)$].
- iii Describe the boundary and initial conditions necessary to complete the specification of the problem.
- iv Solve the one-speed transport equation for the rod assuming an incident current of one particle per second on the left end and zero

reentrant current on the right end. Assume that this current begins at time $t=0$, and prior to that time there are no particles in the rod.

1.8 Develop the particular form of the transport equation in (i) plane geometry, (ii) geometries with spherical symmetry, and (iii) geometries with cylindrical symmetry. For convenience, disregard the energy and time dependence.

1.9 Expand the solution to the transport equation in one-dimensional plane geometry in the first two Legendre polynomials:

$$\varphi(x, E, \mu) \cong \varphi_0(x, E) \left(\frac{1}{2}\right) P_0(\mu) + \varphi_1(x, E) \left(\frac{3}{2}\right) P_1(\mu)$$

where $P_0(\mu) = 1$ and $P_1(\mu) = \mu$. Substitute this expansion into the transport equation, multiply by $P_0(\mu)$ and $P_1(\mu)$, respectively, and integrate over μ to obtain a set of equations for the unknown expansion coefficients $\varphi_0(x, E)$ and $\varphi_1(x, E)$. These are known as the P_1 equations.

1.10 Derive the Liouville equation (1.13) for the ensemble density function $\rho(\Gamma_N, t)$ by using Hamilton's equations (1.12) along with the conservation of the total number of systems in the ensemble. [Refer to any text on statistical mechanics for assistance.]

1.11 Demonstrate the equivalence of the two expressions given for the ensemble average $\langle A(t) \rangle$ in Eq. 1.14.

1.12 Derive the Klimontovich equation (1.16) by directly computing the time derivative of the microscopic phase space density function $\hat{n}(\mathbf{r}, \mathbf{v}, t)$ defined in Eq. 1.15.

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□ 2 □

Exact Solutions for Simple, Modeled Theories of Particle Transport

The transport equation for the phase space density $n(\mathbf{r}, \mathbf{v}, t)$ is an essentially exact description of particle transport processes, provided one allows for a sufficiently general interpretation of the interaction cross sections $\Sigma(\mathbf{r}, \mathbf{v})$. The solution of this equation contains all the information (actually considerably more information) that we might require concerning a transport process. All we have to do is *solve* this equation.

But therein lies the difficulty. For the transport equation contains seven independent variables, $\mathbf{r}$, $\mathbf{v}$, and t . Furthermore, the dependence of the collision cross sections $\Sigma(\mathbf{r}, \mathbf{v}' \rightarrow \mathbf{v})$ on the particle velocity $\mathbf{v}$ (or kinetic energy, $E = mv^2/2$) is usually extremely complicated because of the collision dynamics of the colliding particles. These cross sections may also contain a complicated dependence on position $\mathbf{r}$ if the medium is sufficiently inhomogeneous. We have seen that in some cases they may even depend on the density $n(\mathbf{r}, \mathbf{v}, t)$ itself and lead to a nonlinear transport equation.

These considerations immediately suggest that any attempt to solve the transport equation for a realistic system must involve extensive use of the digital computer. Unfortunately no computer is sufficiently large or fast enough (yet) to solve this equation in the very general form in which we have derived it. Therefore we must introduce approximations to simplify this general description of transport processes, generally by attempting to reduce the number of independent variables that are significant in a given problem.

There are several different paths available to us. (i) We could approximate the form of the transport equation itself in an effort to allow its application to the study of realistic (and therefore, almost by definition, complicated) problems. (ii) We could consider only model problems for which the appropriate form of the transport equation becomes sufficiently simple to allow analytical, closed form solutions. (iii) We could attempt to solve a restricted form of the transport equation directly by using numerical or statistical simulation techniques.

Into the first class would fall methods such as diffusion theory or hydrodynamics (or their generalizations such as the P_N or Chapman-Enskog expansions), which seek to approximate the structure of the streaming operator $\partial/\partial t + \mathbf{v} \cdot \nabla$. Although these methods are extremely important and serve as the cornerstone for most treatments of transport phenomena in engineering applications (e.g., nuclear reactor design or aeronautical engineering), they effectively mutilate the transport character of the theory and as such are generally not classified as “transport theories.”

An alternative approach is to apply the exact form of the transport equation to “modeled” problems that are sufficiently simple to allow detailed analysis. For example, one might consider transport only in very simple geometries, or one might introduce approximations in the energy or angle variables:

Common Approximations of Geometry

- i Isotropic, homogeneous media.
- ii Infinite or semi-infinite geometries (half-spaces).
- iii One-dimensional symmetry (plane, spherical, or cylindrical).
- iv Periodic symmetry (lattices).
- v No symmetry (use a computer).

Common Approximations of Energy Dependence

- i One-speed approximation in which all particles are characterized by a single kinetic energy or speed.
- ii Multigroup energy descriptions in which the particle energy range is broken into intervals or groups, and each group is characterized by a single energy.
- iii Simple models of the cross section energy dependence (e.g., expansion in polynomial functions of energy).
- iv Simple models of the collision kernels (e.g., separable or degenerate kernels).

Common Approximations of the Angular Dependence

- i Isotropic sources.
- ii Isotropic scattering (angle-independent collision kernels).
- iii Expansion of the collision kernels in a finite set of Legendre polynomials in angle.

We have attempted to classify the various “solvable” problems of transport theory (such as there are) along with the appropriate method of solution (analytical vs. numerical) in Table 2.1.

Table 2.1 □ The “Solvable” Problems of Transport Theory

Problem	Geometry ^a					
	One-Dimensional		Two-Dimensional		Three-Dimensional	
	∞ -Medium	Half-Space	Finite	x - y	r - z	General
Energy						
One-speed	A	A	A	N	N	N
Multigroup	A	A, N	N	N	N	N
Continuous E	A	A, N	N	U	U	U
Angle						
Isotropic	A	A	A	N	N	N
Anisotropic	A	A	N	N	N	N
Material						
Vacuum	A	A	A	A	A	A
Pure absorption	A	A	A	A	A	A
Uniform media	A	A	A	N	N	N
Nonuniform media	N	N	N	N	N	N
Sources						
Localized (point, plane, line)	A	A	A	N	N	N
Green's function	A	A	A	N	N	N
Pulsed or oscillating	A	A	A	N	N	U
None (inhomogeneous boundary conditions or critical)	—	A	N	N	N	N
Time dependence						
Static with source	A	A	A	N	N	N
Critical	A	A	A	N	N	N
Oscillating sources	A	A	A	U	U	U
Pulsed sources	A	A	A	U	U	U
General time dependence	A	A	N	U	U	U

^aA = analytical solution available, N = numerical solution available, U = Ugh!

In fact, given a modeled problem that is simple enough, it is occasionally (but not frequently) possible to obtain an exact analytical solution to the appropriate form of the transport equation. We examine this small subset of modeled problems in this chapter, not so much because they provide an adequate description of real, physical phenomena, but rather because they reveal a good deal about the structure of the transport equation and the nature of its solutions for more complicated problems. Moreover they occasionally provide sufficient insight into the character of more complicated problems to allow their efficient numerical solution or provide exact (or “bench-mark”) solutions against which numerical approximation schemes can be tested.

2.1 □ PARTICLE STREAMING IN THE ABSENCE OF SCATTERING □

We begin our study of the solvable class of problems by considering transport in media in which interaction events (if they occur) produce no secondary particles, that is, media for which $c=0$. In such media *all* transport or kinetic equations take the form

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial n}{\partial \mathbf{v}} + v \Sigma_a n(\mathbf{r}, \mathbf{v}, t) = s(\mathbf{r}, \mathbf{v}, t) \quad (2.1)$$

Since the only interaction process allowed is absorption, we have replaced the total cross section Σ by the absorption cross section Σ_a .

Although the neglect of scattering events might appear at first to lead to a rather idealized and uninteresting problem, it turns out to be of very considerable use in studying a variety of physical processes. It is actually of far more use than most of the other models presented in this chapter. For example, such a model would characterize particle streaming in a vacuum; neutrons streaming in gas channels in nuclear reactors or intense radiation produced by sources surrounded by air would be described by this theory. Highly absorbing media such as nuclear reactor fuel elements or optically thick plasmas can also be described by such a model.

In addition, the solution of Eq. 2.1 plays an important role in problems in which scattering processes are allowed. This is because the particle density characterizing a purely absorbing medium can be interpreted as the uncollided or “first-flight” density in more general transport problems. We will find that these solutions can be used as Green’s functions (“first-flight kernels”) to transform the integrodifferential form of the transport equation into an integral equation representation. Moreover, such solutions can be used to calculate the “escape probabilities” or “collision probabilities” characterizing particles streaming through lumped absorbers (which are of significance in the theory of resonance neutron capture in

fission chain reactors or line emission and absorption in radiative transfer processes).

2.1.1 □ General Solution □ We can integrate the particular form of the transport equation appropriate for streaming, Eq. 2.1, by first rewriting it in a more concise (and abstract) notation as

$$\frac{\partial n}{\partial t} + \mathcal{L}n = s \quad (2.2)$$

where we define the “streaming” operator

$$\mathcal{L} \equiv \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial}{\partial \mathbf{v}} + v \Sigma_a$$

If we pretend for the moment that $\mathcal{L}$ is simply a constant, not an operator, we can easily integrate Eq. 2.2 with respect to time from some initial instant, say $t=0$, to find

$$n(\mathbf{r}, \mathbf{v}, t) = e^{-t\mathcal{L}} n(\mathbf{r}, \mathbf{v}, 0) + \int_0^t d\tau e^{-(t-\tau)\mathcal{L}} s(\mathbf{r}, \mathbf{v}, \tau) \quad (2.3)$$

But of course $\mathcal{L}$ is not a constant but rather an operator; thus we must be a bit more careful in our definition of $\exp(-t\mathcal{L})$. We can define this quantity by using a series expansion of the exponential

$$\exp(-t\mathcal{L}) \equiv 1 - t\mathcal{L} + \frac{1}{2}t^2\mathcal{L}^2 - \dots \quad (2.4)$$

disregarding for the moment questions of convergence and other annoying mathematical subtleties. It is apparent that $\exp(-t\mathcal{L})$ is the “time evolution operator” or “time propagator” that propagates a function from its value at the initial time $t=0$ to its value at a later time t as governed by Eq. 2.2.

To make this solution less abstract, suppose for the moment that we consider transport in a vacuum for which $\Sigma_a \equiv F \equiv 0$. Then $\mathcal{L} = \mathbf{v} \cdot \nabla$, and the application of Eq. 2.4 to a function $f(\mathbf{r})$ yields a Taylor expansion such that

$$\exp(-t\mathbf{v} \cdot \nabla) f(\mathbf{r}) = f(\mathbf{r} - \mathbf{v}t)$$

Therefore we can write our general solution given by Eq. 2.3 as

$$n(\mathbf{r}, \mathbf{v}, t) = n(\mathbf{r} - \mathbf{v}t, \mathbf{v}, 0) + \int_0^t d\tau s(\mathbf{r} - \mathbf{v}(t-\tau), \mathbf{v}, \tau) \quad (2.5)$$

Obviously this solution merely tells us that in a vacuum the distribution

function $n(\mathbf{r}, \mathbf{v}, t)$ at time t is found by looking back along the direction $-\mathbf{v}/|\mathbf{v}|$ a distance $v t$ to see what particles are going to stream along this trajectory to the position $\mathbf{r}$ in direction $+\mathbf{v}/|\mathbf{v}|$.

The case of transport in a purely absorbing, spatially uniform medium (in which we continue to ignore external forces) is almost as trivial:

$$n(\mathbf{r}, \mathbf{v}, t) = e^{-v\Sigma_a t} n(\mathbf{r} - \mathbf{v}t, \mathbf{v}, 0) + \int_0^t d\tau e^{-v\Sigma_a(t-\tau)} s(\mathbf{r} - \mathbf{v}(t-\tau), \mathbf{v}, \tau) \quad (2.6)$$

This result has an interpretation similar to that of Eq. 2.5 except that it takes into account the time decay in the density due to particle absorption.

We can relax the assumption of spatial uniformity [i.e., allow $\Sigma = \Sigma(\mathbf{r})$] and the neglect of external forces with only a modest increase in complexity (but no significant gain in understanding).¹ We could use these results to examine stationary problems as well, simply by demanding that the source terms be time independent and extending the limit on the time integration to $t \rightarrow \infty$. However it is useful to rederive the form of the distribution characterizing particle streaming for time-independent problems in a somewhat different fashion.

For the moment we ignore the external force term and introduce the particle flux $\varphi = v n$ as the dependent variable to rewrite Eq. 2.1 as

$$\frac{1}{v} \frac{\partial \varphi}{\partial t} + \hat{\Omega} \cdot \nabla \varphi + \Sigma_a \varphi(\mathbf{r}, \hat{\Omega}, t) = s(\mathbf{r}, \hat{\Omega}, t) \quad (2.7)$$

Here we have suppressed $v = |\mathbf{v}|$ as an independent variable, since there are no physical processes (i.e., no operators in the equation) that will act to change the particle speed or energy. If a particle suffers a collision, then by definition ($c = 0$) it disappears. Thus v appears only as a parameter, not as an independent variable. This will no longer be true if external forces are present, of course.

2.1.2 □ Stationary Transport in a Vacuum □ If we just set $\Sigma = 0$ and $\partial/\partial t = 0$ in the form of the transport equation given by Eq. 2.7, we arrive at an equation describing particle streaming in a vacuum:

$$\hat{\Omega} \cdot \nabla \varphi(\mathbf{r}, \hat{\Omega}) = s(\mathbf{r}, \hat{\Omega}) \quad (2.8)$$

To solve this equation, we simply note that $\hat{\Omega} \cdot \nabla$ is just the directional derivative along the particle flight direction $\hat{\Omega}$. Hence if we define the variable R along the particle trajectory as shown in Figure 2.1, we can rewrite Eq. 2.8 as

$$-\frac{d}{dR} \varphi(\mathbf{r} - R\hat{\Omega}, \hat{\Omega}) = \hat{\Omega} \cdot \nabla \varphi(\mathbf{r} - R\hat{\Omega}, \hat{\Omega}) = s(\mathbf{r} - R\hat{\Omega}, \hat{\Omega})$$

But we can easily integrate this equation over all R to arrive at an

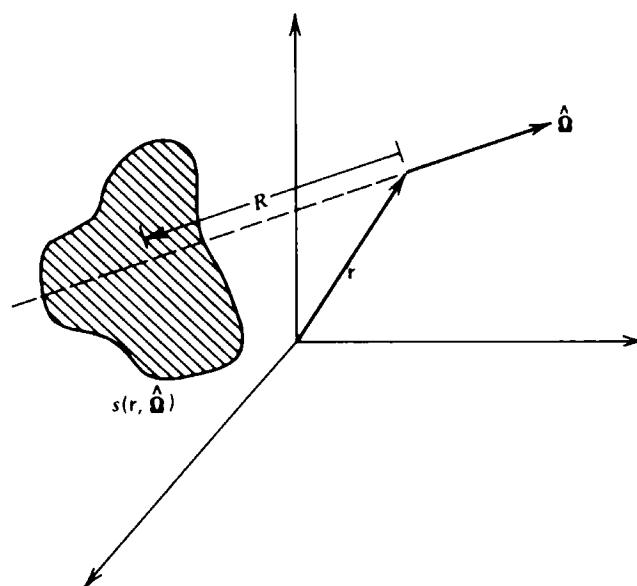


Fig. 2.1 □ Particle streaming from a distributed source in a vacuum.

expression that describes the angular flux $\varphi(\mathbf{r}, \hat{\Omega})$ resulting from a distributed source $s(\mathbf{r}, \hat{\Omega})$ in a vacuum:

$$\varphi(\mathbf{r}, \hat{\Omega}) = \int_0^\infty dR s(\mathbf{r} - R\hat{\Omega}, \hat{\Omega}) \quad (2.9)$$

Of course this solution is intuitively obvious, since it merely expresses the fact that the neutron flux at a position $\mathbf{r}$ can be obtained by adding up all the source neutrons produced in that direction that can pass through point $\mathbf{r}$.

To illustrate this result, suppose we consider a cavity² with a surface source $s_s(\mathbf{r}, \hat{\Omega})$ distributed on its walls (see Figure 2.2). We must be careful here, since we have to modify our volume source term to account for a distributed surface source. If x is the coordinate normal to the surface, we can write

$$s(\mathbf{r}, \hat{\Omega}) = s_s(\mathbf{r}, \hat{\Omega})\delta(x)$$

Then we can substitute this into our general result Eq. 2.9 to find

$$\begin{aligned} \varphi(\mathbf{r}, \hat{\Omega}) &= \int_0^\infty dR s_s(\mathbf{r} - R\hat{\Omega}, \hat{\Omega})\delta(x) = \int_0^\infty dx \left| \frac{dR}{dx} \right| s_s(\mathbf{r} - R\hat{\Omega}, \hat{\Omega})\delta(x) \\ &= \frac{s_s(\mathbf{r} - R_s\hat{\Omega}, \hat{\Omega})}{|\hat{\Omega} \cdot \hat{\mathbf{e}}_s|} \end{aligned}$$

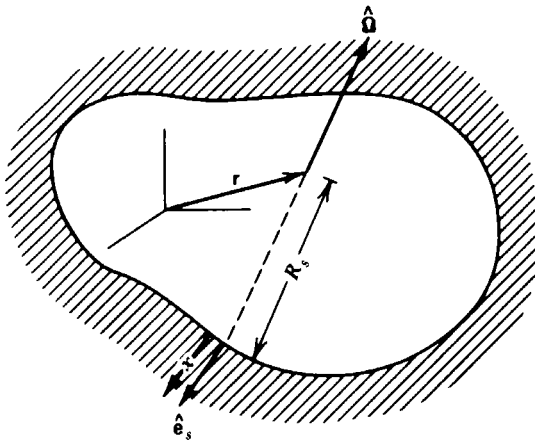


Fig. 2.2 □ The angular flux resulting from a distributed surface source in a cavity.

This result could have been written down almost by inspection—with the possible exception of the factor $|\hat{\Omega} \cdot \hat{e}_s|$ introduced by the surface source distribution.

As a variation on this theme, we can calculate the particle flux that results from a given flux distribution on the surface, $\varphi(\mathbf{r}_s, \hat{\Omega}) = \varphi_s(\mathbf{r}_s, \hat{\Omega})$ as

$$\varphi(\mathbf{r}, \hat{\Omega}) = \varphi_s(\mathbf{r} - R_s \hat{\Omega}, \hat{\Omega})$$

In particular, it should be noted that if the surface flux is isotropic and independent of the position on the surface, the flux at any point in the cavity will similarly be isotropic and position independent.

2.1.3 □ Stationary Transport in Purely Absorbing Media □ We can easily modify the foregoing solution to include the effect of absorption. To this end, consider the appropriate generalization of Eq. 2.8:

$$\hat{\Omega} \cdot \nabla \varphi + \Sigma_a \varphi(\mathbf{r}, \hat{\Omega}) = s(\mathbf{r}, \hat{\Omega}) \quad (2.10)$$

If we assume that $\Sigma_a(\mathbf{r})$ is independent of $\mathbf{r}$, we can use an integrating factor $\exp(\Sigma_a \mathbf{r} \cdot \hat{\Omega})$ to write the solution to Eq. 2.10 as follows:

$$\varphi(\mathbf{r}, \hat{\Omega}) = \int_0^\infty dR s(\mathbf{r} - R \hat{\Omega}, \hat{\Omega}) e^{-\Sigma_a R} \quad (2.11)$$

Since we can identify $\exp(-\Sigma_a R)$ as simply an attenuation factor due to particle absorption, it is apparent that this result is a natural generalization of our vacuum result Eq. 2.9.

We can extend this result even further to account for nonuniform media in which $\Sigma_a = \Sigma_a(\mathbf{r})$ by generalizing the integrating factor

$$\exp(-\Sigma_a R) \longrightarrow \exp[-\alpha(\mathbf{r}, \mathbf{r} - R\hat{\Omega})]$$

where

$$\alpha(\mathbf{r}, \mathbf{r}') \equiv \int_0^{|\mathbf{r}-\mathbf{r}'|} ds \Sigma_a \left(\mathbf{r} - \frac{s(\mathbf{r}-\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \right) \quad (2.12)$$

is known as the *optical thickness*^{2,3} of the medium and characterizes the effective absorption between two points $\mathbf{r}$ and $\mathbf{r}'$. Then the general solution of Eq. 2.10 can be written as follows:

$$\varphi(\mathbf{r}, \hat{\Omega}) = \int_0^\infty dR s(\mathbf{r} - R\hat{\Omega}, \hat{\Omega}) \exp[-\alpha(\mathbf{r}, \mathbf{r} - R\hat{\Omega})] \quad (2.13)$$

2.1.4 □ First-Flight Kernels □ Notice that if we replace Σ_a by the total cross section Σ_t , our solutions for purely absorbing media will describe the distribution of uncollided or “first-flight” particles emitted by a source. As we see later, the solution describing the distribution of first-flight particles for a point source can be very useful because it will serve as the Green’s function for an arbitrary source distribution. That is, it will appear as the “kernel” in an integral equation yielding the particle density due to an arbitrary source.

However before we develop this point source kernel, it is useful to modify our general solution Eq. 2.11 by converting the line integral that appears in this result into a volume integral. For this purpose, we introduce an *angular Dirac δ -function* $\delta_2(\hat{\Omega} \cdot \hat{\Omega}')$,^{1,2} defined by

$$\int_{4\pi} d\hat{\Omega}' \delta_2(\hat{\Omega} \cdot \hat{\Omega}') f(\hat{\Omega}') = f(\hat{\Omega})$$

Notice that this quantity can be expressed in terms of the usual Dirac δ -function as $\delta_2(\hat{\Omega} \cdot \hat{\Omega}') = (2\pi)^{-1} \delta(\hat{\Omega} \cdot \hat{\Omega}' - 1)$. If we insert this function into Eq. 2.11, we can write

$$\varphi(\mathbf{r}, \hat{\Omega}) = \int_{4\pi} d\hat{\Omega}_R \delta_2(\hat{\Omega} \cdot \hat{\Omega}_R) \int_0^\infty dR s(\mathbf{r} - R\hat{\Omega}_R, \hat{\Omega}) e^{-\Sigma_t R} \quad (2.14)$$

where we have defined a dummy integration variable $\hat{\Omega}_R \equiv \mathbf{R}/|\mathbf{R}|$. If we recall that the volume element in R -space is just $d^3R = R^2 dR d\hat{\Omega}_R$, we can

rewrite Eq. 2.14 as a volume integral:

$$\varphi(\mathbf{r}, \hat{\Omega}) = \int d^3R s(\mathbf{r} - \mathbf{R}, \mathbf{R}/|\mathbf{R}|) \delta_2(\hat{\Omega} \cdot \mathbf{R}/|\mathbf{R}|) e^{-\Sigma R} R^{-2} \quad (2.15)$$

Here we should note that although the integration is over all space, the δ_2 -function admits only those vectors $\mathbf{R}$ along $\hat{\Omega}$.

As an application of this result, let us calculate the angular flux resulting from a point source at position $\mathbf{r}_0$ emitting a beam of particles in a direction $\hat{\Omega}_0$ (see Figure 2.3):

$$s(\mathbf{r}, \hat{\Omega}) = s_0 \delta_2(\hat{\Omega} \cdot \hat{\Omega}_0) \delta(\mathbf{r} - \mathbf{r}_0)$$

If we substitute this source into our general result Eq. 2.15, we find

$$\varphi(\mathbf{r}, \hat{\Omega}) = \frac{s_0}{|\mathbf{r} - \mathbf{r}_0|^2} \delta_2(\hat{\Omega}_0 \cdot \hat{\Omega}) \delta_2\left[\frac{(\mathbf{r} - \mathbf{r}_0)}{|\mathbf{r} - \mathbf{r}_0|} \cdot \hat{\Omega}\right] e^{-\Sigma|\mathbf{r} - \mathbf{r}_0|} \equiv s_0 G_{\text{pt}}(\mathbf{r}, \hat{\Omega}; \mathbf{r}_0, \hat{\Omega}_0) \quad (2.16)$$

as the uncollided angular flux at position $\mathbf{r}$ in direction $\hat{\Omega}$ due to a point source at $\mathbf{r}_0$ radiating in direction $\hat{\Omega}_0$. We identify this result as the *first-flight kernel* or Green's function for a point source and denote it by $G_{\text{pt}}(\mathbf{r}, \hat{\Omega}; \mathbf{r}_0, \hat{\Omega}_0)$. Then, consistent with the usual interpretation of a Green's function, we would calculate the uncollided angular flux from an arbitrary source distribution $s(\mathbf{r}, \hat{\Omega})$ as follows:

$$\varphi(\mathbf{r}, \hat{\Omega}) = \int d^3r_0 \int d\hat{\Omega}_0 G_{\text{pt}}(\mathbf{r}, \hat{\Omega}; \mathbf{r}_0, \hat{\Omega}_0) s(\mathbf{r}_0, \hat{\Omega}_0) \quad (2.17)$$

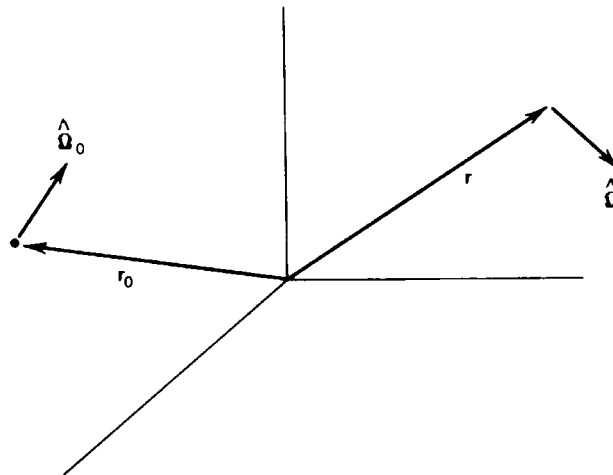


Fig. 2.3 □ The angular flux from a beam source at $\mathbf{r}_0$ radiating in direction $\hat{\Omega}_0$.

As a special case, we can calculate the uncollided flux resulting from an isotropic point source located at the origin

$$\varphi_{\text{pt}}(\mathbf{r}, \hat{\Omega}) = \int d^3r_0 \int d\hat{\Omega}_0 G_{\text{pt}}(\mathbf{r}, \hat{\Omega}; \mathbf{r}_0, \hat{\Omega}_0) \frac{s_0}{4\pi} \delta(\mathbf{r}_0) = s_0 \delta_2\left(\frac{\mathbf{r}}{|\mathbf{r}|} \cdot \hat{\Omega}\right) \frac{e^{-\Sigma_r r}}{4\pi r^2}$$

As a check, we can integrate this to find the flux from a point source

$$\phi_{\text{pt}}(\mathbf{r}) = \int d\hat{\Omega} \varphi_{\text{pt}}(\mathbf{r}, \hat{\Omega}) = s_0 \frac{e^{-\Sigma_r r}}{4\pi r^2}$$

which agrees with our physical intuition, which expects an exponential attenuation $\exp(-\Sigma_r r)$ due to collisions and a $(4\pi r^2)^{-1}$ falloff in the flux due to the geometric spreading of the source particles as they fly away from the source.

We can use the point source kernel to calculate the first-flight kernels characterizing other geometries. Consider, for example, the plane source kernel characterizing plane geometries. If we build up the contribution from a plane source by integrating over a distribution of isotropic point sources (see Figure 2.4), we find

$$\phi_{\text{pl}}(x) = \int_0^\infty \phi_{\text{pt}}(R) 2\pi r dr$$

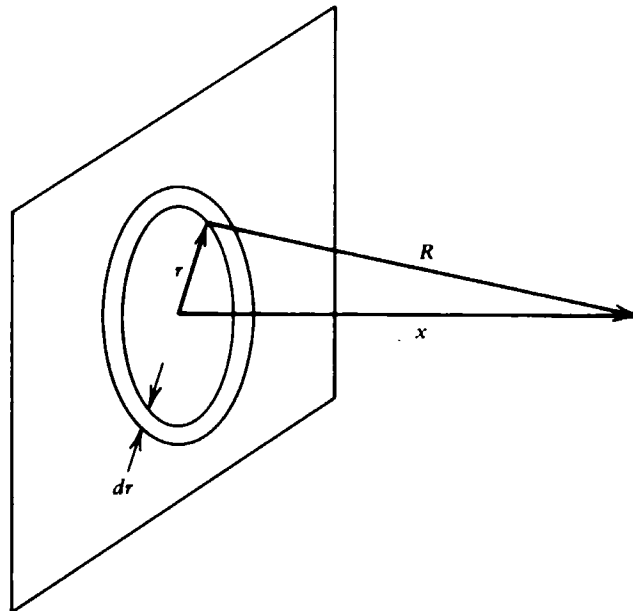


Fig. 2.4 □ Determination of the flux from an isotropic plane source.

Now let $R^2 = r^2 + x^2$, $2R dR = 2r dr$ to write

$$\phi_{\text{pl}}(x) = \int_x^\infty \phi_{\text{pt}}(R) 2\pi R dR = \frac{s_0}{2} \int_x^\infty e^{-\Sigma_t R} \frac{dR}{R} = \frac{s_0}{2} E_1(\Sigma_t x)$$

where we have introduced the exponential integral function

$$E_n(x) \equiv \int_1^\infty du e^{-xu} u^{-n} = \int_0^1 d\mu \mu^{n-2} e^{-x/\mu}$$

In a very similar fashion we can use the point source kernel to build up first-flight kernels for other geometries of interest (see Figure 2.5)^{1,2}

Spherical Shell Source Kernel:

$$\phi_{\text{pt}}(r) = \frac{s_0 a}{2r} [E_1(\Sigma |r-a|) - E_1(\Sigma |r+a|)]$$

Cylindrical Shell Source Kernel:

$$\phi_{\text{cl}}(r) = \frac{2s_0 a}{\pi} \int_{|r-a|}^{r+a} d\lambda \frac{Ki_1(\Sigma \lambda)}{[(r+a)^2 - \lambda^2]^{1/2} [\lambda^2 - (r-a)^2]^{1/2}},$$

$$Ki_1(\Sigma \lambda) \equiv \int_{\Sigma \lambda}^\infty ds K_0(s)$$

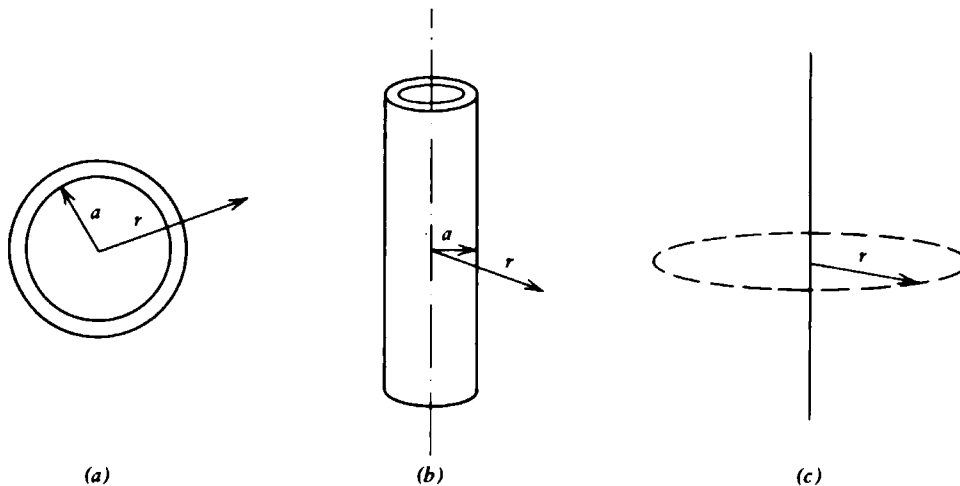


Fig. 2.5 □ Common source distributions. (a) Shell source. (b) Cylindrical source. (c) Line source.

Line Source Kernel:

$$\phi_1(r) = \frac{s_0}{2\pi r} K_1(\Sigma r)$$

It is important to note from Eq. 2.16 that the point source kernel exhibits a rather interesting symmetry property:

$$G_{\text{pt}}(\mathbf{r}, \hat{\Omega}; \mathbf{r}_0, \hat{\Omega}_0) = G_{\text{pt}}(\mathbf{r}_0, -\hat{\Omega}_0; \mathbf{r}, -\hat{\Omega})$$

That is, the flux at $\mathbf{r}$ in direction $\hat{\Omega}$ from a source at $\mathbf{r}_0$ radiating in direction $\hat{\Omega}_0$ is identical to that resulting from a switch of source and observer positions and directions. This “restricted” reciprocity relation plays an important role in the calculation of the escape and collision probabilities, defined in Section 2.2.6. It can also be generalized to apply to particle transport processes that include scattering events.¹

2.1.5 □ Integral Forms of the Transport Equation □ As yet another application of the point source kernel, suppose we return to the more general form of the transport equation characterizing a stationary transport process

$$\begin{aligned} \hat{\Omega} \cdot \nabla \varphi + \Sigma_t \varphi &= \int_0^\infty dE' \int d\hat{\Omega}' \Sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \varphi(\mathbf{r}, E', \hat{\Omega}') + s \\ &\equiv s'(\mathbf{r}, E, \hat{\Omega}) \end{aligned} \quad (2.18)$$

Here we have defined the right-hand side of this equation as an effective source term $s'(\mathbf{r}, E, \hat{\Omega})$. If we pretend for the moment that this source is known [although it depends on the unknown angular flux $\varphi(\mathbf{r}, E, \hat{\Omega})$, of course], we can solve Eq. 2.18 using our general result Eq. 2.17 to find

$$\begin{aligned} \varphi(\mathbf{r}, E, \hat{\Omega}) &= \int d^3r' \int d\hat{\Omega}' \left\{ \frac{\exp[-\Sigma_t(E)|\mathbf{r}-\mathbf{r}'|]}{|\mathbf{r}-\mathbf{r}'|^2} \delta_2(\hat{\Omega} \cdot \hat{\Omega}') \delta_2\left[\frac{(\mathbf{r}'-\mathbf{r}) \cdot \hat{\Omega}}{|\mathbf{r}'-\mathbf{r}|}\right] \right\} \\ &\times \left\{ \int d\hat{\Omega}'' \int_0^\infty dE'' \Sigma_s(E'' \rightarrow E, \hat{\Omega}'' \rightarrow \hat{\Omega}') \varphi(\mathbf{r}', E'', \hat{\Omega}'') + s(\mathbf{r}', E, \hat{\Omega}') \right\} \end{aligned} \quad (2.19)$$

Thus we have arrived at an alternative form of the transport equation—an *integral equation* form, although the kernel is rather singular to be sure. This equation simplifies very considerably if we can assume that both the

source and the scattering process are isotropic:

$$s(\mathbf{r}, E, \hat{\Omega}) = (4\pi)^{-1} S(\mathbf{r}, E), \quad \Sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) = (4\pi)^{-1} \Sigma_s(E' \rightarrow E)$$

Then we can integrate Eq. 2.19 over angle to find an integral equation for the angle-integrated flux

$$\begin{aligned} \phi(\mathbf{r}, E) = \int d^3r' \frac{\exp[-\Sigma_t(E)|\mathbf{r}-\mathbf{r}'|]}{4\pi|\mathbf{r}-\mathbf{r}'|^2} \\ \times \left[\int_0^\infty dE' \Sigma_s(E' \rightarrow E) \phi(\mathbf{r}', E') + S(\mathbf{r}', E) \right] \quad (2.20) \end{aligned}$$

This form of the transport equation is known as the *Peierls equation*,⁴ and it plays an extremely important role in the study of transport processes. It can be specialized to other geometries by using the appropriate form of the first-flight kernel for that geometry:

Plane Symmetry:

$$\phi(x, E) = \int_{-\infty}^{\infty} dx' \frac{1}{2} E_1(\Sigma_t|x-x'|) \left[\int_0^\infty dE' \Sigma_s(E' \rightarrow E) \phi(x', E') + S(x', E) \right] \quad (2.21)$$

Spherical Symmetry:

$$\begin{aligned} \phi(r, E) = \int_0^\infty dr' \frac{r'}{2} [E_1(\Sigma_t|r-r'|) - E_1(\Sigma_t|r+r'|)] \\ \times \left[\int_0^\infty dE' \Sigma_s(E' \rightarrow E) \phi(r', E') + S(r', E) \right] \quad (2.22) \end{aligned}$$

Here we note in passing how similar the integral forms of the transport equation are for plane and spherical geometries. We comment further on this similarity in Section 2.2.

We can develop somewhat different forms of the integral transport equation (2.20) by introducing alternative dependent variables. For example, if we define the particle *collision rate density*

$$F(\mathbf{r}, E) = \Sigma_t(\mathbf{r}, E) \phi(\mathbf{r}, E)$$

we can find an integral equation for $F(\mathbf{r}, E)$ by simply multiplying Eq. 2.20

by $\Sigma_i(\mathbf{r}, E)$:

$$F(\mathbf{r}, E) = \int d^3r' \frac{\exp[-\Sigma_i(E)|\mathbf{r}-\mathbf{r}'|]}{4\pi|\mathbf{r}-\mathbf{r}'|^2} \Sigma_i(E) \\ \times \left[\int_0^\infty dE' \frac{\Sigma_s(E' \rightarrow E)}{\Sigma_i(E')} F(\mathbf{r}', E') + S(\mathbf{r}', E) \right] \quad (2.23)$$

A second variation is obtained by defining the particle *emission rate density*

$$\chi(\mathbf{r}, E) = \int_0^\infty dE' \Sigma_s(E' \rightarrow E) \phi(\mathbf{r}, E') + S(\mathbf{r}, E) \quad (2.24)$$

—that is, the rate density of particles leaving a source or emerging from a collision with coordinates $(\mathbf{r}, E)$. Then obviously Eq. 2.20 can be written as

$$\phi(\mathbf{r}, E) = \int d^3r' \frac{\exp[-\Sigma_i(E)|\mathbf{r}-\mathbf{r}'|]}{4\pi|\mathbf{r}-\mathbf{r}'|^2} \chi(\mathbf{r}', E)$$

But if we substitute this into Eq. 2.24, we arrive at an integral equation for $\chi(\mathbf{r}, E)$

$$\chi(\mathbf{r}, E) = \int_0^\infty dE' \Sigma_s(E' \rightarrow E) \int d^3r' \frac{\exp[-\Sigma_i(E')|\mathbf{r}-\mathbf{r}'|]}{4\pi|\mathbf{r}-\mathbf{r}'|^2} \chi(\mathbf{r}', E') + S(\mathbf{r}, E) \quad (2.25)$$

It should be apparent that equations analogous to Eq. 2.19 can be derived in a similar fashion for the comparable angle-dependent quantities $f(\mathbf{r}, \hat{\Omega}, E)$ and $\chi(\mathbf{r}, \hat{\Omega}, E)$. We can easily generalize these derivations as well to include time dependence. If we utilize the coordinate system defined in Figure 2.6 to write $\mathbf{r}' \equiv \mathbf{r} - R\hat{\Omega}$ and $t' \equiv t - R/v$, we can note

$$-\frac{d}{dR} \varphi(\mathbf{r}', E, \hat{\Omega}, t') = \hat{\Omega} \cdot \nabla \varphi + \frac{1}{v} \frac{\partial \varphi}{\partial t'}$$

to write the transport equation (1.4) as

$$-\frac{d\varphi}{dR} + \Sigma_t(\mathbf{r}') \varphi(\mathbf{r}', t') = \int_0^\infty dE' \int d\hat{\Omega}' \Sigma_s(\mathbf{r}', E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \varphi(\mathbf{r}', E', \hat{\Omega}', t') \\ + s(\mathbf{r}', E, \hat{\Omega}, t')$$

But if we introduce the integrating factor $\exp[-\int_0^R dR' \Sigma_t(\mathbf{r} - R'\hat{\Omega}, E)]$, we

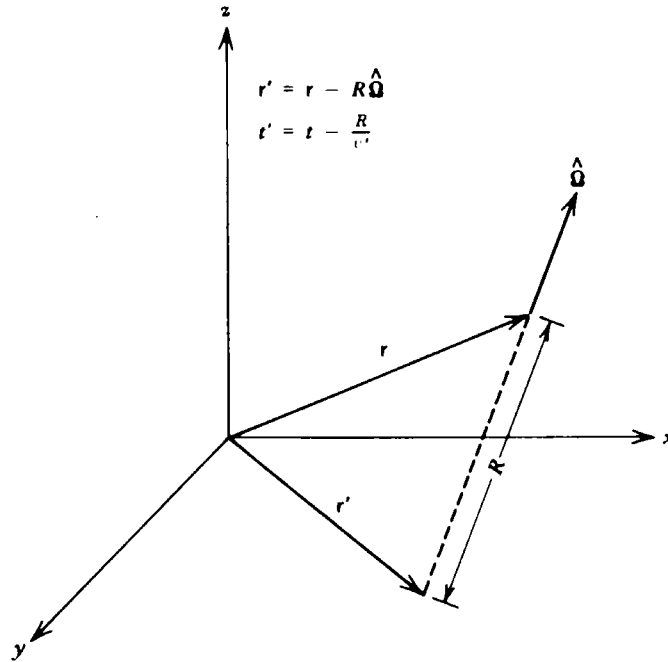


Fig. 2.6 □ Coordinate system for integrating the transport equation.

can integrate this equation directly to find the integral form of the transport equation for the angular flux as

$$\begin{aligned} \varphi(\mathbf{r}, E, \hat{\Omega}, t) = & \int_0^\infty dR \exp[-\alpha(\mathbf{r}, R, \hat{\Omega}, E)] \\ & \times \left\{ \int_0^\infty dE' \int d\hat{\Omega}' \Sigma_s(\mathbf{r}', E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \varphi(\mathbf{r}', E', \hat{\Omega}', t') \right. \\ & \left. + s(\mathbf{r}', E, \hat{\Omega}, t') \right\} \end{aligned}$$

where we have identified the energy-dependent optical thickness

$$\alpha(\mathbf{r}, R, \hat{\Omega}, E) \equiv \int_0^R dR' \Sigma_t(\mathbf{r} - R' \hat{\Omega}, E)$$

When working with the integral form of the time-dependent transport equation, it is generally more convenient to leave the equation in a line integration form rather than converting to volume integration.

2.1.6 □ Escape Probabilities and Collision Probabilities □ The concepts of escape and collision probabilities are frequently introduced to describe the transport of particles in highly absorbing media.^{2,5,6} To be more

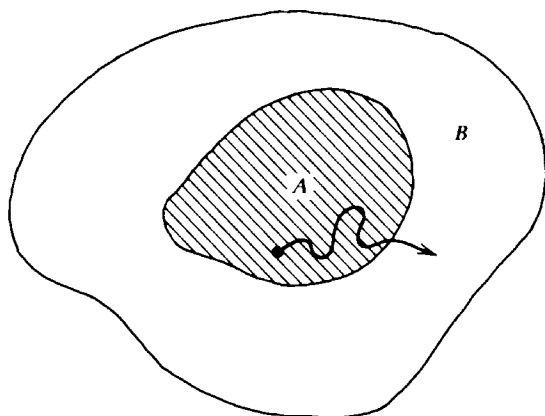


Fig. 2.7 □ Particle escape from region A .

specific, consider a system characterized by two regions as shown in Figure 2.7. Then we can define the *escape probability* for a region, say region A , as

P_A = probability that a particle born uniformly and isotropically in region A will escape into region B before being absorbed

Of course, in the process of escaping from region A , the particle will generally suffer a number of scattering collisions. If the region is highly absorbing, then P_A can be calculated in terms of a much simpler quantity, the *first-flight escape probability*, P_{A0}

P_{A0} = probability that a particle originating uniformly and isotropically in region A will make its next collision in region B (i.e., will escape region A without making a collision)

The calculation of P_{A0} is simply a geometrical problem, since one need only determine the probability that a particle will stream out of region A before it collides with anything. A closely related quantity is the *collision probability* characterizing a region:

P_{AC} = probability that a particle originating uniformly and isotropically in region A will make its first collision in region A

From this definition, it is apparent that $P_{AC} = 1 - P_{A0}$.

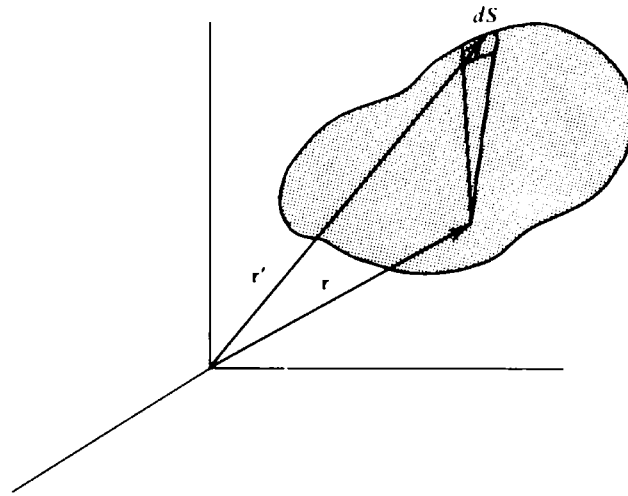


Fig. 2.8 □ Coordinates for escape probability calculation.

There are a variety of geometrical schemes available for calculating the first-flight escape probability. We will consider the *chord method* first introduced by Dirac.^{2,7} To this end, consider a uniform source distribution S_0 emitting particles isotropically in a body of volume V (see Figure 2.8). Then we can calculate the number of particles produced in a volume element d^3r that pass through a surface element dS at point $\mathbf{r}'$ as

$$\text{number from } d^3r \text{ passing through } dS = S_0(4\pi)^{-1} d^3r d\hat{\Omega} \exp[-\Sigma_t|\mathbf{r}' - \mathbf{r}|]$$

Using this, we can calculate the rate at which particles escape from the volume by integrating both over the source distribution and the surface area

$$\text{rate of particle escape from volume} = \frac{S_0}{4\pi} \int_V d^3r \int_{4\pi} d\hat{\Omega} \exp[-\Sigma_t|\mathbf{r}' - \mathbf{r}|]$$

Therefore the first-flight escape probability is just

$$P_0 = \frac{\text{escape rate}}{VS_0} = \frac{1}{4\pi V} \int_V d^3r \int_{4\pi} d\hat{\Omega} \exp[-\Sigma_t|\mathbf{r}' - \mathbf{r}|] \quad (2.26)$$

Now to perform these integrations, it is convenient to introduce a variable transformation as shown in Figure 2.9 such that $d^3r = \hat{\Omega} \cdot \hat{\mathbf{e}}_s dS dR$. Then we

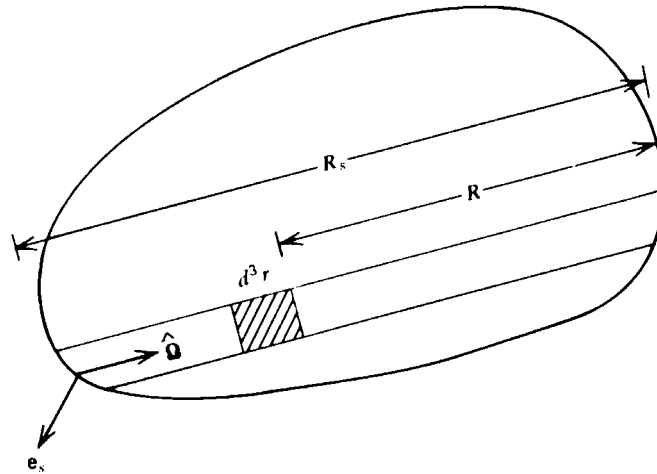


Fig. 2.9 □ Calculation of the chord distribution function.

can rewrite Eq. 2.26 as

$$P_0 = \frac{1}{4\pi V} \int dS \int_0^{R_s} dR \int d\hat{\Omega} e^{-\Sigma_i R} \hat{\Omega} \cdot \hat{e}_s = \frac{1}{4\pi V} \int dS \int d\hat{\Omega} (1 - e^{-\Sigma_i R_s}) (\hat{\Omega} \cdot \hat{e}_s) \quad (2.27)$$

If we now introduce the concept of the chord length distribution function $\Phi(R)$ characterizing the body:

$\Phi(R) dR$ = probability that a chord will have a length R in dR

$$= \frac{4\pi V}{\langle R \rangle} \int_{R_i=R} dS \int d\hat{\Omega} (\hat{\Omega} \cdot \hat{e}_s)$$

we can rewrite Eq. 2.27 (see Ref. 2 for details) as

$$P_0 = \frac{1}{\Sigma_i \langle R \rangle} \int_{R_{\min}}^{R_{\max}} dR (1 - e^{-\Sigma_i R}) \Phi(R) \quad (2.28)$$

where the average chord length of a body $\langle R \rangle$ can be shown to be

$$\langle R \rangle = \int dR R \Phi(R) = \frac{4V}{S}$$

Thus our task is to calculate the chord length distribution function $\Phi(R)$ for the geometry of interest and then perform the integral in Eq. 2.28.

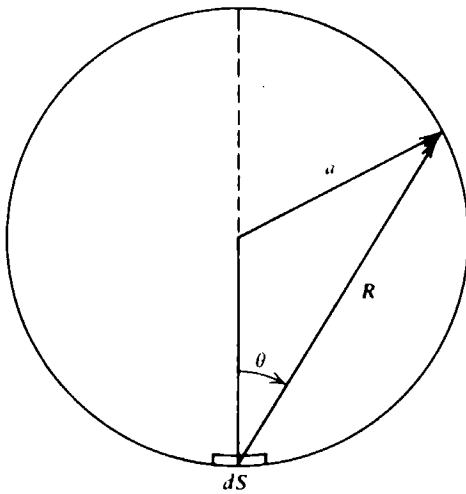


Fig. 2.10 □ Calculation of the first-flight escape probability for a sphere.

Example. Consider the calculation of the first-flight escape probability for a sphere (see Figure 2.10). Then

$$\Phi(R) dR = (\pi S)^{-1} S 2\pi\mu d\mu = 2\mu d\mu$$

where $\mu = \cos\theta = R/2a$ and $d\mu = dR/2a$. Thus

$$\Phi(R) dR = \left(\frac{R}{2a^2} \right) dR$$

We can also find $\langle R \rangle = 4V/S = (4/3)a$. Therefore

$$\begin{aligned} P_0 &= \frac{3}{4a\Sigma_t} \int_0^{2a} dR \frac{R}{2a^2} (1 - e^{-\Sigma_t R}) \\ &= \frac{3}{8(\Sigma_t a)^3} [2(\Sigma_t a)^2 - 1 + (1 + 2\Sigma_t a)e^{-2\Sigma_t a}] \end{aligned}$$

The first-flight escape probabilities P_0 have been calculated and tabulated for most of the common geometries.² Table 2.2 lists several of the more important cases. We should note two particularly useful results that apply to any geometry. Using Eq. 2.28 we can show that in the limit of small volumes,

$$P_0 \xrightarrow[\text{small volumes}]{} 1$$

(since the probability of leaking out before suffering a collision must then

Table 2.2 □ First-Flight Escape Probabilities P_0 in Common Geometries*Slab of width a*

$$P_0 = (2\Sigma a)^{-1} [1 - 2E_3(\Sigma a)]$$

Sphere of radius a

$$P_0 = \frac{3}{8} (\Sigma a)^{-3} [2(\Sigma a)^2 - 1 + (1 + 2\Sigma a)e^{-2\Sigma a}]$$

Infinite cylinder of radius a

$$P_0 = \left(\frac{\Sigma a}{3} \right) \{ 2[\Sigma a K_1(\Sigma a) I_1(\Sigma a) + K_0(\Sigma a) I_0(\Sigma a) - 1] \\ + (\Sigma a)^{-1} K_1(\Sigma a) I_1(\Sigma a) - K_0(\Sigma a) I_1(\Sigma a) + K_1(\Sigma a) I_0(\Sigma a) \}$$

approach unity). For volumes with dimension large compared to a mean free path,

$$P_0 \xrightarrow{\text{large volumes}} \frac{S}{4V\Sigma_t}$$

We return to consider such escape probabilities in Section 8.4.

2.2 □ ONE-SPEED TRANSPORT THEORY □

2.2.1 □ The One-Speed Approximation □ In this section we develop and study a model of particle transport in which we assume that all particles can be characterized by a single speed v or kinetic energy $E = \frac{1}{2}mv^2$. To introduce this approximation, it is natural to begin with the particle transport equation for $\varphi(\mathbf{r}, E, \hat{\Omega}, t)$ so that the energy E and angle $\hat{\Omega}$ variables are explicitly separated

$$\frac{1}{v} \frac{\partial \varphi}{\partial t} + \hat{\Omega} \cdot \nabla \varphi + \Sigma_t \varphi = \int_0^\infty dE' \int d\hat{\Omega}' \Sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \varphi(\mathbf{r}, E', \hat{\Omega}', t) + s \quad (2.29)$$

To remove the energy dependence in this equation, we simply integrate Eq.

2.29 over energy and define the energy-averaged parameters

$$\begin{aligned}
 (\bar{v})^{-1} &\equiv \frac{\int_0^\infty dE (v)^{-1} \varphi(E)}{\int_0^\infty dE \varphi(E)} \\
 \bar{\Sigma}_t &\equiv \frac{\int_0^\infty dE \Sigma_t(E) \varphi(E)}{\int_0^\infty dE \varphi(E)} \\
 \bar{\Sigma}_s(\hat{\Omega}' \rightarrow \hat{\Omega}) &\equiv \frac{\int_0^\infty dE \int_0^\infty dE' \Sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \varphi(E', \hat{\Omega}')}{\int_0^\infty dE' \varphi(E', \hat{\Omega}')} \\
 \bar{s} &\equiv \int_0^\infty dE s(E)
 \end{aligned} \tag{2.30}$$

and the energy-integrated angular flux

$$\varphi(\mathbf{r}, \hat{\Omega}, t) \equiv \int_0^\infty dE \varphi(\mathbf{r}, E, \hat{\Omega}, t)$$

Then the energy-integrated transport equation can be written as

$$\frac{1}{\bar{v}} \frac{\partial \varphi}{\partial t} + \hat{\Omega} \cdot \nabla \varphi + \bar{\Sigma}_t \varphi(\mathbf{r}, \hat{\Omega}, t) = \int d\hat{\Omega}' \bar{\Sigma}_s(\hat{\Omega}' \rightarrow \hat{\Omega}) \varphi(\mathbf{r}, \hat{\Omega}', t) + \bar{s}(\mathbf{r}, \hat{\Omega}, t) \tag{2.31}$$

This energy-averaged equation is known as the *one-speed* or *one (energy) group transport equation*. Of course it has only a formal significance, since the energy averaged parameters such as $\bar{\Sigma}_t$ that appear in the equation depend on the unknown energy-dependent angular flux $\varphi(\mathbf{r}, E, \hat{\Omega}, t)$. However in studying this model we assume that it is possible to guess or approximately calculate these parameters so that they can be regarded as known. For example, if all the particles were to possess only a single energy E , and if $\Sigma_s(E' \rightarrow E) \sim \delta(E' - E)$, then of course the averages in Eq. 2.30 merely would reduce to the value of the cross sections evaluated at the energy E . In the more general case, we might consider using some suitable approximation of $\varphi(\mathbf{r}, E, \hat{\Omega}, t)$ to calculate these quantities,⁸ for example, a

Maxwell-Boltzmann distribution $\varphi(E) \sim vM(E)$. In any event, we assume henceforth that the energy-averaged cross sections (the so-called one-group constants) can be determined and therefore are specified in advance in our study of the one-speed transport equation.

There are actually several problems in transport theory that can be described by such a crude treatment of the particle energy dependence. For example, in nuclear reactor applications, the description of either very fast⁹ or very thermal¹⁰ neutron assemblies can be characterized by such a model. Furthermore, nuclear systems analysis requires a number of neutron transport calculations in which energy effects are of secondary importance (e.g., calculation of the escape probability of fast neutrons in a fuel pin or determination of the flux depression that occurs near a control rod in a nuclear reactor).

The one-speed transport equation also arises in the study of radiative transfer. The general form of the radiative transfer equation for the radiant intensity $I_\nu(\mathbf{r}, \hat{\Omega}, t)$ in which scattering is included can be written as

$$\frac{1}{c} \frac{\partial I_\nu}{\partial t} + \hat{\Omega} \cdot \nabla I_\nu + \Sigma_{\nu} I_\nu(\mathbf{r}, \hat{\Omega}, t) = \Sigma_{\nu} \int d\hat{\Omega}' f_\nu(\hat{\Omega}' \rightarrow \hat{\Omega}) I_\nu(\mathbf{r}, \hat{\Omega}', t) + s_\nu(\mathbf{r}, \hat{\Omega}, t) \quad (2.32)$$

where we have defined the photon interaction cross sections characterizing absorption and scattering, $\Sigma_{av} \equiv \rho \kappa_\nu$ and $\Sigma_{sv} \equiv \gamma_\nu \Sigma_{av}$. In certain applications (the so-called grey atmosphere¹¹ model) one can effectively ignore the frequency dependence of these cross sections. Then if Eq. 2.32 is integrated over frequency, an equation identical to the one-speed transport model Eq. 2.31 results:

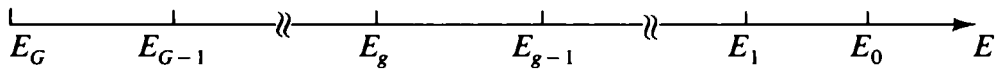
$$\frac{1}{c} \frac{\partial I}{\partial t} + \hat{\Omega} \cdot \nabla I + \Sigma I(\mathbf{r}, \hat{\Omega}, t) = \Sigma \int d\hat{\Omega}' f(\hat{\Omega}' \rightarrow \hat{\Omega}) I(\mathbf{r}, \hat{\Omega}', t) + s(\mathbf{r}, \hat{\Omega}, t)$$

One-speed models also arise in some studies of electron transport, since the elastic collision of electrons with nuclei or atoms is essentially a one-speed process (although, as we noted in Section 1.3, this description must be coupled with a continuous slowing down treatment of the frequent inelastic collision events that cause the electrons to rapidly lose energy as they travel through matter).¹²

On a more fundamental level, one of the most important problems in theoretical physics is the Lorentz gas or fixed scattering center model in which one studies the diffusion of particles through a random array of fixed scattering centers.¹³ Obviously, since the scattering centers are not allowed to recoil, there is no energy exchange in a collision event, and a

one-speed description is appropriate. Of course this problem is essentially just a form of the random walk problem familiar from statistical physics.¹⁴

It is not surprising that the one-speed transport equation has been exhaustively studied in transport theory as an idealized model of various physical phenomena. But there is one additional application of this model that takes on a far more practical (and useful) flavor. In any accurate description of particle transport, it is necessary to consider the particle energy dependence in more detail, and this usually requires a numerical approach. The most popular scheme^{8,15} for treating the particle energy dependence involves a generalization of the one-speed or one-group model in which the energy range is broken into a number of intervals or energy groups:



and then the transport equation is integrated over a given group, $E_g < E < E_{g-1}$. The “backward” group indexing is chosen to correspond to the fact that in most transport processes the particles lose energy in collisions, progressively scattering to lower energies. If we now define the angular flux characterizing a given energy group as

$$\varphi_g(\mathbf{r}, \hat{\Omega}, t) \equiv \int_{E_g}^{E_{g-1}} dE \varphi(\mathbf{r}, E, \hat{\Omega}, t) \equiv \int_g dE \varphi(E)$$

and the corresponding energy-averaged cross sections or group constants characterizing that group as

$$\begin{aligned} v_g^{-1} &\equiv \phi_g^{-1} \int_g dE v^{-1} \varphi(E), & \Sigma_{t,g} &\equiv \phi_g^{-1} \int_g dE \Sigma_t(E) \varphi(E) \\ \Sigma_{s,g} &\equiv \phi_g^{-1} \int_g dE \int_{g'} dE' \Sigma_s(E' \rightarrow E) \varphi(E'), & s_g &\equiv \int_g dE s(E) \end{aligned}$$

then it is apparent that we can integrate the transport equation over a given energy group g to find

$$\frac{1}{v_g} \frac{\partial \varphi_g}{\partial t} + \hat{\Omega} \cdot \nabla \varphi_g + \Sigma_{t,g} \varphi_g = \sum_{g'=1}^G \int d\hat{\Omega}' \Sigma_{s,g'}(\hat{\Omega}' \rightarrow \hat{\Omega}) \varphi_{g'}(\mathbf{r}, \hat{\Omega}', t) + s_g(\mathbf{r}, \hat{\Omega}, t),$$

$$g = 1, \dots, G \quad (2.33)$$

These equations are known as the *multigroup transport equations*, and such

a multigroup approach is the most common method for obtaining accurate solutions to realistic (complex) transport problems in which energy-dependent effects must be included.

But how is this related to our one-speed model? Suppose that we rearrange all the terms in the multigroup transport equation (2.33) that involve groups $g' \neq g$ over to the right-hand side of the equation

$$\frac{1}{v_g} \frac{\partial \varphi_g}{\partial t} + \hat{\Omega} \cdot \nabla \varphi_g + \Sigma_{t_g} \varphi_g - \int d\hat{\Omega}' \Sigma_{s_{gg}} \varphi_g = \sum_{g' \neq g} \int d\hat{\Omega}' \Sigma_{s_{g'g}} \varphi_{g'} + s_g \equiv s'_g \quad (2.34)$$

Now note that if we knew the group fluxes $\varphi_{g'}$, the terms involving these fluxes would appear as *source* terms in an effective one-group transport equation characterizing group g . But this is exactly how the multigroup equations are solved in practice! In the vast majority of transport problems, one can effectively assume that the particles will only lose energy in a collision, since their energy is usually considerably in excess of the thermal energy of the atoms comprising the host medium. Hence we can start at the highest energy group $g=1$ and solve a successive series of one-group problems for the group fluxes. At each stage of this process, the only group fluxes $\varphi_{g'}$ that appear involve higher energy groups and therefore are known from earlier stages of the calculation. Even if “upscattering” in energy occurs, and the $\varphi_{g'}$ then involve both higher and lower energy groups, it is still most efficient to solve the multigroup equations in an iterative fashion by assuming that the $\varphi_{g'}$ are known, solve the effective one-group equations (2.34) down the group structure, and repeat the calculation using the computed values of φ_g .

Hence it should be evident that the one-speed or one-group transport equation is not only significant for simple modeled theories of particle transport, but it also plays a pivotal role in more accurate numerical solutions of transport problems using multigroup methods. It is therefore apparent why this simple form of the transport equation warrants a very thorough study in any development of the subject of transport theory.

We introduce several additional simplifications into the one-speed model we intend to study in this section. First we consider only *stationary* transport processes (deferring the study of time-dependent phenomena to Section 2.3). Next we restrict ourselves to transport processes occurring in *homogeneous, isotropic* media for which the interaction parameters become independent of position and direction, [i.e., $\Sigma(\mathbf{r}, \hat{\Omega}) = \Sigma, c(\mathbf{r}) = c$]. Then the corresponding form of the one-speed transport equation becomes

$$\hat{\Omega} \cdot \nabla \varphi + \Sigma_t \varphi(\mathbf{r}, \hat{\Omega}) = c \Sigma_s \int d\hat{\Omega}' f(\hat{\Omega}' \rightarrow \hat{\Omega}) \varphi(\mathbf{r}, \hat{\Omega}', t) + s(\mathbf{r}, \hat{\Omega}, t)$$

where we recall that $f(\hat{\Omega}' \rightarrow \hat{\Omega})$ is defined to be the probability distribution characterizing particle scattering from directions $\hat{\Omega}'$ to $\hat{\Omega}$.

It occasionally proves convenient to restrict our study to isotropic scattering processes and source distributions for which $f(\hat{\Omega}' \rightarrow \hat{\Omega}) = (4\pi)^{-1}$ and $s(\mathbf{r}, \hat{\Omega}) = S(\mathbf{r})/4\pi$. Under these assumptions, the one-speed transport equation simplifies still further to

$$\hat{\Omega} \cdot \nabla \varphi + \Sigma_t \varphi(\mathbf{r}, \hat{\Omega}) = \frac{c \Sigma_t}{4\pi} \int d\hat{\Omega}' \varphi(\mathbf{r}, \hat{\Omega}') + \frac{S(\mathbf{r})}{4\pi} \quad (2.35)$$

It is useful to note the corresponding form of the integral transport equation in the one-speed approximation

$$\phi(\mathbf{r}) = \int d^3r' \frac{\exp(-\Sigma_t |\mathbf{r} - \mathbf{r}'|)}{4\pi |\mathbf{r} - \mathbf{r}'|^2} [c \Sigma_t \phi(\mathbf{r}') + S(\mathbf{r}')] \quad (2.36)$$

Table 2.3 presents the specific forms taken by these equations in the more common geometries (plane, spherical, and cylindrical).

2.2.2 □ A Formal Solution of the One-Speed Transport Equation □ We begin our study of the one-speed transport equation by solving it in a very formal fashion for the case of isotropic scattering and sources. For this purpose we consider the integral form of the transport equation or Peierls equation as given by Eq. 2.36. This equation is classified mathematically as an inhomogeneous Fredholm equation of the second kind with a displacement kernel.¹⁶ The theory of such equations is rather well developed (see, e.g., Courant and Hilbert¹⁷ or Morse and Feshbach¹⁸). In fact from a historical viewpoint, much more was known about the mathematical properties of this form of the transport equation than the original integro-differential equation derived by Boltzmann, and therefore most of the early “classical” work in transport theory was based on Eq. 2.36. Only comparatively recently has the theory of the integrodifferential form of the transport equation reached a comparable stage of development.

Let us begin by defining an integral operator K

$$K \circ \equiv \int d^3r' \frac{\exp[-\Sigma_t |\mathbf{r} - \mathbf{r}'|]}{4\pi |\mathbf{r} - \mathbf{r}'|^2} c \Sigma_t \circ \quad (2.37)$$

Then we can rewrite our inhomogeneous integral equation (2.36) in operator form as

$$(I - K)\phi = K\left(\frac{S}{c \Sigma_t}\right)$$

Table 2.3 □ The One-Speed Transport Equation for Various Geometries

<i>General form</i>	
$\hat{\Omega} \cdot \nabla \varphi + \Sigma_i \varphi = \frac{c \Sigma_i}{4\pi} \int d\hat{\Omega}' \varphi(r, \hat{\Omega}') + \frac{S(r)}{4\pi}$	$\phi(r) = \int d^3r' \frac{e^{-\Sigma_i r-r' }}{4\pi r-r' ^2} [c \Sigma_i \phi(r') + S(r')]$
<i>Plane symmetry</i>	
$\mu \frac{\partial \varphi}{\partial x} + \Sigma_i \varphi = \frac{c \Sigma_i}{2} \int_{-1}^{+1} d\mu' \varphi(x, \mu') + \frac{S(x)}{2}$	$\phi(x) = \int_{-\infty}^{\infty} dx' \frac{1}{2} E_1(\Sigma_i x-x') [c \Sigma_i \phi(x') + S(x')]$
<i>Spherical symmetry</i>	
$\frac{\mu}{r^2} \frac{\partial}{\partial r} (r^2 \varphi) + \frac{1}{r} \frac{\partial}{\partial \mu} (1-\mu^2) \varphi = \frac{c \Sigma_i}{2} \int_{-1}^{+1} d\mu' \varphi(r, \mu') + \frac{S(r)}{2}$	$\phi(r) = \frac{1}{2r} \int_0^{\infty} r' dr' [E_1(\Sigma_i r-r') - E_1(\Sigma_i r+r')] [c \Sigma_i \phi(r') + S(r')]$
<i>Cylindrical symmetry</i>	
$\frac{\mu}{r} \frac{\partial}{\partial r} (r \varphi) - \frac{1}{r} \frac{\partial}{\partial \omega} (\eta \varphi) = \frac{c \Sigma_i}{4\pi} \int d\hat{\Omega}' \varphi(r, \hat{\Omega}') + \frac{S(r)}{4\pi}$	$\phi(r) = \frac{2}{\pi} \int_0^{\infty} r' dr' \int_{ r-r' }^{r+r'} d\lambda \left\{ \frac{K_1(\Sigma_i \lambda)}{\sqrt{[(r+r')^2 - \lambda^2][\lambda^2 - (r-r')^2]}} \right\} [c \Sigma_i \phi(r') + S(r')]$

where I is the identity operator. The formal solution to this equation can then be written as

$$\phi = (I - K)^{-1} K \left(\frac{S}{c \Sigma_t} \right) \quad (2.38)$$

If K were just a scalar, we could expand the inverse $(I - K)^{-1}$ as

$$(I - K)^{-1} = 1 + K + K^2 + \cdots = \sum_{n=0}^{\infty} K^n, \quad |K| < 1 \quad (2.39)$$

Let us suppose for the moment that we can write a similar expansion for the operator inverse $(I - K)^{-1}$ in Eq. 2.38 to find

$$\phi = \sum_{n=0}^{\infty} K^n \left(\frac{S}{c \Sigma_t} \right) \quad (2.40)$$

Such an expansion is known as a *Neumann series*¹⁶ solution of the integral equation, and it is useful for solving (formally) a wide class of problems, provided the series converges. This form of solution can also be generated using an iterative method (a *Neumann iteration*) defined by

$$\phi^{(n+1)} = K \phi^{(n)} + K \left(\frac{S}{c \Sigma_t} \right), \quad \phi^{(0)} = K \left(\frac{S}{c \Sigma_t} \right)$$

But when is such an expansion valid? From analogy with the power series expansion (Eq. 2.39) we might expect

$$(I - K)^{-1} = \sum_{n=0}^{\infty} K^n \quad \text{for } \|K\| < 1$$

where $\|K\|$ is some appropriate operator norm defined by

$$\|K\| = \max \left\{ \frac{\|Kf\|}{\|f\|} : f \in \text{class of admissible functions} \right\}$$

where the function norm might be, for example, the Hilbert norm

$$\|f\| = \left[\int dx f^*(x) f(x) \right]^{1/2}$$

But when might we expect $\|K\| < 1$? If we examine the first few terms in

the expansion Eq. 2.40, we can assign a physical interpretation to each term as representing a sequence of collision events:

$$\begin{aligned}
 \phi(\mathbf{r}) = & \int d^3r' \frac{\exp(-\Sigma_t|\mathbf{r}-\mathbf{r}'|)}{4\pi|\mathbf{r}-\mathbf{r}'|^2} S(\mathbf{r}') \\
 & \text{virgin source} \\
 & \text{particles} \\
 & \text{arriving at } \mathbf{r} \\
 & + \int d^3r' \frac{\exp(-\Sigma_t|\mathbf{r}-\mathbf{r}'|)}{4\pi|\mathbf{r}-\mathbf{r}'|^2} c\Sigma_t \int d^3r'' \frac{\exp(-\Sigma_t|\mathbf{r}'-\mathbf{r}''|)}{4\pi|\mathbf{r}'-\mathbf{r}''|^2} S(\mathbf{r}'') + \dots \\
 & \text{second generation source} \\
 & \text{particles that have scattered} \\
 & \text{once at } \mathbf{r}' \text{ before arriving at } \mathbf{r}
 \end{aligned}
 \tag{2.41}$$

Hence the Neumann expansion is nothing more than an expansion in the number of times a particle has suffered a collision (i.e., a “collision” expansion). In the light of this physical interpretation, we might expect convergence to depend on whether the system of interest tends to deplete (absorb) or multiply particle numbers in collision events. For example, we might suspect that for neutron transport in a fission chain reaction, $\|K\| < 1$ for a subcritical reactor, $\|K\| = 1$ for a critical reactor, and $\|K\| > 1$ for a supercritical reactor.

To be a bit more precise, in bounded systems we can estimate the norm of K as:

$$\|K\| = \left\| \int d^3r' \frac{\exp(-\Sigma_t|\mathbf{r}-\mathbf{r}'|)}{4\pi|\mathbf{r}-\mathbf{r}'|^2} c\Sigma_t \right\| = O(c\Sigma_t l)$$

where l is some characteristic dimension of the system (e.g., an average chord length, $\langle R \rangle$). Hence if

$$\|K\| = O(c\Sigma_t l) \ll 1$$

that is, if $l \ll \text{mfp}$ or $c \ll 1$, the expansion Eq. 2.41 should converge rapidly. For very small systems or highly absorbing systems, the particles will experience very few collisions before leaking out or being absorbed. Then naturally the Neumann or collision expansion should converge rapidly.

2.2.3 □ General Methods for Solving Boundary Value Problems in Transport Theory □ The collision expansion method is particularly useful for the study of transport in small, highly absorbing systems such as neutron transport in fuel pins or control rods.⁸ However for systems in which scattering interactions are dominant, the expansion will converge very slowly and a more direct method for solving the transport equation must be utilized. The particular method will depend sensitively on the details of the transport problem we wish to consider (e.g., the geometry, type of boundary condition, source distribution).

To illustrate the various methods available for solving the transport equation, let us consider a very simple problem, that of a plane source of infinite extent emitting particles isotropically at the origin of an infinite medium. Then the appropriate forms of the transport equation we wish to solve are the one-dimensional (plane symmetry) integrodifferential or integral forms of the transport equation (refer to Table 2.3) with a source term $S(x) = S_0\delta(x)$. We must augment the integrodifferential equation with appropriate boundary conditions—for example, by requiring $\phi(x, \mu)$ to be bounded as $|x| \rightarrow \infty$. A similar condition requiring $\phi(x) < \infty$ as $|x| \rightarrow \infty$ will be necessary for the solution of the integral equation (see Figure 2.11).

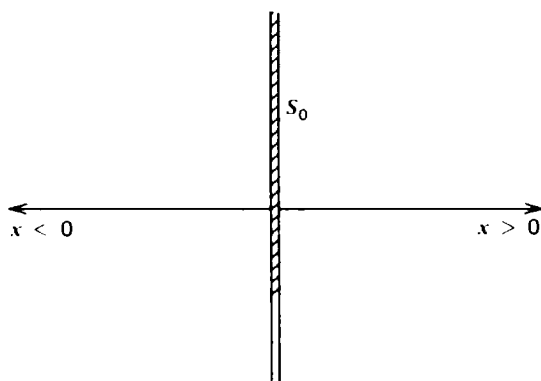


Fig. 2.11 □ An isotropic plane source in an infinite medium.

How might we solve such transport equations? Perhaps we can take a hint from methods used to solve the more familiar diffusion equation for a similar boundary value problem. To this end, consider the plane source problem in diffusion theory:

$$-D \frac{d^2\phi}{dx^2} + \Sigma_a \phi(x) = S_0 \delta(x) \quad (2.42)$$

with boundary conditions:

$$\begin{aligned} \text{i} \quad & \lim_{|x| \rightarrow 0} -D \frac{d\phi}{dx} = \frac{S_0}{2} \\ \text{ii} \quad & \lim_{|x| \rightarrow \infty} \phi(x) = 0 \end{aligned}$$

The two most common methods available for solving such boundary value problems involve integral transforms and separation of variables (or elementary solutions).

Method 1. Integral Transform Method. The infinite domain $x \in (-\infty, \infty)$ suggests that we define the Fourier transform pair

$$\tilde{\phi}(k) = \int_{-\infty}^{\infty} dx e^{ikx} \phi(x), \quad \phi(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{-ikx} \tilde{\phi}(k)$$

If we now multiply Eq. 2.42 by $\exp(ikx)$ and integrate by parts, we arrive at the transformed equation

$$(k^2 D + \Sigma_a) \tilde{\phi}(k) = S_0$$

which we can solve for the transformed solution $\tilde{\phi}(k)$

$$\tilde{\phi}(k) = \frac{S_0}{k^2 D + \Sigma_a} = \frac{S_0/D}{k^2 + L^{-2}}, \quad L \equiv \left(\frac{D}{\Sigma_a} \right)^{1/2}$$

We now must invert this transform. For most boundary value problems, this must be accomplished directly using contour integration methods. That is, one writes the Fourier inversion integral as

$$\phi(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{-ikx} \frac{S_0/D}{k^2 + L^{-2}}$$

then locates the singularities of the integrand in the complex k -plane, performs an appropriate contour deformation, and evaluates the contributions from each of these singularities (e.g., residues from simple poles, line integrals from branch cuts). For our particular problem this procedure yields (see Figure 2.12)

$$\phi(x) = \frac{S_0/D}{2\pi} \oint_C dk \frac{e^{-ikx}}{(k + i/L)(k - i/L)} = \frac{S_0 L}{2D} e^{-x/L}, \quad x > 0$$

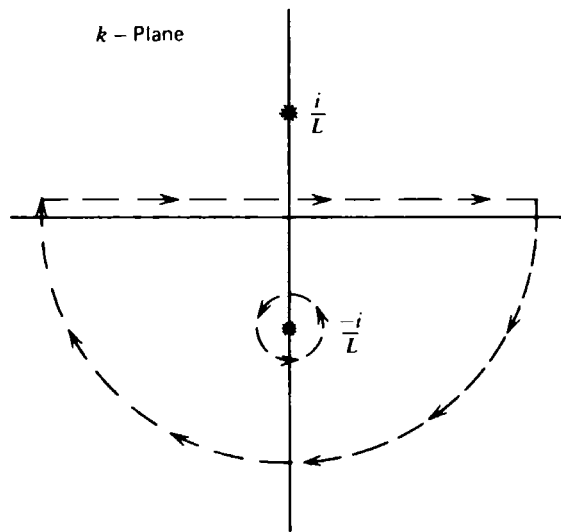


Fig. 2.12 □ Integration contour for plane source problem as described by diffusion theory.

Method 2. Separation of Variables. We first seek elementary solutions to the homogeneous equation counterpart of Eq. 2.42. For an equation in several independent variables, we would seek these elementary solutions as separable products of functions of each variable. However for the simple ordinary differential equation (2.42) we can bypass this step by noting immediately that the elementary solutions must be of the form $\phi(x) \sim \exp(-\kappa x)$ where κ is an unknown parameter. If we substitute this form into the homogeneous equation, we can evaluate this parameter as

$$-\kappa^2 D + \Sigma_a = 0 \Rightarrow \kappa = \pm \left(\frac{\Sigma_a}{D} \right)^{1/2} = \pm L^{-1}$$

to find the general form of the solution to the boundary value problem as

$$\phi(x) = a_1 e^{x/L} + a_2 e^{-x/L}$$

Then the expansion coefficients a_1 and a_2 can be determined by applying the boundary conditions: i $\Rightarrow a_1 = 0$ for $x > 0$, ii $\Rightarrow a_2 = S_0 L / 2D$ to find the solution

$$\phi(x) = \frac{S_0 L}{2D} e^{-x/L}, \quad x > 0$$

Note that the unknown parameters κ that appear in the separation of

variables approach (or “method of elementary solutions”) play the role of relaxation parameters. We later find that they are intimately related to the eigenvalues of the operator governing the diffusion (or transport) process of interest.

With this background, let us return to consider how we might attack the more general transport problems. We can apply the same techniques we used to solve the simple diffusion problem: integral transforms and separation of variables. The integral transform approach has been applied to the solution of transport problems for many years, and aside from a minor complication due to the nature of the boundary conditions imposed in certain types of transport problem (which necessitates the use of the Wiener-Hopf method to perform the transform inversion), its application to these problems is very similar to that characterizing more familiar boundary value problems for partial differential equations.

The separation of variables approach or method of elementary solutions is of more recent vintage in transport theory applications because the elementary solutions to the transport equation tend to be somewhat singular (and tend to involve distributions such as δ -functions and Cauchy principal values). However once some additional mathematics is introduced to facilitate the manipulation of these singular solutions (or, as we will see, singular eigenfunctions), this method can also be applied to transport problems in a straightforward fashion.

Although integral transform and separation of variables methods in transport theory are equivalent, both in power and ease of application, we discuss both approaches for completeness. We begin with the integral transform approach, in keeping with historical precedent, and also because it involves somewhat less in the way of unusual mathematics.

2.2.4 □ Integral Transform Methods □

Plane Source in an Infinite Medium □ In considering the problem of determining the angular flux produced by an isotropic plane source located at the origin of an infinite medium, recall that the form taken by the one-speed transport equation for this problem is

$$\mu \frac{\partial \varphi}{\partial x} + \Sigma_t \varphi(x, \mu) = \frac{c \Sigma_s}{2} \int_{-1}^{+1} d\mu' \varphi(x, \mu') + \frac{S_0}{2} \delta(x) \quad (2.43)$$

with boundary conditions:

$$\lim_{|x| \rightarrow \infty} \varphi(x, \mu) = 0$$

The infinite domain $x \in (-\infty, \infty)$ suggests that a Fourier transform^{2, 18, 19} is appropriate for this problem. To this end we define the Fourier transform pair

$$\tilde{\varphi}(k, \mu) \equiv \int_{-\infty}^{\infty} dx e^{ikx} \varphi(x, \mu), \quad \varphi(x, \mu) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{-ikx} \tilde{\varphi}(k, \mu)$$

If we now multiply the transport equation (2.43) by $\exp(ikx)$ and integrate over x , using integration by parts to handle the derivative term (and noting the boundary conditions at $x \rightarrow \pm \infty$), we find the transformed equation

$$-ik\mu\tilde{\varphi} + \Sigma_t\tilde{\varphi} = \frac{c\Sigma_t}{2} \int_{-1}^{+1} d\mu' \tilde{\varphi}(k, \mu') + \frac{S_0}{2} \quad (2.44)$$

Now divide this equation through by $(\Sigma_t - ik\mu)$ and integrate over μ

$$\tilde{\phi}(k) \equiv \int_{-1}^{+1} d\mu \tilde{\varphi}(k, \mu) = \left[c\Sigma_t\tilde{\phi}(k) + S_0 \right] \frac{1}{2} \int_{-1}^{+1} d\mu (\Sigma_t - ik\mu)^{-1}$$

Therefore we can solve for the angle-integrated flux as

$$\tilde{\phi}(k) = \frac{(S_0/2) \int_{-1}^{+1} d\mu (\Sigma_t - ik\mu)^{-1}}{1 - (c\Sigma_t/2) \int_{-1}^{+1} d\mu (\Sigma_t - ik\mu)^{-1}} \equiv \frac{\chi(k)}{\Lambda(k)} \quad (2.45)$$

If we substitute this back into Eq. 2.44 we can solve for the angular flux as

$$\tilde{\varphi}(k, \mu) = \frac{(c\Sigma_t/2)\chi(k)}{(\Sigma_t - ik\mu)\Lambda(k)} + \frac{S_0/2}{(\Sigma_t - ik\mu)}$$

Therefore all that remains is to invert the transform to find

$$\phi(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{-ikx} \tilde{\phi}(k)$$

Before we attempt this inversion, let us briefly digress to consider how the analogous problem would be attacked using the integral transport equation

$$\phi(x) - \int_{-\infty}^{\infty} dx' E_1(\Sigma_t|x-x'|) \left(\frac{c\Sigma_t}{2} \right) \phi(x') = \left(\frac{S_0}{2} \right) E_1(\Sigma_t, x)$$

We can again use Fourier transforms if we recall the convolution theorem

$$\mathcal{F}\left\{\int_{-\infty}^{\infty} dy f(x-y)g(y)\right\} = \mathcal{F}\{f\} \mathcal{F}\{g\} = \tilde{f}(k)\tilde{g}(k)$$

so that the transformed equation becomes

$$\tilde{\phi}(k) - \left(\frac{c\Sigma_t}{2}\right)\tilde{E}_1(k)\tilde{\phi}(k) = \left(\frac{S_0}{2}\right)\tilde{E}_1(k)$$

A little work (or integral tables) will show that

$$\int_{-\infty}^{\infty} dx e^{ikx} E_1(\Sigma_t|x|) = 2k^{-1} \tan^{-1}\left(\frac{k}{\Sigma_t}\right) = \frac{1}{ik} \ln\left(\frac{\Sigma_t + ik}{\Sigma_t - ik}\right) = \int_{-1}^{+1} \frac{d\mu}{\Sigma_t - ik\mu}$$

Therefore we arrive at a solution identical to that resulting from the transformed integrodifferential transport equation:

$$\tilde{\phi}(k) = \frac{(S_0/k) \tan^{-1}(k/\Sigma_t)}{1 - (c\Sigma_t/k) \tan^{-1}(k/\Sigma_t)} = \frac{\frac{S_0}{2ik} \ln\left(\frac{\Sigma_t + ik}{\Sigma_t - ik}\right)}{1 - \frac{c\Sigma_t}{2ik} \ln\left(\frac{\Sigma_t + ik}{\Sigma_t - ik}\right)} = \frac{\chi(k)}{\Lambda(k)} \quad (2.46)$$

Thus our only remaining task is to perform the Fourier transform inversion. To accomplish this, we utilize contour integration in the complex k -plane. The general scheme is as follows:

- i Note that the Fourier transform we have been utilizing is defined for real k . Therefore we must analytically continue the definition of $\tilde{\phi}(k)$ to the complex k -plane. Then we examine the analytic behavior of $\phi(k)$ in the k -plane.
- ii Deform the original inversion contour around the singularities of $\tilde{\phi}(k)$.
- iii Evaluate the contributions from these singularities, including residues from poles and line integrals from branch cuts.

Therefore let us begin by analytically continuing $\tilde{\phi}(k)$ into the complex k -plane by simply interpreting the explicit form given by Eq. 2.46 as a function of complex k . We note that $\tilde{\phi}(k)$ has a pair of branch point singularities at $k = \pm i\Sigma_t$, because of the $\ln[(\Sigma_t + ik)/(\Sigma_t - ik)]$ term. To

define this logarithm function as a single-valued function, therefore, we must insert branch cuts. The choice of a branch cut arises very frequently in mathematical physics, and it is almost never uniquely determined by the mathematics of the problem alone, but in addition usually requires a dash of physics. In our case we can merely recall the form of the angular integration in Eq. 2.45 that led to the logarithm term. If we notice that this integral is "singular" for $k = \Sigma_t / i\mu$ for $\mu \in [-1, +1]$, we find that we must choose the branch cut along the imaginary axis as shown in Figure 2.13.

Now that we have taken care of the branch points, we look for isolated singularities such as poles. At first it appears that the origin $k=0$ is a candidate, but if we note that $\ln[(\Sigma_t + ik)/(\Sigma_t - ik)] \sim 2ik/\Sigma_t$ for small k , it is apparent that $(1/ik)$ times this quantity is analytic in the cut-plane. Therefore the only possibility for poles of $\tilde{\phi}(k)$ involves zeros of the denominator $\Lambda(k)$:

$$\Lambda(k) = 1 - \frac{c\Sigma_t}{2ik} \ln\left(\frac{\Sigma_t + ik}{\Sigma_t - ik}\right) = 1 - \frac{c\Sigma_t}{k} \tan^{-1}\left(\frac{k}{\Sigma_t}\right) = 0 \quad (2.47)$$

In fact, since $k^{-1} \tan^{-1}(k/\Sigma_t)$ is even in k , then if k_0 is a zero of $\Lambda(k)$, so also is $k = -k_0$. A more detailed analysis reveals the presence of two zeros, $\pm k_0$, of $\Lambda(k)$ [and therefore two poles of $\tilde{\phi}(k)$]. Using graphical techniques, we can identify three possible cases depending on the value

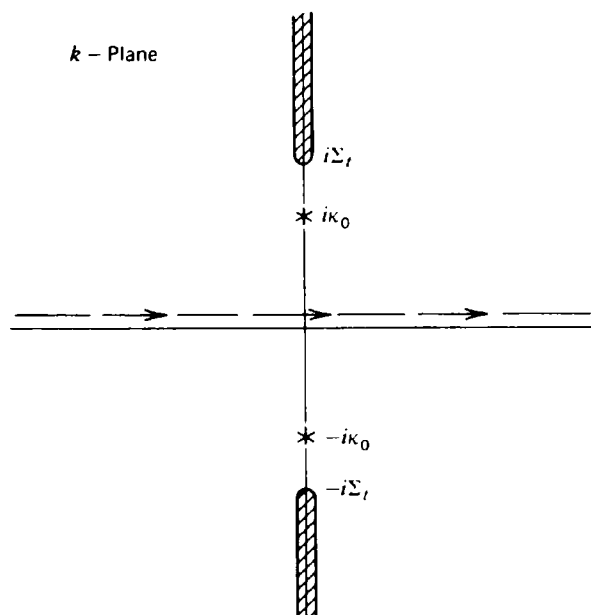


Fig. 2.13 □ k -Plane structure for plane source problem.

of c :

- $c > 1$ There are two real roots, $\pm k_0$, which lie on the real axis and will correspond to solutions of the form $\exp(\pm ik_0x)$.
- $c = 0$ In this case, $k = 0$ is a double root.
- $c < 1$ There are two imaginary zeros $\pm i\kappa_0$, which correspond to solutions of the form $\exp(\pm \kappa_0x)$.

Actually, as we show later, in the case $c < 1$ we obtain solutions $\exp(\pm \kappa_0x)$ similar to those obtained in diffusion theory (cf. Section 2.2.4). In fact, κ_0 is essentially just the inverse of the "diffusion length" $L = (D/\Sigma_a)^{1/2}$. That is, for small absorption such that $c \lesssim 1$, we can expand the root of Eq. 2.47 to find

$$\kappa_0 = \Sigma_t [3(1-c)]^{1/2} \left[1 - \left(\frac{2}{5} \right) (1-c) + \cdots \right], \quad |1-c| \ll 1$$

But since we can identify $L^2 = [3(1-c)\Sigma_t^2]^{-1}$, we find that this expansion yields the diffusion theory relaxation length L to lowest order in $1-c$.

Armed with this information, we now return to the inversion of the Fourier transformed flux $\tilde{\phi}(k)$

$$\phi(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{-ikx} \frac{\chi(k)}{\Lambda(k)}$$

We have determined the singularities of $\tilde{\phi}(k)$ to be as shown in Figure 2.13 (for $c < 1$). Suppose that k is in the lower half-plane. Then for large $x > 0$, $\exp[-i(-i\kappa)x] \rightarrow \exp(-\kappa x) \rightarrow 0$. Thus for positive values of x , we can deform the inversion contour into the lower half k -plane as follows. Apply the residue formula to the closed contour shown in Figure 2.14. Then symbolically we would find

$$\oint = 2\pi i \operatorname{Res}(k = -i\kappa_0) = 2\pi i \left(\frac{\partial \Lambda}{\partial k} \right) \chi(i\kappa_0) e^{-\kappa_0 x} \equiv 2\pi a_0 e^{-\kappa_0 x}$$

If we shrink the smaller radius to zero and expand the larger radius to infinity, we can identify

$$\phi(x) = \frac{1}{2\pi} \left[- \lim_{R \rightarrow \infty} \int_{C_2 + C_3 + C_5 + C_6} - \lim_{r \rightarrow 0} \int_{C_4} \right] dk e^{-ikx} \frac{\chi(k)}{\Lambda(k)} + a_0 e^{-\kappa_0 x} \quad (2.48)$$

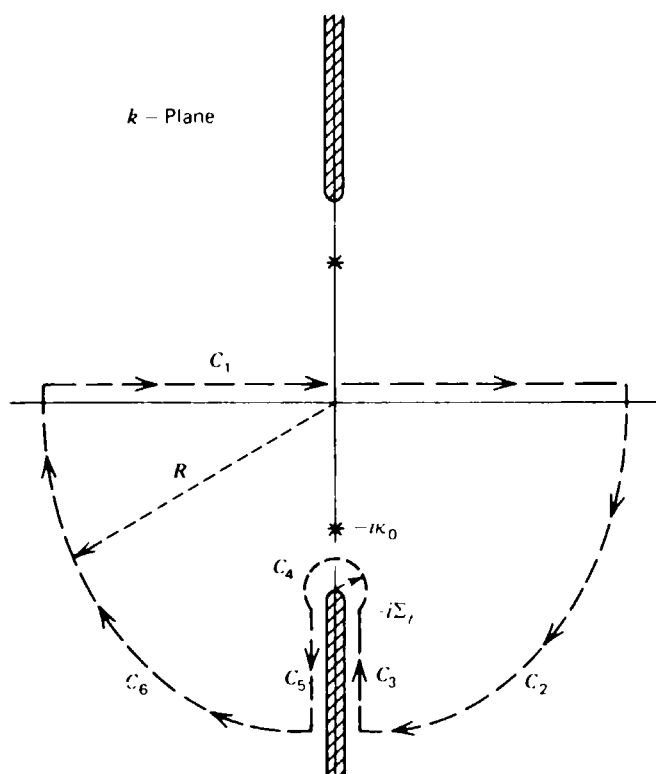


Fig. 2.14 □ Integration contour for Fourier transform inversion.

Let us proceed more carefully to evaluate each of the contributions to this integral.

C_4 Since $k = -i\Sigma_i$ is not a pole, $\int_{C_4} \rightarrow 2\pi r \rightarrow 0$ as $r \rightarrow 0$.

C_2, C_6 For large $k = R \exp(i\theta)$, $\ln[(1 + iR e^{i\theta})/(1 - iR e^{i\theta})] \rightarrow \ln(-1) = \pm i\pi$. Hence we find $\chi(k)/\Lambda(k) \rightarrow O(1/R)$ as $R \rightarrow \infty$. At this point, it is easiest to recall a “well-known” fact concerning Laplace transforms (which are, of course, a special form of Fourier transforms):

$$\int_C ds e^{sf}(s) \rightarrow 0 \quad \text{as } R \rightarrow \infty \quad \text{when } f(x) = O(R^{-\nu}), \nu > 0$$

This fact (known in the trade as “Jordan’s lemma”)²⁰ implies that the integrals over C_2 and C_6 vanish as $R \rightarrow \infty$. [For the analogous point source problem, $\phi(k) \sim O(1)$ as $R \rightarrow \infty$, and life becomes a bit more complicated. Then a special limit procedure due to Cesàro^{2,19} must be used.]

C_3, C_5 We can calculate the limiting value of the logarithm function as $k \rightarrow i\kappa$ from either side of the branch cut as

$$\ln\left(\frac{\Sigma_t + ik}{\Sigma_t - ik}\right) \rightarrow \ln\left|\frac{\Sigma_t + \kappa}{\Sigma_t - \kappa}\right| \pm \pi \quad \text{on} \quad \begin{matrix} C_3 \\ C_5 \end{matrix}$$

Then after some manipulation, we find

$$\begin{aligned} \frac{1}{2\pi} \int_{C_3 + C_5} &= \int_{\Sigma_t}^{\infty} d\kappa (2\kappa)^{-1} e^{-\kappa x} \left\{ \left[1 - \frac{c\Sigma_t}{2\kappa} \ln\left|\frac{\Sigma_t + \kappa}{\Sigma_t - \kappa}\right| \right]^2 + \left(\frac{c\Sigma_t \pi}{2\kappa} \right)^2 \right\}^{-1} \\ &\equiv \int_{\Sigma_t}^{\infty} d\kappa A(\kappa) e^{-\kappa x} \end{aligned}$$

Therefore, after collecting together all these bits and pieces, we find that we can write our inverted solution from Eq. 2.48 as

$$\phi(x) = a_0 e^{-\kappa_0 |x|} + \int_{\Sigma_t}^{\infty} d\kappa A(\kappa) e^{-\kappa |x|} \quad (2.49)$$

Let us recall that $\kappa_0 < \Sigma_t$. Hence the “discrete” exponential mode is spatially damped less than the branch cut contribution, and we would expect that for large distances from the source plane, the solution will assume an asymptotic form

$$\phi(x) \sim a_0 e^{-\kappa_0 x} \equiv \phi_{\text{asy}}(x) \quad \text{for } x \gg \Sigma_t^{-1} = \text{mfp}$$

But if we note that for $c \sim 1$, $\kappa_0 \sim L^{-1}$, this asymptotic form is similar to that given by diffusion theory. Close to the source plane we must retain the branch cut term; therefore the terms “asymptotic” and “transient” are frequently applied to each of the contributions in Eq. 2.49. The relative magnitudes of each of these components depends on the value of c (e.g., the amount of absorption relative to scattering). For $c \ll 1$, we find that the integrand $A(\kappa)$ due to the branch cut contribution becomes more and more peaked near $\kappa = \Sigma_t$, while the root κ_0 approaches the branch point at $k = \pm i\Sigma_t$. This causes the transient term to approach the asymptotic term in magnitude.

Point Source in an Infinite Medium □ A very similar approach can be used to determine the flux resulting from an isotropic point source at the origin of an infinite medium as described by the integral transport equation¹⁹

$$\phi(\mathbf{r}) = \int d^3r' \frac{\exp(-\Sigma_t |\mathbf{r} - \mathbf{r}'|)}{4\pi |\mathbf{r} - \mathbf{r}'|^2} [c\Sigma_t \phi(\mathbf{r}') + S_0 \delta(\mathbf{r}')] \quad (2.50)$$

We now define a three-dimensional Fourier transform pair:

$$\tilde{\phi}(\mathbf{k}) \equiv \int d^3r e^{i\mathbf{k}\cdot\mathbf{r}} \phi(\mathbf{r}), \quad \phi(\mathbf{r}) = \frac{1}{(2\pi)^3} \int d^3k e^{-i\mathbf{k}\cdot\mathbf{r}} \tilde{\phi}(\mathbf{k})$$

If we apply this to the integral transport equation (2.50), we find an equation for the transformed flux

$$\tilde{\phi}(\mathbf{k}) = c \frac{\Sigma_t}{k} \tan^{-1}\left(\frac{k}{\Sigma_t}\right) \tilde{\phi}(\mathbf{k}) + \frac{S_0}{k} \tan^{-1}\left(\frac{k}{\Sigma_t}\right)$$

or solving,

$$\tilde{\phi}(k) = \frac{S_0 k^{-1} \tan^{-1}(k/\Sigma_t)}{1 - (c\Sigma_t/k) \tan^{-1}(k/\Sigma_t)}$$

Then we can write the Fourier transform inversion as

$$\phi(\mathbf{r}) = \frac{1}{(2\pi)^3} \int d^3k e^{-i\mathbf{k}\cdot\mathbf{r}} \tilde{\phi}(\mathbf{k}) = \frac{1}{(2\pi^2)} \int_0^\infty dk k^2 \left(\frac{\sin kr}{kr} \right) \tilde{\phi}(k)$$

Once again we can use contour integration in the complex k -plane to evaluate this inversion integral. Since the details of this inversion calculation are very similar to those we described for the plane source problem, we give only the final result here:

$$\phi(r) = (2\pi r)^{-1} \left[a_0 \kappa_0 e^{-\kappa_0 r} + \int_{\Sigma_t}^\infty d\kappa A(\kappa) \kappa e^{-\kappa r} \right]$$

This result is quite similar to that of the plane source problem. Indeed, if we recognize that the plane source can be represented as a superposition of point sources, it is not surprising that we can relate these two solutions by

$$\phi_{\text{pt}}(r) = -(2\pi r)^{-1} \frac{d\phi_{\text{pl}}}{dx} \Big|_{x=r}$$

or

$$\phi_{\text{pl}}(x) = 2\pi \int_{|x|}^\infty dR R \phi_{\text{pt}}(R)$$

The Milne Problem: Solution by Way of the Wiener-Hopf Technique □ We have just demonstrated how integral transforms (in particular, Fourier transforms) can be used to obtain the solution to the problem of an

isotropic plane (or point) source in an infinite medium. The general procedure was to transform the transport equation, solve the transformed equation for the transformed solution, study the analytic structure of the transformed solution in the k -plane, and finally invert the transform using contour integration. But most problems in transport theory are not nearly so simple. In particular, the second step of solving the transformed equation frequently becomes rather difficult.

The infinite medium problems we have considered are examples of so-called full-range boundary value problems in that the source and boundary conditions are given for all values of $\mu \in [-1, +1]$. By way of contrast, consider a half-space problem with a free surface in which we require a boundary condition of zero reentrant flux

$$\varphi(x_0, \mu) = 0, \quad \mu \in [0, 1]$$

Notice that this boundary condition implies nothing about $\varphi(x_0, \mu)$ for $\mu \in [-1, 0]$. Such “partial-range” boundary value problems are considerably more difficult to treat. (In fact, they are the analogues to mixed boundary value problems²¹ that arise in partial differential equations.)

To illustrate how these problems must be approached, we now turn our attention to what is perhaps the most famous problem of transport theory, the *Milne problem*. The essence of the problem is to determine the emerging flux from a free surface, given a source at infinity. Typical applications include the determination of the neutron distribution emerging from a thick shield⁸ or the distribution of light emerging from the surface of a star.²²

To be more precise, consider the integral equation for the half-space geometry illustrated in Figure 2.15:

$$\phi(x) = \frac{c\Sigma_t}{2} \int_0^\infty dx' E_1(\Sigma_t|x-x'|)\phi(x'), \quad 0 \leq x < \infty \quad (2.51)$$

Here we have simply truncated the integration in the more general form of the equation. There is no source term in this equation, since one imagines in the Milne problem that all sources are placed at infinity. To implement the source condition, we recall from our study of the plane source problem that far away from a source we expect to find an asymptotic flux behavior of the form $\exp(-\kappa_0 x)$. Thus we can attach a source condition by merely requiring that any solutions that we obtain for Eq. 2.51 behave as

$$\phi(x) \sim C \exp(\kappa_0 x) \quad \text{as } x \rightarrow \infty$$

Therefore we now have an integral equation to solve with an accompanying condition on the solution for large x . Such integral equations arise

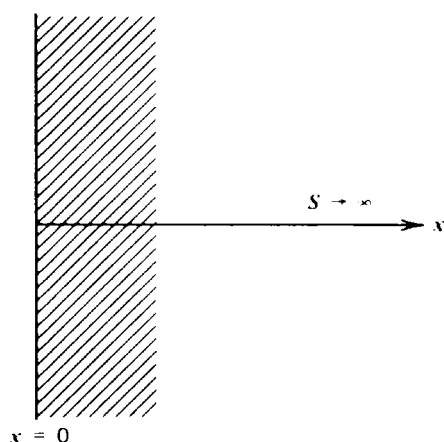


Fig. 2.15 □ Half-space geometry for the Milne problem.

very frequently in physics, and the procedure we now describe for treating the Milne problem can be used to find the solution to many such equations. Suppose the range of integration in Eq. 2.51 ran from $-\infty$ to $+\infty$. Then, just as in the plane source problem, we could use a Fourier transform and run through the standard procedure of transforming the original equation, solving the transformed equation, then performing a transform inversion. But the difficulty in such partial-range problems is that the unknown $\phi(x)$ in Eq. 2.51 is not defined for $x < 0$.

Let us ignore this fact for the moment and forge ahead by taking a Fourier transform, but take care to decompose it in a special way:

$$\tilde{\phi}(k) = \int_{-\infty}^0 dx e^{ikx} \phi(x) + \int_0^{\infty} dx e^{ikx} \phi(x) \equiv \tilde{\phi}_-(k) + \tilde{\phi}_+(k)$$

Since $\phi(x)$ for $x > 0$ is defined as the solution to the integral equation (2.51), $\tilde{\phi}_+(k)$ is presumably determinable. But we have no definition of $\phi(x)$ for $x < 0$. In lieu of a definition, we simply use the integral equation (2.51) itself to formally define $\phi(x)$ for $x < 0$ by extending the range of the independent variable to $x < 0$. (Although it may make mathematical sense to extend the integral equation in this way, it makes no physical sense, since the region $x < 0$ is a vacuum and is not described by Eq. 2.51.)

With this worry pushed aside for the present, we can go ahead and Fourier transform the integral equation (using a modified version of the convolution theorem) to find

$$\tilde{\phi}_+(k) + \tilde{\phi}_-(k) = \left[\frac{c \Sigma_t}{2ik} \ln \left(\frac{\Sigma_t + ik}{\Sigma_t - ik} \right) \right] \tilde{\phi}_+(k)$$

or rearranging

$$\Lambda(k) \tilde{\phi}_+(k) = -\tilde{\phi}_-(k) \quad (2.52)$$

where we define as before

$$\Lambda(k) \equiv 1 - \frac{c\Sigma_t}{2ik} \ln \left(\frac{\Sigma_t + ik}{\Sigma_t - ik} \right)$$

Now the next step in our standard integral transform procedure would be to solve Eq. 2.52 for $\tilde{\phi}(k)$. But how? This is one equation for two unknowns, $\phi_+(k)$ and $\phi_-(k)$! Fortunately, the Wiener-Hopf technique was devised to solve just such a problem.²¹⁻²³

We begin by studying the analytic structure of Eq. 2.51. First note that from our source condition at $x \rightarrow \infty$, $\phi(x) \rightarrow 0(\exp(+\kappa_0 x))$, we can determine that

$$\tilde{\phi}_+(k) \equiv \int_0^\infty dx e^{ikx} \phi(x)$$

is analytic in the upper half k -plane, $\text{Im } k > \kappa_0$.

We next try to arrive at a similar statement for $\tilde{\phi}_-(k)$ by examining the limiting behavior of $\phi(x)$ as $x \rightarrow -\infty$. Of course, although we are not really interested in the physical interpretation of $\phi(x)$ for $x < 0$, we can go ahead and use the integral equation (2.51) to find

$$\phi(x) = \frac{c\Sigma_t}{2} \int_0^\infty dx' E_1(\Sigma_t |x - x'|) \phi(x') \sim 0(e^{\Sigma_t x}), \quad x \rightarrow -\infty$$

Hence we conclude that

$$\tilde{\phi}_-(k) \equiv \int_{-\infty}^0 dx e^{ikx} \phi(x)$$

is analytic in the lower half k -plane, $\text{Im } k < \Sigma_t$.

As a final piece of information, we know that $\Lambda(k)$ is analytic in the k -plane cut from $(-i\infty, -i\Sigma_t]$ and $[i\Sigma_t, i\infty)$ with zeros at $k = \pm i\kappa_0$. Hence the regions of analyticity of $\phi_+(k)$, $\phi_-(k)$, and $\Lambda(k)$ overlap in a strip: $\kappa_0 < \text{Im } k < \Sigma_t$ (see Figure 2.16).

Now *suppose* we could decompose $\Lambda(k)$ into a quotient of two functions

$$\Lambda(k) = \frac{\lambda_+(k)}{\lambda_-(k)}$$

where $\lambda_+(k)$ is analytic in some upper half-plane and $\lambda_-(k)$ is analytic in some lower half-plane, and these half-planes have a common strip of

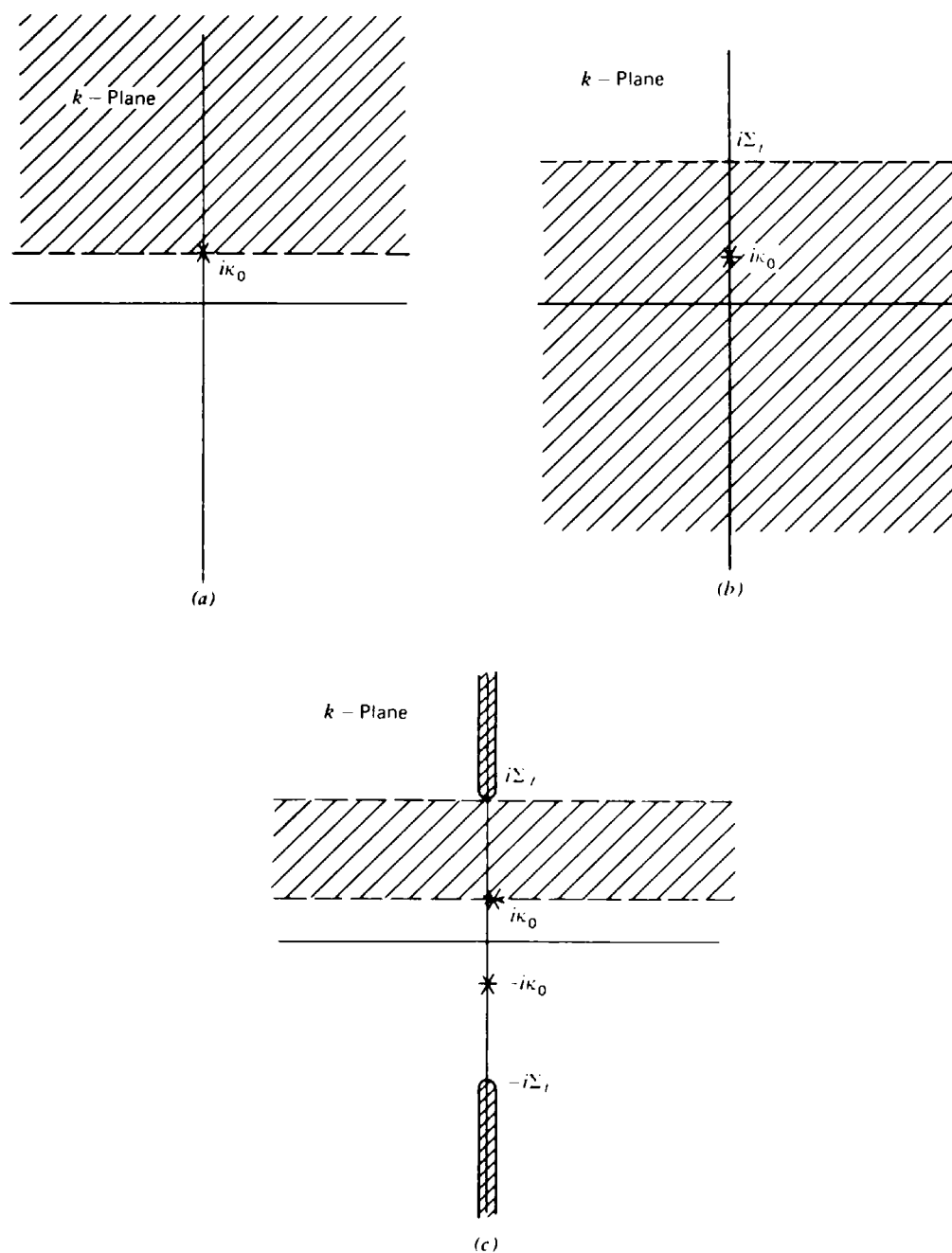


Fig. 2.16 $\square$ Regions of analyticity of functions in the Wiener-Hopf problem. (a) $\tilde{\phi}_+(k)$. (b) $\tilde{\phi}_-(k)$. (c) $\Lambda(k)$.

analyticity within the strip $\kappa_0 < \text{Im } k < \Sigma_t$. Then we could write Eq. 2.52 as

$$\lambda_+(k)\tilde{\phi}_+(k) = -\lambda_-(k)\tilde{\phi}_-(k) \quad (2.53)$$

for k in this strip.

Next, suppose we define a function

$$J(k) \equiv \begin{cases} \lambda_+(k)\tilde{\phi}_+(k), & \text{Im } k > \kappa_0 \\ -\lambda_-(k)\tilde{\phi}_-(k), & \text{Im } k < \Sigma_t \end{cases}$$

First note that by construction, $J(k)$ is analytic in the upper half-plane $\text{Im } k > \kappa_0$ and lower half-plane $\text{Im } k < \Sigma_t$. Furthermore, these two representations are each analytic and equal in the common strip by Eq. 2.53. Therefore we conclude that $J(k)$ must be an entire function of k . (One can use the identity theorem for analytic functions or analytic continuation to show this.) We can now apply Liouville's theorem²⁴ to completely determine $J(k)$ by using its behavior at infinity. Then, once we know $J(k)$, we can solve for

$$\tilde{\phi}_\pm(k) = \pm \frac{J(k)}{\lambda_\pm(k)}$$

and find

$$\phi(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{-ikx} [\tilde{\phi}_+(k) + \tilde{\phi}_-(k)]$$

with the integration path confined to the strip $\kappa_0 < \text{Im } k < \Sigma_t$.

The key step in this procedure is the decomposition of an analytic function into a quotient (or sum) of functions, each analytic in a different half-plane with an overlapping strip of analyticity. This decomposition can sometimes be accomplished by inspection. However for the Milne problem (and most transport problems) it cannot, and we must employ two general theorems due to Wiener and Hopf, which provide the detailed form of the decomposition. These are stated and proved in Appendix A.

We note here only that the detailed application of the Wiener-Hopf decomposition theorems to $\Lambda(k)$ yields the result

$$\lambda_+(k) = \left[\frac{(k^2 + \kappa_0^2)}{(k + i\Sigma_t)} \right] \exp[\psi_+(k)]$$

$$\lambda_-(k) = (k - i\Sigma_t)^{-1} \exp[\psi_-(k)]$$

where we define

$$\psi_+(k) \equiv \frac{1}{2\pi i} \int_{-\infty + ia_1}^{\infty + ia_1} dz \frac{\psi(z)}{z - k}, \quad \text{Im } k > a_1 > \kappa_0$$

$$\psi_-(k) \equiv \frac{1}{2\pi i} \int_{-\infty + ib_1}^{\infty + ib_1} dz \frac{\psi(z)}{z - k}, \quad \text{Im } k < b_1 < \Sigma_t$$

and

$$\psi(z) \equiv \ln \left[\left(\frac{z^2 + \Sigma_t^2}{z^2 + \kappa_0^2} \right) \Lambda(z) \right]$$

The detailed construction of $\lambda_{\pm}(k)$ is given in Appendix A.

We can now use these explicit forms for $\lambda_{\pm}(k)$ to examine the behavior of $J(k)$ for large k and complete the solution of the problem. Since one can show that $\psi(k) \rightarrow \text{constant}$ for large k , then $\exp[\psi_{\pm}(k)] \rightarrow 1$ as $k \rightarrow \infty$. Furthermore, since $\tilde{\phi}_+(k)$ is integrable, it must tend to zero at large k . Hence we conclude

$$\lambda_+(k) \tilde{\phi}_+(k) \rightarrow k \tilde{\phi}_+(k) \sim 0(1) \quad \text{as } k \rightarrow \infty$$

Similarly we can show that $\lambda_-(k) \tilde{\phi}_-(k) \sim 0(1)$ as $k \rightarrow \infty$. Hence by Liouville's theorem [i.e., if $f(z)$ is an entire function and $|f(z)|$ is bounded for all values of z in the complex plane, then $f(z)$ is a constant], we find

$$J(k) = \text{constant} = A$$

Thus we have now used the Wiener-Hopf technique to find

$$\tilde{\phi}_+(k) = A \left[\frac{(k + i\Sigma_t)}{(k^2 + \kappa_0^2)} \right] \exp[-\psi_+(k)]$$

$$\tilde{\phi}_-(k) = -A(k - i\Sigma_t) \exp[-\psi_-(k)]$$

The final step involves the inversion

$$\phi(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{-ikx} \tilde{\phi}_-(k) + \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{-ikx} \tilde{\phi}_+(k)$$

As before, we can use contour deformation into the lower half-plane for $x > 0$. But since $\tilde{\phi}_-(k)$ is analytic in the lower half-plane, it will yield no

contribution to the inversion. Thus we need only calculate

$$\phi(x) = \frac{A}{2\pi} \int_{-\infty + i\Sigma_l}^{\infty + i\Sigma_l} dk e^{-ikx} \left(\frac{k + i\Sigma_l}{k^2 + \kappa_0^2} \right) e^{-\psi_+(k)}$$

where

$$\psi_+(k) = \frac{1}{2\pi i} \int_{-\infty + ia_l}^{\infty + ia_l} \frac{dz}{z - k} \ln \left[\left(\frac{z^2 + \Sigma_l^2}{z^2 + \kappa_0^2} \right) \Lambda(z) \right]$$

If we deform our inversion contour as shown in Figure 2.17, we find that our final solution takes the form

$$\begin{aligned} \phi(x) = & \frac{A}{2} \left(\frac{\Sigma_l + \kappa_0}{\kappa_0} \right) e^{-\psi_+(i\kappa_0)} e^{\kappa_0 x} - \frac{A}{2} \left(\frac{\Sigma_l - \kappa_0}{\kappa_0} \right) e^{-\psi_-(-i\kappa_0)} e^{-\kappa_0 x} \\ & + \frac{iA}{\pi} \int_{\Sigma_l}^{\infty} ds e^{-sx} \left(\frac{s - \Sigma_l}{s^2 - \kappa_0^2} \right) [\exp(-\psi_+(is)) - \exp(-\psi_-(-is))] \end{aligned}$$

where $\psi_{\pm}^{\pm}$ is the limit of $\psi_{\pm}(k)$ as $k \rightarrow \pm is$.

Although the expression is rather ugly, this is the “solution,” the *exact* solution, to the Milne problem. There are many manipulations one can use to simplify this expression.²⁵ However we defer a detailed analysis of the solution until we re-solve the Milne problem in the next section, using the separation of variables method.

The procedure we have just outlined looks rather cumbersome and complex. And indeed it is! But even so, it is in many ways a more direct approach to solving the types of boundary value problem that arise in transport theory than the separation of variables method. It is an unfortunate fact of life that transport problems that involve partial-range boundary conditions are hard to solve!

The Milne problem could also have been approached by application of integral transforms directly to the integrodifferential form of the transport equation:^{26,27}

$$\mu \frac{\partial \varphi}{\partial x} + \Sigma_l \varphi(x, \mu) = \frac{c\Sigma_l}{2} \int_{-1}^{+1} d\mu' \varphi(x, \mu') \quad (2.54)$$

subject to boundary conditions:

$$\begin{aligned} \text{i } & \varphi(x, \mu) \sim O(e^{\kappa_0 x}), \quad x \rightarrow \infty \\ \text{ii } & \varphi(0, \mu) = 0, \quad 0 \leq \mu \leq 1 \end{aligned}$$

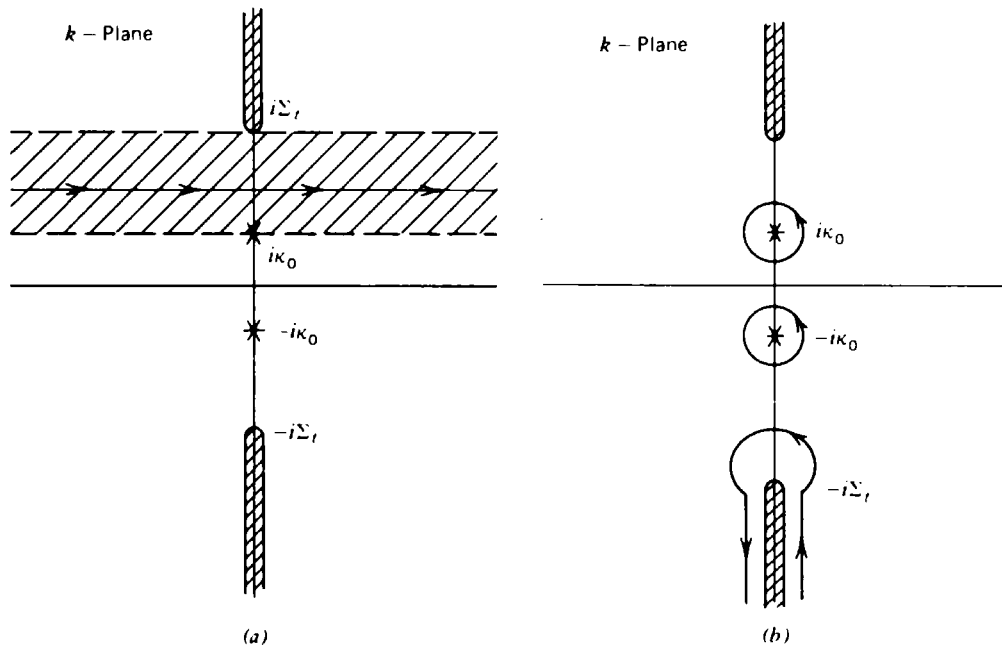


Fig. 2.17 □ The original (a) and deformed (b) inversion contours for the Milne problem.

Since Eq. 2.54 is defined on the domain $[0, \infty)$, it is appropriate to select a Laplace transform pair

$$\tilde{\varphi}(s, \mu) \equiv \int_0^\infty dx e^{-sx} \varphi(x, \mu), \quad \varphi(x, \mu) = \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} ds e^{sx} \tilde{\varphi}(s, \mu)$$

Then if we Laplace transform the transport equation (2.54), we find

$$\mu [s\tilde{\varphi}(s, \mu) - \varphi(0, \mu)] + \Sigma_t \tilde{\varphi}(s, \mu) = \frac{c\Sigma_t}{2} \int_{-1}^{+1} d\mu' \tilde{\varphi}(s, \mu')$$

or after division by $(\Sigma_t + s\mu)$,

$$\tilde{\varphi}(s, \mu) = \left(\frac{c\Sigma_t/2}{\Sigma_t + s\mu} \right) \int_{-1}^{+1} d\mu' \tilde{\varphi}(s, \mu') + \frac{\mu\varphi(0, \mu)}{\Sigma_t + s\mu}$$

Next, we can integrate over μ and rearrange to find

$$\Lambda(s) \tilde{\phi}(s) = \int_{-1}^0 d\mu \frac{\mu\varphi(0, \mu)}{\Sigma_t + s\mu} \equiv g(s) \quad (2.55)$$

Now note that $\tilde{\phi}(s)$ is analytic in the right half-plane $\text{Re } s > \kappa_0$, and $g(s)$ is

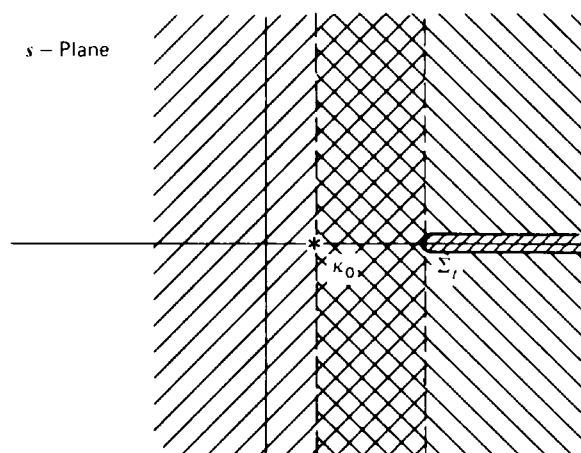


Fig. 2.18 □ s -Plane structure for the Milne problem solved by way of Laplace transforms.

analytic in the left half-plane $\text{Re } s < \Sigma_l$. Furthermore, Eq. 2.55 is satisfied in an overlapping strip of analyticity $\kappa_0 < \text{Re } s < \Sigma_l$. Thus we can identify the usual type of function equation in complex variables which is amenable to the Wiener-Hopf technique (see Figure 2.18).

Half-space problems of several different types can be approached in a very similar manner (e.g., the study of the flux in the neighborhood of the interface between two dissimilar media or the albedo problem in which one calculates the flux resulting from a source incident on the free surface of a half-space geometry). However since the cataloguing of the solvable plane geometry problems in one-speed transport theory can be accomplished more efficiently using the singular eigenfunction method (once we have constructed these functions and determined their properties for half-space geometries, we can immediately obtain the solutions for any of the “solvable” problems), we avoid further applications of the integral transform method at this time.

2.2.4 □ Separation of Variables (Singular Eigenfunction Method) □ An alternative approach to integral transforms for solving the integrodifferential form of the transport equation is the analogue to the separation of variables method commonly employed in solving partial differential equations (PDEs). Recall that the general approach is as follows:

- i Seek a separable solution, say $\varphi(x, \mu) = \chi(x)\psi(\mu)$, to the homogeneous PDE of interest.

- ii This will yield ordinary differential equations (ODEs) for $\chi(x)$ and $\psi(\mu)$. These ODEs actually take the form of eigenvalue problems $A\psi_\lambda = \lambda\psi_\lambda$, where λ is the separation constant. The idea now is to solve the ODEs—the eigenvalue problem—for all the elementary solutions or eigenfunctions.
- iii Finally one seeks the general solution to the original PDE as a linear combination of these eigenfunctions

$$\varphi(x, \mu) = \sum_{\lambda} a_{\lambda} \chi_{\lambda}(x) \psi_{\lambda}(\mu)$$

and uses the boundary or initial conditions to determine the expansion coefficients a_{λ} (using a property such as orthogonality).

This procedure can also be applied to the transport equation in a very similar manner—with one exception. Now the eigenvalue problem is not an ODE, but rather an integral equation in μ . Furthermore, the eigenfunctions are of a rather singular type—in fact, they are not even “functions” at all, but rather generalized functions or distributions (e.g., δ -functions). For this reason the separation of variables approach in transport theory is sometimes referred to as the *singular eigenfunction method*. It is also occasionally referred to as *Case’s method*, after K. M. Case who developed the technique for neutron transport problems.²⁸

Actually the general idea of expanding the solution to the transport equation in a set of singular elementary solutions or eigenfunctions can be traced back to Davison (1945).²⁹ It was first applied to the study of electron density oscillations in plasmas by Van Kampen,³⁰ who also extended the method to neutron transport. However in 1960 Case³¹ provided a very detailed analysis of the properties of the singular eigenfunctions, including not only proofs of their completeness for a variety of boundary value problems, but also prescriptions for determining the expansion coefficients, which greatly enhanced the power and versatility of the method.³²

Before we begin our discussion, however, it is useful to make one slight change in notation. It has become customary to recast the transport equation into dimensionless form when applying singular eigenfunction methods. To this end we will measure length in units of mfp, Σ_t^{-1} , so that the integrodifferential form of the transport equation can be written as

$$\mu \frac{\partial \varphi}{\partial x} + \varphi(x, \mu) = \frac{c}{2} \int_{-1}^{+1} d\mu' \varphi(x, \mu') + s(x, \mu) \quad (2.56)$$

Separation of Variables □ We seek a separable solution of the form $\varphi(x, \mu) = \chi(x)\psi(\mu)$ to the homogeneous form of the transport equation (2.56). If we substitute this form into the equation, we find

$$\mu \frac{d\chi}{dx} \psi + \chi \psi = \frac{c}{2} \chi \int_{-1}^{+1} d\mu' \psi(\mu')$$

or dividing by $\chi(x)\psi(\mu)$ and rearranging

$$\frac{1}{\chi} \frac{d\chi}{dx} = -\frac{1}{\mu} + \frac{c}{2\mu\psi} \int_{-1}^{+1} d\mu' \psi(\mu') = \text{constant} = -\frac{1}{\nu} \quad (2.57)$$

where we have defined the separation constant, $1/\nu$. We can now solve the spatial part of Eq. 2.57 immediately to find

$$\chi(x) = e^{-x/\nu}$$

This leaves us with an integral equation for $\psi(\mu)$ of the form

$$\left(1 - \frac{\mu}{\nu}\right) \psi_\nu(\mu) = \frac{c}{2} \int_{-1}^{+1} d\mu' \psi_\nu(\mu') \quad (2.58)$$

Frequently one just uses translation invariance²⁸ of the transport equation $\varphi(x, \mu) \rightarrow \varphi(x + a, \mu)$ to suggest an “ansatz” or guess that

$$\varphi(x, \mu) = e^{-x/\nu} \psi_\nu(\mu)$$

Equation 2.58 is now our advertised eigenvalue problem for the eigenvalue ν and corresponding eigenfunction $\psi_\nu(\mu)$. Before considering this problem, let us make one further simplification. Since the normalization of the ψ_ν 's is arbitrary (we are solving a homogeneous equation), it is convenient and customary to normalize $\psi_\nu(\mu)$ such that

$$\int_{-1}^{+1} d\mu' \psi_\nu(\mu') = 1 \quad (2.59)$$

The Eigenvalue Problem □ Rewrite the eigenvalue problem (2.58) using the choice of normalization (2.59) as

$$(\nu - \mu) \psi_\nu(\mu) = \frac{c\nu}{2} \quad (2.60)$$

To be more precise, we wish to find those values of ν for which there exist nontrivial solutions $\psi_\nu(\mu)$ to this equation.

But this is simply an algebraic equation for $\psi_\nu(\mu)$. So why not just divide through to find

$$\psi_\nu(\mu) = \frac{c\nu}{2(\nu - \mu)}$$

and then apply the normalization condition (2.59) to determine the values of ν that will allow such a solution? But we must be very careful here, since if $\nu \in [-1, +1]$, then $\nu = \mu$ for some $\mu \in [-1, +1]$, and this division makes no sense. Therefore we consider two separate cases, depending on whether or not ν lies in the interval $[-1, +1]$.

Case 1: $\nu \notin [-1, +1]$. Then $\nu \neq \mu$ for any value of $\mu \in [-1, +1]$, and we can divide Eq. 2.60 by $(\nu - \mu)$ to find

$$\psi_\nu(\mu) = \frac{c\nu}{2(\nu - \mu)}$$

If we apply the normalization condition (2.59),

$$\int_{-1}^{+1} d\mu \psi_\nu(\mu) = 1 = \frac{c\nu}{2} \int_{-1}^{+1} \frac{d\mu}{\nu - \mu} = \frac{c\nu}{2} \ln \frac{\nu + 1}{\nu - 1}$$

we arrive at a condition on ν that is necessary if nontrivial solutions (i.e., eigenfunctions) $\psi_\nu(\mu)$ to Eq. 2.58 are to exist:

$$1 - \frac{c\nu}{2} \ln \frac{\nu + 1}{\nu - 1} = 0$$

But notice that if we reinsert the mfp Σ_t^{-1} into the transport equation and let $\nu = (ik)^{-1}$, we find that this condition is just that which characterized the presence of poles of our Fourier transform solution (cf. Eq. 2.47), $\Lambda(k) = 0$. Hence we can immediately identify two zeros or eigenvalues, $\pm \nu_0 = \pm 1/ik_0$, which shift about in the complex ν -plane as shown in Figure 2.19. Hence for $\nu \notin [-1, +1]$, we have found that there are two eigenfunctions

$$\psi_{0\pm}(\mu) = \pm \frac{\nu_0}{2} c \frac{1}{\pm \nu_0 - \mu} = \frac{c\nu_0}{2(\nu_0 \mp \mu)}$$

The values $\pm \nu_0$ are sometimes referred to as “discrete” eigenvalues, and the corresponding eigenfunctions as “discrete” eigenfunctions or modes (for reasons that will become apparent momentarily).

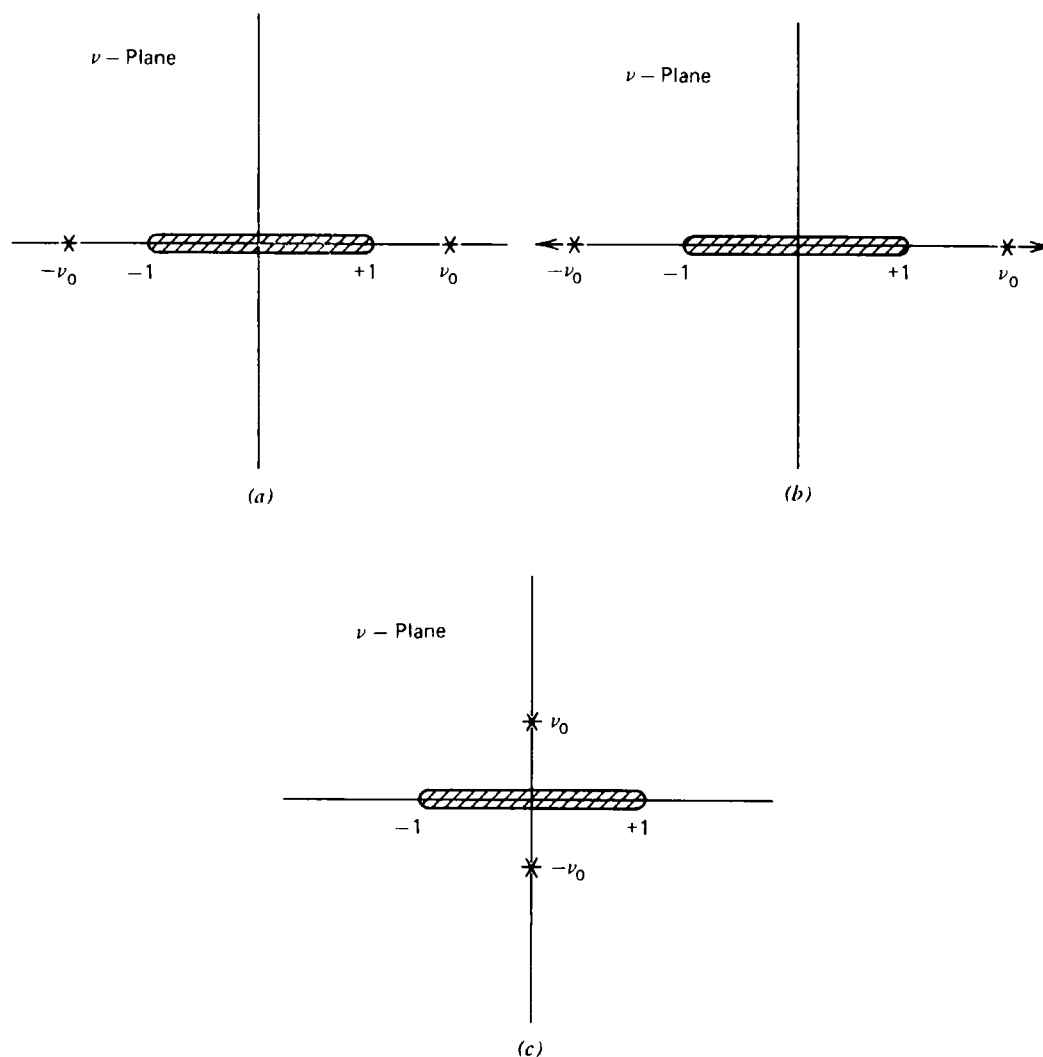


Fig. 2.19 □ Location of the discrete eigenvalues $\pm \nu_0$ in complex ν -plane. (a) $c < 1$. (b) $c \rightarrow 1$. (c) $c > 1$.

The case $c = 1$ is a bit pathological, since the eigenvalues $\nu_0 \rightarrow \infty$, and we find only one eigenfunction, $\psi_0(\mu) = 1/2$. However if we return to the original transport equation, we can find two linearly independent elementary solutions for this case

$$\varphi_1(x, \mu) = \frac{1}{2}, \quad \varphi_2(x, \mu) = \frac{1}{2}(x - \mu)$$

Case 2: $\nu \in [-1, +1]$. Now $(\nu - \mu)$ can vanish for some $\mu \in [-1, +1]$. In connection with the general topic of eigenvalue problems in transport theory, we demonstrate later in Chapter 5 that *every* $\nu \in [-1, +1]$ is an

“eigenvalue” with a corresponding eigenfunction. Because of their continuous distribution, $\nu \in [-1, +1]$ are sometimes referred to as the “continuous eigenvalues” or the “continuous spectrum of eigenvalues.”^{33,34} (We introduce a more precise terminology in Chapter 5.) It should be noted that this set $\nu \in [-1, +1]$ corresponds to the branch cut in the Fourier transform analysis.

The corresponding eigenfunctions are of a very singular type

$$\psi_\nu(\mu) = \frac{c\nu}{2} P \frac{1}{(\nu - \mu)} + \lambda(\nu)\delta(\nu - \mu) \quad (2.61)$$

where P is symbolic for a Cauchy principal value integration whenever $(\nu - \mu)^{-1}$ is integrated, and $\lambda(\nu)$ has yet to be determined. (For a detailed discussion of principal value integration and Cauchy integrals, refer to Appendix B.) Most references^{15,28,35} on the singular eigenfunction method in transport theory give a heuristic motivation for the form taken by these eigenfunctions, but these arguments are usually more confusing than informative. A rigorous derivation of such forms must come from functional analysis and the spectral theory of operators,^{34,36-41} a subject that would take us too far afield at this point (although we return to consider it in Chapter 5). Hence for the present we accept as a fact of life that Eq. 2.58 is an eigenvalue problem with a continuous spectrum $\nu \in [-1, +1]$ and corresponding singular eigenfunctions of the form Eq. 2.61. To determine $\lambda(\nu)$ we apply the normalization condition (2.60), taking note of the principal value integration, to find

$$\lambda(\nu) = 1 - \frac{c\nu}{2} P \int_{-1}^{+1} \frac{d\mu}{\nu - \mu} = 1 - \frac{c\nu}{2} \ln \frac{1 + \nu}{1 - \nu} = 1 - c\nu \tanh^{-1} \nu$$

Therefore in summary we have found that the eigenfunctions of Eq. 2.58 can be written as

$$\begin{aligned} \psi_{0+}(\mu) &= \frac{c\nu_0}{2(\nu_0 - \mu)} \\ \psi_{0-}(\mu) &= \frac{c\nu_0}{2(\nu_0 + \mu)} \\ \psi_\nu(\mu) &= \frac{c\nu}{2} P \frac{1}{\nu - \mu} + \lambda(\nu)\delta(\nu - \mu), \quad \nu \in [-1, +1] \end{aligned} \quad (2.62)$$

(Unless otherwise indicated, we confine ourselves to the case of $c < 1$.)

We are now ready to proceed to the third and final stage of our task, to use an expansion in these eigenfunctions to obtain the solution to boundary value problems. We consider two classes of such problems, as exemplified by the plane source, infinite medium problem and the Milne problem, which we solved in the last section using integral transforms.

Full-Range Boundary Value Problems □ The general idea is to seek a solution to the transport equation plus associated boundary conditions as an eigenfunction expansion

$$\varphi(x, \mu) = a_{0+} \psi_{0+}(\mu) e^{-x/\nu_0} + a_{0-} \psi_{0-}(\mu) e^{+x/\nu_0} + \int_{-1}^{+1} d\nu A(\nu) \psi_\nu(\mu) e^{-x/\nu} \quad (2.63)$$

and then use the specific boundary conditions for the problem of interest to evaluate the expansion coefficients a_{0+} , a_{0-} , and $A(\nu)$. The particular type of boundary value problem we consider first has boundary conditions in which $\varphi(x, \mu)$ is given at a position x for the full range of $\mu \in [-1, +1]$, for example,

$$\varphi(x_0, \mu) = f(\mu), \quad \mu \in [-1, +1]$$

There are two very important questions we must answer if we are to use eigenfunction expansions such as Eq. 2.63 to solve such boundary value problems:

- i Does such an expansion make sense? That is, do the $\{\psi_\nu\}$ form a complete set?
- ii If the $\{\psi_\nu\}$ are complete, how do we determine the expansion coefficients from a given boundary condition?

The answer to the first question is *yes*, as we demonstrate in a moment. However let us first turn our attention to the second question. We recall that the usual trick in PDE boundary value problems is to use the orthogonality of the eigenfunctions. A similar approach can be used in transport problems.

Theorem. Full-Range Orthogonality. The $\{\psi_\nu\}$ are orthogonal in the sense that

$$\int_{-1}^{+1} d\mu \mu \psi_\nu(\mu) \psi_{\nu'}(\mu) = 0, \quad \nu \neq \nu'$$

Proof. The proof is trivial. If we multiply Eq. 2.58 by $\psi_{\nu'}(\mu)$ and integrate, we find

$$\int_{-1}^{+1} d\mu \left\{ \left(1 - \frac{\mu}{\nu} \right) \psi_{\nu} = \frac{c}{2} \int_{-1}^{+1} d\mu' \psi_{\nu'}(\mu') \right\} \psi_{\nu'}(\mu)$$

Similarly, we can find

$$\int_{-1}^{+1} d\mu \left\{ \left(1 - \frac{\mu}{\nu'} \right) \psi_{\nu'} = \frac{c}{2} \int_{-1}^{+1} d\mu' \psi_{\nu'}(\mu') \right\} \psi_{\nu}(\mu)$$

Therefore subtracting these two equations, we can arrive at

$$\left(\frac{1}{\nu'} - \frac{1}{\nu} \right) \int_{-1}^{+1} d\mu \mu \psi_{\nu}(\mu) \psi_{\nu'}(\mu) = 0$$

which implies the orthogonality property.

It is useful to calculate the normalization integrals for $\nu = \nu'$. One can show²⁸

$$N_{0\pm} \equiv \int_{-1}^{+1} d\mu \mu \psi_{0\pm}^2(\mu) = \pm \frac{c}{2} \nu_0^3 \left(\frac{c}{\nu_0^2 - 1} - \frac{1}{\nu_0^2} \right) = \pm \frac{c\nu_0^2}{2} \Lambda'(\nu_0)$$

and

$$N(\nu) = \nu \left[\lambda^2(\nu) + \left(\frac{c\pi\nu}{2} \right)^2 \right]$$

where we define $N(\nu)$ by

$$\int_{-1}^{+1} d\mu \mu \psi_{\nu}(\mu) \left[\int_{-1}^{+1} d\nu' A(\nu') \psi_{\nu'}(\mu) \right] = N(\nu) A(\nu)$$

The calculation of the normalization of the singular eigenfunctions $\psi_{\nu}(\mu)$ is complicated by the presence of a product of Dirac δ -functions. This can be circumvented by use of the Poincaré-Bertrand formula⁴² (see Problem 2.27).

To demonstrate how these orthogonality relations can be used, we solve once again the problem of a plane source at the origin of an infinite medium ($c < 1$):

$$\mu \frac{\partial \varphi}{\partial x} + \varphi(x, \mu) = \frac{c}{2} \int_{-1}^{+1} d\mu' \varphi(x, \mu') + \frac{S_0}{2} \delta(x)$$

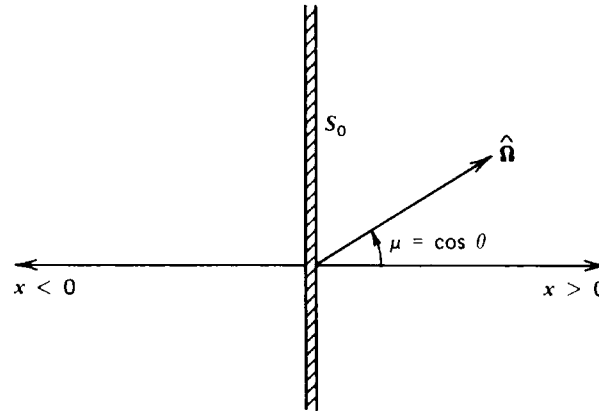


Fig. 2.20 □ Isotropic plane source at the origin of an infinite medium.

subject to boundary conditions: $\lim_{|x| \rightarrow \infty} \varphi(x, \mu) = 0$ (see Figure 2.20). We will seek the solution to this problem as an eigenfunction expansion of the form Eq. 2.63. Then the boundary conditions at infinity demand

$$\varphi(x, \mu) = a_{0+} \psi_{0+}(\mu) e^{-x/\nu_0} + \int_0^{+1} d\nu A(\nu) \psi_\nu(\mu) e^{-x/\nu}, \quad x > 0$$

$$\varphi(x, \mu) = -a_{0-} \psi_{0-}(\mu) e^{+x/\nu_0} - \int_{-1}^0 d\nu A(\nu) \psi_\nu(\mu) e^{-x/\nu}, \quad x < 0$$

If we next integrate the transport equation across the source plane from $0-\varepsilon$ to $0+\varepsilon$ and take the limit as $\varepsilon \rightarrow 0$, we find a source boundary condition

$$\varphi(0^+, \mu) - \varphi(0^-, \mu) = \frac{S_0}{2\mu}$$

We can substitute in our forms for $\varphi(0^+, \mu)$ and $\varphi(0^-, \mu)$ to find

$$\frac{S_0}{2\mu} = a_{0+} \psi_{0+}(\mu) + a_{0-} \psi_{0-}(\mu) + \int_{-1}^{+1} d\nu A(\nu) \psi_\nu(\mu)$$

To evaluate the expansion coefficients, we now multiply through by $\mu \psi_{0\pm}(\mu)$ and integrate over μ , using orthogonality, to find

$$a_{0\pm} = [N_{0\pm}]^{-1} \int_{-1}^{+1} d\mu \mu \psi_{0\pm}(\mu) \frac{S_0}{2\mu}$$

$$A(\nu) = [N(\nu)]^{-1} \int_{-1}^{+1} d\mu \mu \psi_\nu(\mu) \frac{S_0}{2\mu}$$

Hence we can solve full-range boundary value problems rather directly, provided we can verify that an expansion such as that given by Eq. 2.63 is valid. To this end we now prove the following theorem.

Theorem. Full-Range Completeness. The functions $\psi_{0+}(\mu)$, $\psi_{0-}(\mu)$, and $\psi_\nu(\mu)$, $\nu \in [-1, +1]$ are complete for the class of all functions $f(\mu) \in H^*$ defined on the full range $\mu \in [-1, +1]$.

Proof. Here, H^* refers to the class of all Hölder continuous functions⁴² (refer to Appendix B for a precise definition). Our approach to the proof of this completeness theorem is somewhat different from the conventional approaches utilized in mathematical physics. Typically one attempts to demonstrate that a sequence of functions chosen from the set of interest will converge (in some suitable norm) to any function in the class of interest.³³ We adopt instead a constructive approach³¹ and demonstrate that we can represent any function $f(\mu)$ in the class H^* as

$$f(\mu) = a_{0+}\psi_{0+}(\mu) + a_{0-}\psi_{0-}(\mu) + \int_{-1}^{+1} d\nu A(\nu)\psi_\nu(\mu) \quad (2.64)$$

by actually proving that a_{0+} , a_{0-} , and $A(\nu)$ exist and are uniquely determined for any function $f(\mu) \in H^*$. To get a better idea of what is involved in this proof, let us ignore a_{0+} and a_{0-} for the moment by defining

$$f'(\mu) \equiv f(\mu) - a_{0+}\psi_{0+}(\mu) - a_{0-}\psi_{0-}(\mu)$$

If we now substitute our explicit form (2.61) for the singular eigenfunction into Eq. 2.64, we find

$$f'(\mu) = \lambda(\mu)A(\mu) + P \int_{-1}^{+1} d\nu \frac{c\nu}{2(\nu - \mu)} A(\nu) \quad (2.65)$$

Notice that this is an inhomogeneous integral equation for $A(\mu)$, although of a singular type, to be sure, because of the $(\nu - \mu)^{-1}$ in the integrand. One refers to such equations as *singular integral equations of the Cauchy type*. Extensive methods have been developed for the analysis of such equations and these are described in the treatise of Muskhelishvili (and briefly summarized in Appendix C).

Hence all we have to do to prove completeness is to demonstrate the existence and uniqueness of a solution $A(\mu)$ to this singular integral equation for any function $f'(\mu) \in H^*$ and somehow determine $a_{0\pm}$ in the process. We accomplish this in the most direct manner by solving the integral equation for $A(\mu)$ in terms of an arbitrary $f'(\mu)$.

To this end, consider a function defined by

$$n(z) = \frac{1}{2\pi i} \int_{-1}^{+1} d\nu \frac{c\nu A(\nu)}{2(\nu - z)}$$

Now if $A(\nu) \in H^*$, then $n(z)$ is analytic in the plane cut along the real axis from $[-1, +1]$ (see Appendix B for details). Furthermore we can use the Plemelj formula,⁴² which gives the limiting value of a function defined by a Cauchy integral of the form

$$\Phi(z) = \int_C dt \frac{\varphi(t)}{t - z}$$

as z approaches the cut from above or below

$$\Phi^\pm(t_0) \equiv \lim_{z \rightarrow t_0^\pm} \Phi(z) = P \int_C dt \frac{\varphi(t)}{t - t_0} \pm \pi i \varphi(t_0)$$

(see Appendix B) to evaluate the limiting values of $n(z)$ on the cut from $[-1, +1]$ as

$$n^\pm(\mu) = \frac{1}{2\pi i} P \int_{-1}^{+1} d\nu \frac{c\nu A(\nu)}{2(\nu - z)} \pm \frac{c\mu}{4} A(\mu)$$

Using this result, we can rewrite Eq. 2.65 in terms of the boundary values of $n(z)$ on the cut as

$$f'(\mu) = \lambda(\mu) \left(\frac{2}{c\mu} \right) [n^+(\mu) - n^-(\mu)] + \pi i [n^+(\mu) + n^-(\mu)]$$

or rearranging

$$\frac{c\mu}{2} f'(\mu) = \left[\lambda(\mu) + \frac{i\pi c\mu}{2} \right] n^+(\mu) - \left[\lambda(\mu) - \frac{i\pi c\mu}{2} \right] n^-(\mu) \quad (2.66)$$

But if we define

$$\Lambda(z) \equiv 1 - \int_{-1}^{+1} d\nu \frac{cz}{2(z - \nu)}$$

and note that on the cut this function assumes the limiting values

$$\Lambda^\pm(\mu) = 1 - P \int_{-1}^{+1} d\nu \frac{c\mu}{2(\mu - \nu)} \pm \frac{i\pi c\mu}{2} = \lambda(\mu) \pm \frac{i\pi c\mu}{2}$$

it is apparent that we can rewrite Eq. 2.66 as follows:

$$\left(\frac{c\mu}{2}\right)f'(\mu) = \Lambda^+(\mu)n^+(\mu) - \Lambda^-(\mu)n^-(\mu), \quad \mu \in [-1, +1]$$

We now observe that $\Lambda(z)$ and $n(z)$ are analytic in the same cut-plane. (This will not be true in general, as we will find in half-space problems.) Therefore we can regard this as a boundary value problem in complex variables for the product function $\Lambda(z)n(z)$ and solve this problem using the methods described in Appendix B to find

$$\Lambda(z)n(z) = \frac{1}{2\pi i} \int_{-1}^{+1} d\nu \frac{c\nu f'(\nu)}{2(\nu - z)} + P_k(z)$$

where $P_k(z)$ is an arbitrary polynomial in z of order k . But since $\Lambda(z)n(z) \rightarrow (1-c)/z \rightarrow 0$ as $z \rightarrow \infty$, we can apply Liouville's theorem to conclude $P_k(z) = 0$. Therefore we can write

$$n(z) = \frac{1}{2\pi i \Lambda(z)} \int_{-1}^{+1} d\nu \frac{c\nu f'(\nu)}{2(\nu - z)}$$

But $n(z)$, at least as advertised, is supposed to be analytic in the cut-plane. And we know that $\Lambda(z)$ has two zeros, $\pm\nu_0$. Therefore to keep $n(z)$ analytic at these zeros, we must require that

$$\int_{-1}^{+1} d\nu \frac{c\nu f'(\nu)}{2(\nu \mp \nu_0)} = 0$$

or

$$\int_{-1}^{+1} d\nu \frac{c\nu f(\nu)}{2(\nu \mp \nu_0)} = a_{0+} \int_{-1}^{+1} d\nu \frac{c\nu \psi_{0+}(\nu)}{2(\nu \mp \nu_0)} + a_{0-} \int_{-1}^{+1} d\nu \frac{c\nu \psi_{0-}(\nu)}{2(\nu \mp \nu_0)}$$

But these two equations can hold only if we choose

$$a_{0\pm} = (N_{0\pm})^{-1} \int_{-1}^{+1} d\mu \psi_{0\pm}(\mu) f(\mu)$$

Of course these are the same values for the expansion coefficients a_{0+} and a_{0-} we obtained using the full-range orthogonality relations. With this choice of $a_{0\pm}$, $n(z)$ is indeed analytic in the cut-plane, and we can find

$$A(\nu) = \left(\frac{2}{c\nu}\right) [n^+(\nu) - n^-(\nu)] = [N(\nu)]^{-1} \int_{-1}^{+1} d\mu \mu \psi_\nu(\mu) f(\mu)$$

(for the detailed manipulations, see Case and Zweifel,²⁸ pp. 75–76). Thus we have demonstrated the existence and uniqueness of the expansion coefficients $a_{0\pm}$ and $A(\nu)$ for any function $f(\mu) \in H^*$, and our proof is complete.

Although the full-range completeness property was first demonstrated by Case³¹ using the constructive approach we have sketched, several completeness theorems of a more traditional nature have been given in subsequent investigations. For example, Kuščer and Shure^{43,32} have proceeded by demonstrating that the eigenfunctions $\{\psi_\nu\}$ satisfy a closure property, which can be obtained by first writing

$$\delta(\mu - \mu_0) = a_{0+}\psi_{0+}(\mu) + a_{0-}\psi_{0-}(\mu) + \int_{-1}^{+1} d\nu A(\nu)\psi_\nu(\mu)$$

If orthogonality is used to determine the expansion coefficients, one arrives at the closure relation

$$\begin{aligned} \delta(\mu - \mu_0) = & \frac{2\mu_0}{2\nu_0^2\Lambda'(\nu_0)} [\psi_{0+}(\mu_0)\psi_{0+}(\mu) + \psi_{0-}(\mu_0)\psi_{0-}(\mu)] \\ & + \int_{-1}^{+1} d\nu \frac{\mu_0\psi_\nu(\mu_0)\psi_\nu(\mu)}{\nu\Lambda^+(\nu)\Lambda^-(\nu)} \end{aligned}$$

One can demonstrate that this relationship is indeed satisfied by the eigenfunctions $\{\psi_\nu\}$.

A somewhat more formal demonstration of the completeness properties can be given in terms of convergence arguments using methods of functional analysis. We sketch yet another approach using resolvent integration methods in the last section of this chapter.

Half-Range Boundary Value Problems □ Suppose we wish to solve the Milne problem as specified by the integrodifferential form of the transport equation (2.54) and the accompanying boundary conditions given by applying a singular eigenfunction expansion of the form (2.63). Then applying the source boundary condition i at infinity, we find we must choose $a_{0-} = C$ and $A(\nu) = 0$ for $\nu \in [-1, 0]$. The boundary condition ii at the surface implies (after some rearranging)

$$-C\psi_{0-}(\mu) = a_{0+}\psi_{0+}(\mu) + \int_0^1 d\nu A(\nu)\psi_\nu(\mu)$$

But this equation actually implies that we are expanding a function $f(\mu)$

[in this case, $C\psi_{0-}(\mu)$] defined over the half-range $\mu \in [0, 1]$ as

$$f(\mu) = a_{0+}\psi_{0+}(\mu) + \int_0^1 d\nu A(\nu)\psi_\nu(\mu), \quad \mu \in [0, 1] \quad (2.67)$$

Again, two questions arise:

- i Does such an expansion make sense—do we have half-range completeness?
- ii How do we evaluate the expansion coefficients a_{0+} and $A(\nu)$? Here we observe that our earlier orthogonality condition does not apply, since Eq. 2.67 is given over only half the interval $[-1, +1]$.

Again we prove a completeness theorem. Of course we expect life to be more difficult in this case, just as the half-range problem treated by integral transforms was more difficult and necessitated the Wiener-Hopf technique.

Theorem. Half-Range Completeness. The functions $\psi_{0+}(\mu)$ and $\psi_\nu(\mu)$, $\nu \in [0, 1]$ are complete for the class of all functions $f(\mu) \in H^*$ defined on the half-range $\mu \in [0, 1]$.

Proof. In a sense, this theorem is actually more useful than the full-range theorem, since it is the only way of evaluating the expansion coefficients a_{0+} and $A(\nu)$. (There is no direct way to obtain an orthogonality relation⁴⁴ over the half-range without going through the details of the proof.) Again the idea is to demonstrate that the expansion

$$f(\mu) = a_{0+}\psi_{0+}(\mu) + \int_0^1 d\nu A(\nu)\psi_\nu(\mu), \quad \mu \in [0, 1]$$

uniquely determines the a_{0+} and $A(\nu)$ for any $f(\mu) \in H^*$. As before, we define

$$f'(\mu) \equiv f(\mu) - a_{0+}\psi_{0+}(\mu)$$

and use the explicit form for $\psi_\nu(\mu)$ to obtain a singular integral equation of the Cauchy type for $A(\mu)$:

$$f'(\mu) = \lambda(\mu)A(\mu) + \int_0^1 d\nu \frac{c\nu}{2(\nu - \mu)} A(\nu) \quad (2.68)$$

The partial range of this integration complicates the solution of this equation, just as the partial range $x \in [0, \infty)$ complicated the solution of the

Peierls equation by Fourier transforms. We cannot use the Plemelj formula directly as we did for the full-range problem. Fortunately, the theory of such singular integral equations⁴² is well developed, and standard methods are available for solving them.

In Appendix C we demonstrate that the solution of equations such as Eq. 2.68 involves three essential steps:

- i The use of the Plemelj formula to reduce the integral equation to a type of boundary value problem in complex variable theory known as the inhomogeneous Hilbert problem.⁴²
- ii The solution of an associated homogeneous problem known as the Riemann-Hilbert problem.⁴²
- iii The use of this solution to solve the inhomogeneous Hilbert problem and obtain the solution $A(\mu)$ to the singular integral equation.

We briefly summarize each of these steps as it applies to the half-range expansion represented by Eq. 2.68. The details for this and more general problems are provided in Appendix C.

We begin as in the full-range case by defining a function

$$n(z) = \frac{1}{2\pi i} \int_0^1 d\nu \frac{c\nu A(\nu)}{2(\nu - z)}$$

which is analytic in the z -plane cut along $[0, 1]$. Using the Plemelj formula and our earlier manipulation of Eq. 2.66, we can rewrite the integral equation 2.68 as

$$\Lambda^+(\mu)n^+(\mu) - \Lambda^-(\mu)n^-(\mu) = \left(\frac{c\mu}{2}\right)f'(\mu), \quad \mu \in [0, 1] \quad (2.69)$$

Notice that we can no longer directly apply the Plemelj formula to solve Eq. 2.69 as we did for the full-range case Eq. 2.66, since $n(z)$ is analytic in the plane cut along $[0, 1]$, while $\Lambda(z)$ is analytic in a different plane cut along $[-1, +1]$. Therefore we must follow a far more laborious route.

First, divide Eq. 2.69 by $\Lambda^-(\mu)$ to arrive at an equation for $n^+(\mu)$ and $n^-(\mu)$ of the form

$$\frac{\Lambda^+(\mu)}{\Lambda^-(\mu)} n^+(\mu) - n^-(\mu) = \frac{c\mu f'(\mu)}{2\Lambda^-(\mu)}, \quad \mu \in [0, 1] \quad (2.70)$$

Boundary value problems of this type are classified as the *inhomogeneous Hilbert problem*. To solve this problem, we must first solve a related homogeneous boundary value problem known as the *Riemann-Hilbert*

problem, which requires that we determine a function $X(z)$ that is analytic in the plane cut along $[0, 1]$, is nonzero, and has limiting values on the cut that satisfy the following condition:

$$\frac{X^+(\mu)}{X^-(\mu)} = \frac{\Lambda^+(\mu)}{\Lambda^-(\mu)} \equiv \exp[2i\Theta(\mu)], \quad \Theta(\mu) \equiv \tan^{-1} \left[\frac{c\pi\mu}{2\lambda(\mu)} \right]$$

We demonstrate in Appendix C that a suitable candidate for the solution $X(z)$ is given by

$$\exp[\Gamma(z)] = \exp \left[\frac{1}{\pi} \int_0^1 d\nu \frac{\Theta(\nu)}{\nu - z} \right]$$

But to ensure that $\exp[\Gamma(z)]$ is nonzero and analytic, we must examine its endpoint behavior at $z=0$ and $z=1$. Since $\Theta(0) = \tan^{-1} 0$, we take $\Theta(0)=0$ (fixing the branch of $\tan^{-1} z$). Then we have no trouble at $z=0$. By examining the behavior of $c\pi\mu/2\lambda(\mu)$, one can verify that $\Theta(1)=\pi$. Hence we find

$$\exp[\Gamma(z)] \sim (1-z) \exp[\Gamma_1(z)] \quad \text{as } z \rightarrow 1$$

Thus we have to divide out the $(1-z)$ factor to find

$$X(z) = (1-z)^{-1} \exp \left[\frac{1}{\pi} \int_0^1 d\nu \frac{\Theta(\nu)}{\nu - z} \right]$$

Now if we insert $\exp[2i\Theta] = X^+/X^-$ into Eq. 2.70, we find

$$X^+(\mu)n^+(\mu) - X^-(\mu)n^-(\mu) = c\mu X^-(\mu)f'(\mu)/2\Lambda^-(\mu), \quad \mu \in [0, 1]$$

Since $X(z)$ and $n(z)$ are now both analytic in the plane cut from $[0, 1]$, we can apply the Plemelj formula (see Appendix B) to find

$$n(z) = \frac{1}{X(z)} \left[\frac{1}{2\pi i} \int_0^1 d\nu \frac{c\nu X^-(\nu)f'(\nu)}{2\Lambda^-(\nu)(\nu - z)} + P_k(z) \right]$$

The analysis in Appendix C indicates that $P_k(z) \equiv 0$ and we must apply an additional condition

$$\int_0^1 d\nu \frac{c\nu X^-(\nu)f'(\nu)}{2\Lambda^-(\nu)} = 0$$

so that $n(z)$ will vanish like $1/z$ as $z \rightarrow \infty$. This restriction determines a_{0+}

for us as

$$a_{0+} = \left[\int_0^1 d\nu \frac{c\nu X^-(\nu) f(\nu)}{2\Lambda^-(\nu)} \right] \left[\int_0^1 d\nu \frac{c\nu X^-(\nu) \psi_{0+}(\nu)}{2\Lambda^-(\nu)} \right]^{-1}$$

We also have then

$$A(\nu) = \left(\frac{c\nu}{2} \right) [n^+(\nu) - n^-(\nu)], \quad \nu \in [0, 1]$$

Hence we have solved the singular integral equation (2.68) for $A(\mu)$ and have determined a_{0+} in the process. Therefore we have explicitly demonstrated the existence and uniqueness of a_{0+} and $A(\nu)$, and the proof of the half-range completeness property is finished.

We can now return and use these results to complete our solution of the Milne problem. We need only set $f(\mu) = -C\psi_{0-}(\mu)$ in our half-range completeness theorem to find

$$a_{0+} = \left[-C \int_0^1 d\nu \gamma(\nu) \psi_{0-}(\nu) \right] \left[\int_0^1 d\nu \gamma(\nu) \psi_{0+}(\nu) \right]^{-1}$$

where we have defined

$$\gamma(\nu) = \frac{c\nu}{2} \frac{X^-(\nu)}{\Lambda^-(\nu)}$$

(this factor occurs very frequently in algebraic manipulations). Similarly, we can calculate

$$n(z) = \frac{1}{X(z)2\pi i} \int_0^1 d\nu \frac{\gamma(\nu)}{\nu - z} [-C\psi_{0-}(\nu) - a_{0+}\psi_{0+}(\nu)]$$

and then arrive at the continuum expansion coefficient as

$$A(\nu) = \left(\frac{2}{c\nu} \right) [n^+(\nu) - n^-(\nu)], \quad \nu \in [0, 1]$$

Needless to say, these results are still messy. However we can simplify things a little by using some identities involving the $X(z)$ functions, which are proved by Case and Zweifel.²⁸ We simply state results here and refer the reader to other sources for details:

$$A(\nu) = - \frac{c(1-c)\nu_0^2\nu CX(-\nu_0)X(-\nu)}{N(\nu)}$$

and

$$a_{0+} = \frac{CX(-\nu_0)}{X(\nu_0)}$$

If we now use these forms in the eigenfunction expansion

$$\varphi(x, \mu) = C\psi_{0-}(\mu)e^{x/\nu_0} + a_{0+}\psi_{0+}(\mu)e^{-x/\nu_0} + \int_0^1 d\nu A(\nu)\psi_\nu(\mu)e^{-x/\nu}$$

we arrive at the solution to the Milne problem.

This solution is still rather opaque. It does simplify for certain applications, such as the determination of the emerging angular distribution at the surface (for $C = 1$):

$$\begin{aligned} \varphi(0, \mu) = \frac{c\nu_0}{2(\nu_0 + \mu)} + a_{0+} \frac{c\nu_0}{2(\nu_0 - \mu)} + P \int_0^1 d\nu \frac{c\nu A(\nu)}{2(\nu - \mu)} \\ + \int_0^1 d\nu \lambda(\nu) \delta(\nu - \mu) A(\nu) \end{aligned}$$

Since we are interested in $\mu < 0$, we note that the last term in this expression vanishes and furthermore that the principal value integration in the third term is no longer needed. Then if we use our expressions for a_{0+} and $A(\nu)$, a bit of algebra leads to the result:

$$\varphi(0, \mu) = \frac{c\nu_0^2 X(-\nu_0)}{X(\nu)(\nu_0^2 - \mu^2)}, \quad \mu < 0$$

This result is plotted for various values of c in Figure 2.21. As $c \rightarrow 1$, the solution assumes a linear dependence on angle, $\varphi(0, \mu) \sim A + B\mu$. As $c \rightarrow 0$, $\varphi(0, \mu)$ approaches a singular form corresponding to streaming perpendicular to the surface. That is, we find a strong forward peaking in the angular flux for large absorption. We can also evaluate the total flux at the surface as

$$\phi(0) = 2\nu_0(1 - c)^{1/2} X(-\nu_0)$$

One can play around with these solutions indefinitely, proving all kinds of fancy identities and manipulating the solutions like a Chinese puzzle.^{28,32} The only other result we choose to consider here involves the calculation of the “extrapolated endpoint,” which is customarily used to yield a free surface boundary condition in diffusion theory. For large x

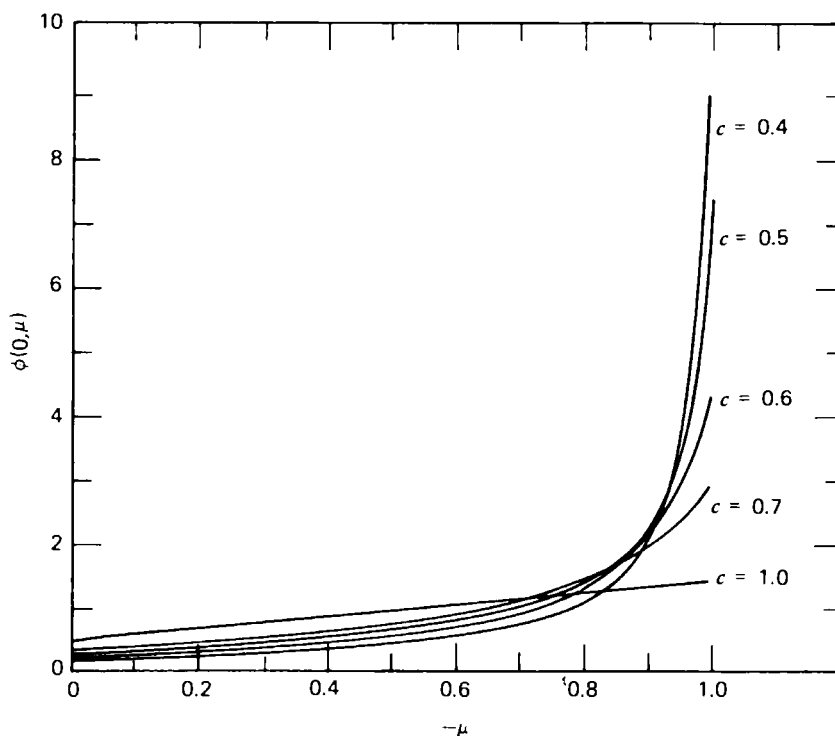


Fig. 2.21 □ Emerging angular flux distribution from a free surface. From Case et al.³

(far away from the boundary), we can ignore the transient term to write

$$\varphi(x, \mu) \sim \psi_{0-} e^{x/\nu_0} + a_{0+} \psi_{0+} e^{-x/\nu_0} + O(e^{-x})$$

or for the total flux

$$\phi(x) \sim e^{x/\nu_0} + a_{0+} e^{-x/\nu_0}$$

We define the “extrapolation length” z_0 as the distance outside the surface at which the flux in the interior extrapolates to zero. To evaluate this, we just set (see Figure 2.22)

$$\phi(-z_0) = e^{-z_0/\nu_0} + a_{0+} e^{z_0/\nu_0} = 0$$

Therefore we can solve for z_0 as

$$z_0 = -\left(\frac{\nu_0}{2}\right) \ln a_{0+} = -\left(\frac{\nu_0}{2}\right) \ln \left[\frac{-X(-\nu_0)}{X(\nu_0)} \right]$$

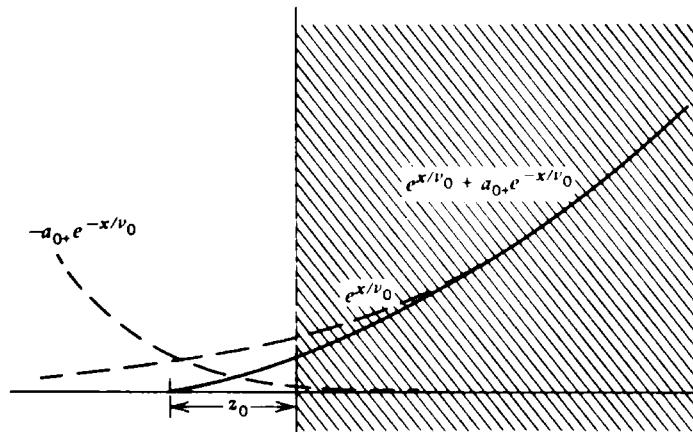


Fig. 2.22 □ Determination of the extrapolated endpoint from the asymptotic solution of the Milne problem.

A detailed evaluation of the $X(z)$ functions yields the familiar result (at least to nuclear engineers and astrophysicists)

$$z_0 = 0.710446 \left[\frac{1}{c} - 0.0199 \frac{(1-c)^2}{c} + O\left(\frac{(1-c)^3}{c}\right) \right]$$

Half-Range Orthogonality Relations □ For several years following the introduction of the singular eigenfunction method by Case, the half-range completeness theorem was the only way to evaluate the expansion coefficients. However in 1965 Kuščer, McCormick, and Summerfield⁴⁴ developed an orthogonality relation that could be used to evaluate the expansion coefficients directly. That is, if we wish to expand some function $f(\mu)$ as

$$f(\mu) = a_{0+} \psi_{0+}(\mu) + \int_0^1 d\nu A(\nu) \psi_\nu(\mu)$$

then to evaluate the a_{0+} and $A(\nu)$, we can use the half-range orthogonality relation

$$\int_0^1 d\mu W(\mu) \psi_\nu(\mu) \psi_{\nu'}(\mu) = 0, \quad \nu \neq \nu'$$

The determination of the weighting factor $W(\mu)$ involves solving a singular integral equation.²⁸ We avoid the detailed construction of $W(\mu)$ here and merely note the orthogonality relations themselves.

If we choose

$$W(\mu) = \gamma(\mu)(\nu_0 - \mu) = \frac{(c\mu/2)(\nu_0 - \mu)X^-(\mu)}{\Lambda^-(\mu)}$$

the corresponding half-range orthogonality relations become

$$\int_0^1 d\mu W(\mu) \psi_\nu(\mu) \psi_{\nu'}(\mu) = W(\nu) \nu^{-1} N(\nu) \delta(\nu - \nu')$$

$$\int_0^1 d\mu W(\mu) \psi_{0\pm}(\mu) \psi_{0+}(\mu) = \mp \left(\frac{c\nu_0}{2} \right)^2 X(\pm \nu_0)$$

$$\int_0^1 d\mu W(\mu) \psi_{0+}(\mu) \psi_\nu(\mu) = 0$$

$$\int_0^1 d\mu W(\mu) \psi_{0-}(\mu) \psi_\nu(\mu) = c\nu\nu_0 X(-\nu_0) \psi_{0-}(\nu)$$

$$\int_0^1 d\mu W(\mu) \psi_{0+}(\mu) \psi_{-\nu}(\mu) = \left(\frac{c^2 \nu \nu_0}{4} \right) X(-\nu)$$

$$\int_0^1 d\mu W(\mu) \psi_{\nu'}(\mu) \psi_{-\nu}(\mu) = \left(\frac{c\nu'}{2} \right) \psi_{-\nu}(\nu') (\nu_0 + \nu) X(-\nu)$$

Note that the half-range weighting function $W(\mu)$ is simply related to the Chandrasekhar H -function,^{32,45,46} which appears in the literature of radiative transfer, by

$$W(\mu) = \mu H(\mu)$$

Example. The Albedo Problem. In this problem we are given the incident beam of particles on a free surface and wish to determine the distribution within the medium. The appropriate form of the transport equation is

$$\mu \frac{\partial \varphi}{\partial x} + \varphi(x, \mu) = \frac{c}{2} \int_{-1}^{+1} d\mu' \varphi(x, \mu')$$

with boundary conditions:

$$\begin{aligned} \text{i} \quad & \lim_{x \rightarrow \infty} \varphi(x, \mu) = 0 \\ \text{ii} \quad & \varphi(0, \mu) = \delta(\mu - \mu_0), \quad \mu \in [0, 1] \end{aligned}$$

The boundary condition i at infinity demands us to seek a solution

$$\varphi(x, \mu) = a_{0+} \psi_{0+}(\mu) e^{-x/\nu_0} + \int_0^1 d\nu A(\nu) \psi_\nu(\mu) e^{-x/\nu}$$

Then applying condition ii, we find

$$\delta(\mu - \mu_0) = a_{0+}(\mu) + \int_0^1 d\nu A(\nu) \psi_\nu(\mu), \quad \mu > 0$$

If we now multiply by $W(\mu)\psi_\nu(\mu)$ and integrate over μ , we find

$$\begin{aligned} W(\mu_0)\psi_\nu(\mu_0) &= a_{0+} \int_0^1 d\mu W(\mu)\psi_{0+}(\mu)\psi_\nu(\mu) \\ &\quad + \int_0^1 d\nu' A(\nu') \int_0^1 d\mu W(\mu)\psi_{\nu'}(\mu)\psi_\nu(\mu) \end{aligned}$$

or

$$A(\nu) = \frac{\nu W(\mu_0)\psi_\nu(\mu_0)}{N(\nu)W(\nu)}$$

Similarly, if we multiply by $W(\mu)\psi_{0+}(\mu)$ and integrate over μ , we find

$$a_{0+} = -\frac{2\gamma(\mu_0)}{c\nu_0 X(\nu_0)}$$

Thus our final solution can be written as

$$\begin{aligned} \varphi(x, \mu) &= -\frac{2\gamma(\mu_0)}{c\nu_0 X(\nu_0)} \psi_{0+}(\mu) e^{-x/\nu_0} \\ &\quad + (\nu_0 - \mu_0) \gamma(\mu_0) \int_0^1 d\nu \frac{\nu \psi_\nu(\mu_0) \psi_\nu(\mu)}{N(\nu) \gamma(\nu) (\nu_0 - \nu)} e^{-x/\nu} \end{aligned}$$

The half-range orthogonality relations have made short work of this half-space problem. All the work has been done for us in the construction of $W(\mu)$.

Unfortunately, the list of problems that can be solved using the half-range completeness and orthogonality properties is rather short.^{28,32,45} One can obtain the Green's function for a half-space, or solve for the flux in a medium composed of two adjacent half-spaces, each composed of different material (see Figure 2.23). It is also possible to formally solve the transport equation characterizing a slab geometry, although in the last case the "solution" eventually yields for the expansion coefficients an integral equation that must be solved numerically.⁴⁷ In effect, singular eigenfunction methods yield explicit solutions of the transport equation only for one-dimensional geometries with at most one boundary.

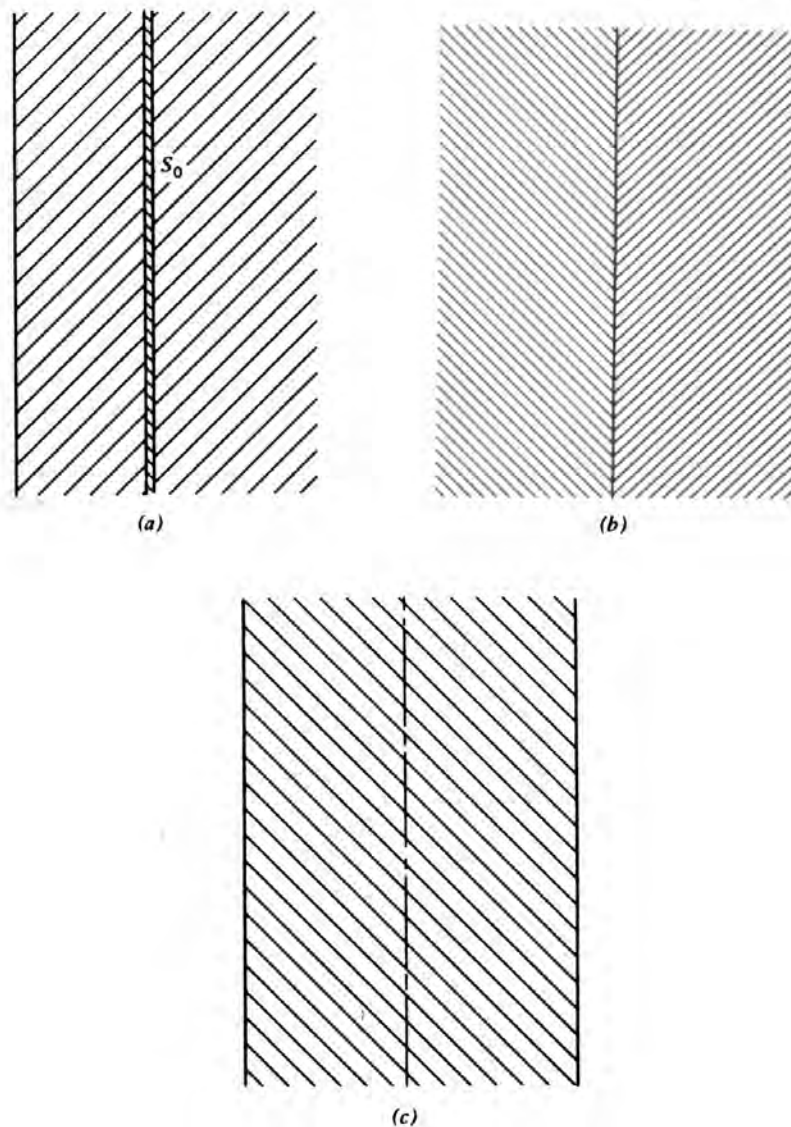


Fig. 2.23 □ The solvable problems in one-speed transport theory. (a) Green's function for a half-space geometry. (b) Two adjacent half-spaces problem. (c) Finite slab geometry.

Some Further Comments on the Singular Eigenfunction Method □ All too frequently one hears claims that the singular eigenfunction method exhibits certain advantages of simplicity and elegance over the more conventional Fourier transform (Wiener-Hopf) method for solving the transport equation. It should be apparent from our discussion, however, that these two approaches are very similar, both in mathematical content and ease of application. But this should not be surprising, since integral transform

methods are intimately related to eigenfunction expansions.

To illustrate this, consider first the case of full-range boundary value problems. If we let $k = \Sigma_i / iv$, the eigenvalues in the singular eigenfunction method become the singularities in the Fourier transform plane (see Figure 2.24). This identity arises for a very fundamental reason. Suppose we consider an operator problem of the form

$$\frac{\partial f}{\partial x} + Af = g$$

where A is an operator and $f(x)$ is the unknown function defined on $x \in (-\infty, \infty)$. If we take a Fourier transform in x , we find

$$(A - ik)\tilde{f} = \tilde{g}$$

or formally

$$\tilde{f} = (A - ik)^{-1} \tilde{g}$$

Then we can invert this expression to find

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{-ikx} (A - ik)^{-1} \tilde{g}(k)$$

But to accomplish this inversion, we must study the singularities of $(A - ik)^{-1}$ in the k -plane. Of course these singularities are just those points at which

$$(A - ik)\psi = 0 \quad \text{or} \quad A\psi_k = ik\psi_k$$

that is, where ik is an eigenvalue of A . Chapter 5, which discusses eigenvalue problems in transport theory from the more general viewpoint of the spectral theory of linear operators, clarifies these ideas.

In half-range boundary value problems, both integral transform and separation of variables methods lead eventually to a functional equation in complex variables. The integral transform approach yields an equation relating the two unknown "halves" of the Fourier transform, $\tilde{\phi}_+(k)$ and $\tilde{\phi}_-(k)$:

$$G(k)\tilde{\phi}_+(k) - \tilde{\phi}_-(k) = f(k)$$

Furthermore, we can show that $\tilde{\phi}_+(k)$ and $\tilde{\phi}_-(k)$ are analytic in complementary half-planes and in a common strip. The Wiener-Hopf method can then be used to solve this equation by a suitable decomposition of known

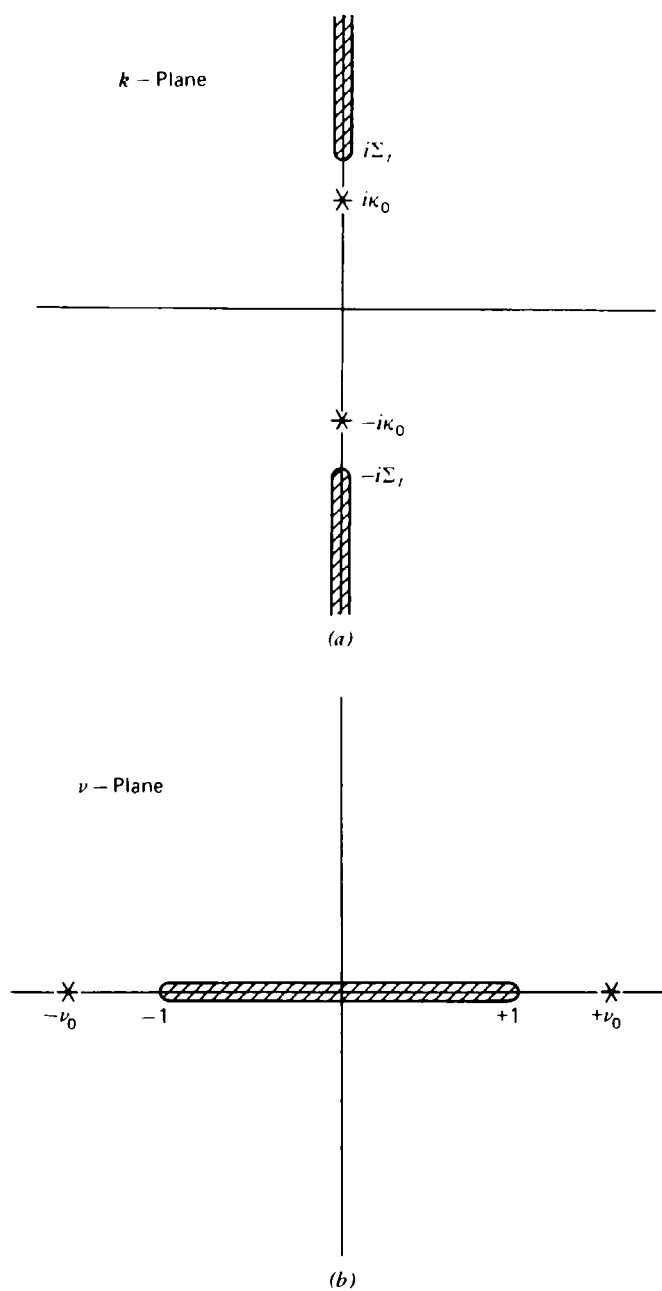


Fig. 2.24 □ Comparison of analytic structure of (a) Fourier transform (k -plane) with (b) eigenvalue spectrum (ν -plane).

functions that allows the application of Liouville's theorem to determine the unknowns.

In the separation of variables method, we identified the evaluation of the expansion coefficients in an eigenfunction expansion using specified boundary conditions as equivalent to solving a singular integral equation of the Cauchy type. Then using the standard techniques of Muskhelishvili, we reduced this equation to a boundary value problem in complex variables—the inhomogeneous Hilbert problem

$$G(\mu)\Phi^+(\mu) - \Phi^-(\mu) = f(\mu), \quad \mu \in [-1, +1]$$

Again a factorization of known functions (the Riemann-Hilbert problem) was used to solve this functional equation.

It is important to recognize that the application of singular integral equation methods could have also been used in the integral transform approach (although this makes for a rather round-about way of solving transport problems).³² Consider by way of example the Milne problem in which a Laplace transform has been applied directly to the integrodifferential form of the transport equation to find

$$\Lambda(s)\tilde{\phi}(s) = \int_{-1}^0 d\mu \frac{\mu\varphi(0, \mu)}{\Sigma_t + s\mu} \quad (2.71)$$

Then if we note that

$$\mu\varphi(0, \mu) = \frac{c\Sigma_t}{2} \int_0^\infty dx \phi(x) \exp\left(\frac{\Sigma_t x}{\mu}\right) = \left(\frac{c\Sigma_t}{2}\right) \tilde{\phi}\left(\frac{-\Sigma_t}{\mu}\right)$$

we can rewrite Eq. 2.71 as

$$\Lambda(s)\tilde{\phi}(s) = \frac{c\Sigma_t}{2} \int_{-1}^0 d\mu \frac{\tilde{\phi}(\Sigma_t/\mu)}{\Sigma_t + s\mu}$$

which is just a singular integral equation of the Cauchy type and therefore is amenable to the methods described in Appendix C.

Therefore one can either use the Wiener-Hopf method to solve the transformed transport equation or recast this as a singular integral equation and then reduce it to a Riemann-Hilbert problem. Both methods eventually obtain a solution by decomposition of the “dispersion function” $\Lambda(z)$ characterizing the spatial relaxation modes of the transport equation and then appealing to Liouville's theorem.

Even the structure of the decomposition of $\Lambda(z)$ in each approach is remarkably similar, as Figure 2.25 should make apparent. Furthermore,

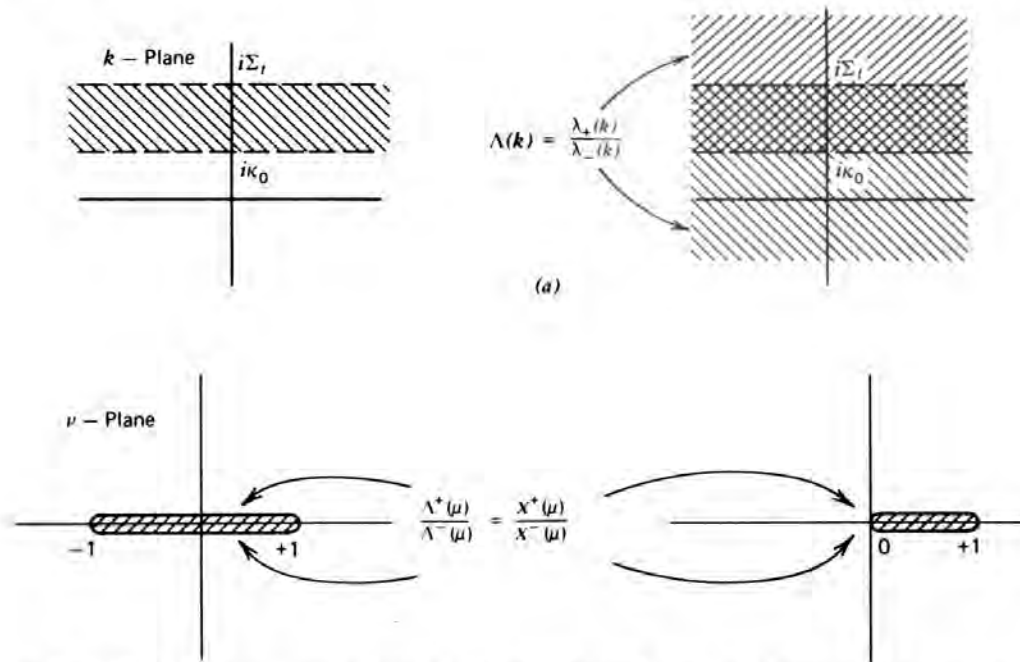


Fig. 2.25 □ Comparison of the (a) Wiener-Hopf and (b) Riemann-Hilbert decompositions of the dispersion function $\Delta(z)$.

the specific forms of the solutions are similar. Thus, in a very real sense, the integral transform (Wiener-Hopf) and singular eigenfunction (Riemann-Hilbert) approaches are almost equivalent. (Of course each of these techniques has its own following of devoted disciples—the “Caseologists” and the “Wiener-Hopf”ers—and most comparisons of the two methods usually include a long discourse on why one method is better than the other. But that is the way the game is sometimes played.) Excellent reviews of the Wiener-Hopf and singular eigenfunction methods (along with a rather detailed comparison of the methods) have been given by Williams²⁶ and by McCormick and Kuščer.³²

2.2.5 □ Some Generalizations □

Anisotropic Scattering □ In our earlier analysis in this chapter we have assumed that the scattering probability was isotropic [i.e., $f(\hat{\Omega}' \rightarrow \hat{\Omega}) = 1/4\pi$]. However in many cases this assumption is inadequate: for example, in the case of fast neutron transport⁴⁸ or photon transport⁴⁹ in atmospheres. To generalize our treatment, we represent the scattering probab-

ity as a finite term expansion in Legendre polynomials of the form

$$f(\hat{\Omega}' \rightarrow \hat{\Omega}) = \sum_{l=0}^N \left(\frac{2l+1}{4\pi} \right) f_l P_l(\hat{\Omega}' \cdot \hat{\Omega})$$

where the expansion coefficients, f_l , are presumed known. Then by substituting this into the one-speed transport equation and using the addition theorem for spherical harmonics (see Chapter 4 for details), we can write the more general one-speed transport equation (in dimensionless notation)

$$\mu \frac{\partial \varphi}{\partial x} + \varphi(x, \mu) = \frac{c}{2} \sum_{l=0}^N (2l+1) f_l P_l(\mu) \int_{-1}^{+1} d\mu' P_l(\mu') \varphi(x, \mu') + s(x, \mu)$$

The extension of the singular eigenfunction method to this equation was first given by Mika.⁵⁰ We seek solutions in the usual form

$$\varphi(x, \mu) = \psi_\nu(\mu) e^{-x/\nu} \quad (2.72)$$

and then substitute this ansatz into Eq. 2.72 to find the eigenvalue problem for ν :

$$(\nu - \mu) \psi_\nu(\mu) = \frac{c\nu}{2} \sum_{l=0}^N (2l+1) f_l P_l(\mu) \int_{-1}^{+1} d\mu' P_l(\mu') \psi_\nu(\mu') \equiv \frac{c\nu}{2} M(\mu, \nu)$$

If we multiply through by $P_k(\mu)$, integrate over μ , and use the orthogonality properties of the Legendre polynomials, we arrive at a three-term recursion relation for

$$\psi_{\nu k} \equiv \int_{-1}^{+1} d\mu' P_k(\mu') \psi_\nu(\mu')$$

of the form

$$\nu(1 - cf_k) \psi_{\nu k} - \left(\frac{k+1}{2k+1} \right) \psi_{\nu k+1} - \left(\frac{k}{2k+1} \right) \psi_{\nu k-1} = 0$$

This can be used to determine $\psi_{\nu k}$, subject to the normalization condition $\psi_{\nu 0} = 1$.

We can restrict $\nu \notin [-1, +1]$ in the usual way to determine a condition for the discrete eigenvalues

$$\Lambda(\nu) = 1 - \frac{c\nu}{2} \sum_{l=0}^N (2l+1) f_l \psi_{\nu l} \int_{-1}^{+1} d\mu \frac{P_l(\mu)}{\nu - \mu} = 0$$

Because we now have a sum of N integrals in this equation, we might expect to find more than just the two zeros $\pm \nu_0$, which occurred for isotropic scattering. One finds $2M$ discrete eigenvalues $\pm \nu_j$ in general, where $M \leq N$, and the corresponding discrete eigenfunctions become

$$\psi_{j\pm}(\mu) = \pm \frac{c\nu_j}{2} \frac{M(\mu, \pm \nu_j)}{\pm \nu_j - \mu}, \quad j = 1, \dots, M$$

(See Mika⁵⁰ or Case and Zweifel²⁸ for details concerning the location of the discrete eigenvalues.)

Just as in the isotropic scattering case, we find that those $\nu \in [-1, +1]$ correspond to the continuous spectrum of eigenvalues with corresponding singular eigenfunctions:

$$\psi_\nu(\mu) = \frac{c\nu}{2} PM(\mu, \nu) \frac{1}{\nu - \mu} + \lambda(\nu) \delta(\mu - \nu)$$

where λ is again determined by the normalization condition. With only a slight complication in algebra, we can prove that these eigenfunctions are orthogonal and complete over the full range $[-1, +1]$ and complete over the half-range $[-1, 0]$ and $[0, +1]$ (for details, refer to Mika⁵⁰).

Hence these eigenfunctions can be used to solve any of the standard problems we have discussed for the case of isotropic scattering—at least formally. However from a practical standpoint, the calculation becomes extremely awkward unless N is small (e.g., $N=0$ or $N=1$).

Finite Geometries with One-Dimensional Symmetry □ We begin by noting that the integral transport equations for slab and sphere geometries are very similar:

SLAB

$$\phi(x) = \frac{c}{2} \int_0^a dx' E_1(|x - x'|) \phi(x') + s_0(x)$$

SPHERE

$$\phi(r) = \frac{c}{2r} \int_0^{a/2} dr' r' [E_1(|r - r'|) - E_1(|r + r'|)] \phi(r') + s_0(r)$$

If we let $\hat{\phi}(r) = r\phi(r)$ and $\phi_0(r) = \hat{\phi}(r - a/2)$ in the equation for a sphere, we find

$$\phi_0(x) = \frac{c}{2} \int_0^a dx' E_1(|x - x'|) \phi_0(x') + \left(x - \frac{a}{2}\right) s_0\left(x - \frac{a}{2}\right)$$

which is identical to the slab equation, except that we have an asymmetric source term. Hence if we can solve the transport equation for a slab, we can also solve it for a sphere.

But how do we solve the problem of the one-speed slab geometry? We could try an expansion in singular eigenfunctions (see Case and Zweifel⁵¹ or the original work by Mitsis⁵²). But this is rather awkward. A more elegant technique, proposed by Leonard and Mullikin,⁵³ is based on integral transforms. Consider the integrodifferential transport equation for a critical slab of width $2a$:

$$\mu \frac{\partial \varphi}{\partial x} + \varphi(x, \mu) = \frac{c}{2} \int_{-1}^{+1} d\mu' \varphi(x, \mu') \quad (2.73)$$

with boundary conditions

$$\varphi(a, -\mu) = \varphi(-a, \mu) = 0, \quad \mu \in [0, 1]$$

Suppose we decompose

$$\phi(x) = \int_{-1}^{+1} d\mu \varphi(x, \mu) = \int_0^1 d\mu [\varphi(x, \mu) + \varphi(x, -\mu)]$$

Then if we integrate the transport equation (2.73) over space, we find

$$\varphi(x, \mu) = \frac{c}{2\mu} \int_{-a}^x dx' \phi(x') e^{-(x-x')/\mu} \quad (2.74)$$

$$\varphi(x, -\mu) = \frac{c}{2\mu} \int_x^a dx' \phi(x') e^{-(x'-x)/\mu} \quad (2.75)$$

But we can regard equations (2.74) and (2.75) as defining an integral transform pair. If we now insert Eq. 2.74 into Eq. 2.75 and integrate over x , we find an integral equation

$$\begin{aligned} \varphi(x, \mu) = & \frac{c}{2} \int_{-1}^{+1} d\nu \frac{\varphi(x, \nu) - \mu \varphi(x, \mu)}{\nu - \mu} \\ & + \frac{c}{2} \int_0^1 d\nu \frac{\mu \varphi(x, \mu) + \nu \varphi(x, -\nu) - \nu \exp[-(a+x)/\mu]}{\nu + \mu} \end{aligned}$$

or collecting terms,

$$\lambda(\mu) \varphi(x, \mu) = \frac{c}{2} P \int_{-1}^{+1} d\nu \frac{\nu \varphi(x, \nu)}{\nu - \mu} - \frac{c}{2} e^{-(a+x)/\mu} \int_0^1 d\nu \frac{\nu \varphi(a, \nu)}{\nu + \mu} \quad (2.76)$$

But we recognize this as a singular integral equation of the Cauchy type, very similar to those we encountered in the half-range completeness proofs. (In a sense, Eq. 2.76 turns out to be adjoint to the singular integral equation we solved earlier.) The same techniques (i.e., reduction to an inhomogeneous Hilbert problem in complex variables) can be used to solve Eq. 2.76 for $\varphi(a, \mu)$, and this form can be inserted into Eq. 2.77 to find $\varphi(x, \mu)$. Very similar techniques can be used to solve transport problems in periodic geometries (e.g., one-dimensional lattices).

Multidimensional Transport Problems □ Both the integral transform (Wiener-Hopf) and singular eigenfunction methods are essentially restricted to one-dimensional boundary value problems in transport theory. Although there have been many attempts to extend these methods to two- and three-dimensional problems (e.g., the “corner” Milne problem), these extensions have usually encountered extreme mathematical complexity and have met with only marginal success.⁵⁴

Consider, for example, the application of a two-dimensional Fourier transform that results in a transformed flux $\tilde{\phi}(k_x, k_y)$, which is defined in the neighborhood of the real k_x and k_y axes. We can analytically continue the integral definition of $\tilde{\phi}(k_x, k_y)$ as four components, analytic in the upper-upper $k_x - k_y$ planes, upper-lower $k_x - k_y$ planes, and so on. Hence it is apparent that we must solve one functional equation for four unknowns ϕ_{++} , ϕ_{+-} , ϕ_{-+} , and ϕ_{--} using the analogue to the Wiener-Hopf decomposition (known as the Bochner theorem).⁵⁵ But an explicit scheme for constructing this decomposition is not yet available.

Singular eigenfunction methods have fared no better. Indeed, even the determination of the singular eigenfunctions⁵⁶ is a far from trivial task—much less their application to solve actual multidimensional boundary value problems. Therefore we must conclude that the solution of even simple modeled transport problems in more than one space dimension is beyond the capability of existing methods of analysis.

There has been limited success in studying boundary value problems in which the additional dimensions are treated in an asymptotic sense. In these schemes one seeks to represent the angular flux in the form

$$\varphi(x, y, z, \hat{\Omega}) = \varphi(z, \hat{\Omega}) e^{iB_x x} e^{iB_y y}$$

where the parameters B_x and B_y that characterize the transverse directions are regarded as real, fixed parameters. One then arrives at an effectively one-dimensional problem (dependent on the parameters B_x and B_y) that can be solved using the usual integral transform or singular eigenfunction methods.

2.3 □ TIME-DEPENDENT PROBLEMS IN TRANSPORT THEORY

□ In principle at least, one can easily extend either integral transform or singular eigenfunction methods to the analysis of time-dependent problems in one-speed transport theory. We illustrate with an initial value problem involving the time-dependent, one-speed transport equation characterizing a slab of width a :

$$\frac{1}{v} \frac{\partial \varphi}{\partial t} + \mu \frac{\partial \varphi}{\partial x} + \Sigma_t \varphi(x, \mu, t) = \frac{c \Sigma_t}{2} \int_{-1}^{+1} d\mu' \varphi(x, \mu', t)$$

with boundary conditions

$$\varphi(0, \mu, t) = 0 = \varphi(a, -\mu, t), \quad \mu > 0$$

and initial condition

$$\varphi(x, \mu, 0) = \varphi_0(x, \mu)$$

We begin by taking a Laplace transform in time

$$\tilde{\varphi}(x, \mu, s) = \int_0^\infty dt e^{-st} \varphi(x, \mu, t)$$

to find the transformed transport equation

$$\mu \frac{\partial \tilde{\varphi}}{\partial x} + \left(\Sigma_t + \frac{s}{v} \right) \tilde{\varphi}(x, \mu, s) = \frac{c \Sigma_t}{2} \int_{-1}^{+1} d\mu' \tilde{\varphi}(x, \mu', s) + \frac{1}{v} \varphi_0(x, \mu)$$

But this can be identified as just a steady-state problem with a “complex” mean free path or cross section $\Sigma_t + s/v = (mfp)^{-1}$. Hence we can apply the usual integral transform or eigenfunction expansion methods to solve this effectively one-speed, time-independent problem (treating s as an arbitrary complex parameter). But of course the most difficult task follows, when the Laplace-transformed solution must be inverted.

A variety of half-space problems have been approached in this manner. Kuščer and Zweifel⁵⁷ analyzed the time-dependent albedo problem in which a beam of particles is reflected off a half-space. A similar problem with two adjacent half-spaces was studied by Erdmann and Lurie.⁵⁸ Perhaps the most elegant work has been Bowden's solution⁵⁹ of the time-dependent slab problem. As a general rule, any stationary problem that can be solved with one-speed transport theory can also be solved as a time-dependent problem, if one has enough patience (tedious, but straightforward).

Although the detailed mathematical manipulation involved in solving such time-dependent boundary value problems can become rather ugly, some rather amusing physics that occurs in such problems can be illustrated by solving a somewhat simpler problem. Consider the initial value problem for the transport equation in which we specify the spatial dependence of the flux by assuming a form:

$$\varphi(x, \mu, t) = \varphi(\mu, t) e^{iBx} \quad (2.77)$$

where B is a fixed parameter. For example, if Eq. 2.77 is used to simulate the fundamental spatial mode of a slab geometry, we would choose $B = \pi/a$. Substituting this form into the transport equation, we find, after taking a Laplace transform,

$$\left(iB\mu + \Sigma_t + \frac{s}{v}\right) \tilde{\varphi}(\mu, s) = \frac{c\Sigma_t}{2} \int_{-1}^{+1} d\mu' \tilde{\varphi}(\mu', s) + \frac{1}{v} \varphi_0(\mu) \quad (2.78)$$

where $\varphi_0(\mu)$ is the initial value of the flux [also assumed to be of the form $\exp(iBx)$]. We can now solve Eq. 2.78 in the usual way for

$$\tilde{\phi}(s) = \int_{-1}^{+1} d\mu \tilde{\varphi}(\mu, s) = \frac{\int_{-1}^{+1} d\mu \frac{\varphi_0(\mu)}{(iB\mu + \Sigma_t + s/v)}}{1 - \frac{c\Sigma_t}{2} \int_{-1}^{+1} \frac{d\mu}{iB\mu + \Sigma_t + s/v}} \equiv \frac{\chi(B, s)}{\Lambda(B, s)} \quad (2.79)$$

Here we have explicitly indicated that this solution depends on the value B chosen to characterize the spatial dependence. We can now attempt the inversion of the Laplace transform

$$\phi(t) = \frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} ds e^{st} \frac{\chi(B, s)}{\Lambda(B, s)}$$

by studying the analytic structure of the transformed flux given by Eq. 2.79.

We begin by noting the presence of branch point singularities at $s = -v\Sigma_t \pm iBv$. If we note the integration over μ that gives rise to these singularities, it is apparent that we must draw in the branch cut as shown in Figure 2.26.

The poles of the transformed flux will correspond to zeros of $\Lambda(B, s)$:

$$\Lambda(B, s) = 1 - \frac{c\Sigma_t}{2} \int_{-1}^{+1} \frac{d\mu}{iB\mu + \Sigma_t + s/v} = 0 \quad (2.80)$$

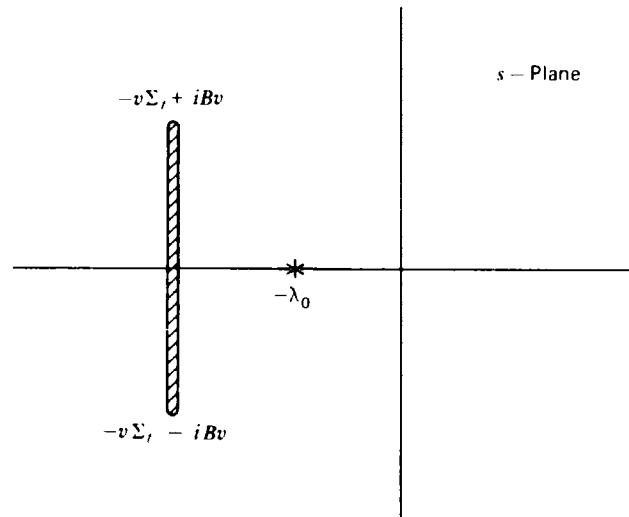


Fig. 2.26 □ Laplace transform s-plane structure.

Notice here that these zeros will depend on the parameter B . A relationship such as Eq. 2.80, which gives the characteristic “frequencies” of a process, $s_0(B)$, in terms of the “wave number” B is referred to as a *dispersion law* or *dispersion relation*.⁶⁰

But how many zeros does $\Lambda(B, s)$ have? A clue is provided by the case $B=0$, for then

$$\Lambda(0, s) = 1 - \frac{c\Sigma_i}{\Sigma_i + s/v} = 0 \Rightarrow s_0 = -(1-c)v\Sigma_i$$

One can easily demonstrate that for $B > 0$, there continues to be only one zero, which we label as $s_0 = -\lambda_0(B)$. It can also be shown that this zero is real and is located on the negative real axis $-v\Sigma_i < -\lambda_0(B) < \infty$.

Therefore we expect a general solution of the form

$$\phi(t) = a_0 e^{-\lambda_0 t} + e^{-\lambda^* t} \int_0^{vB} d\lambda A(B, \lambda) \sin \lambda t$$

where we have introduced the definition $\lambda^* \equiv v\Sigma_i$. In particular, for large t [more precisely, for $t \gg (v\Sigma_i)^{-1}$], we find the expected exponential behavior

$$\phi(t) \sim a_0 e^{-\lambda_0 t}, \quad t \gg \lambda^*{}^{-1}$$

But something rather interesting can occur here. We recall that the exponential decay constant $\lambda_0(B)$ depends on the parameter B which, in turn, characterizes the size of the system (e.g., the width of the slab). If we

were to make the system smaller, B would increase and $\lambda_0(B)$ would change. It can be demonstrated that $\lambda_0(B)$ is a monotonically increasing function of B (actually, of B^2) as Figure 2.27 illustrates. But what happens if we make the system sufficiently small that we drive $\lambda_0(B)$ to λ^* [i.e., we push the pole $-\lambda_0(B)$ over to the cut]? If we note that

$$\int_{-1}^{+1} \frac{d\mu}{iB\mu + \Sigma_i + s/v} = \frac{2}{B} \tan^{-1} \left(\frac{B}{\Sigma_i + s/v} \right) < \frac{2}{B} \left(\frac{\pi}{2} \right)$$

then it is apparent that the dispersion law (2.80) will have no zeros for $B > B^* \equiv c\Sigma_i\pi/2$. That is, for $B > B^*$, there will be no pole; therefore, apparently, the time behavior of the flux will assume the form

$$\phi(t) = e^{-\lambda^* t} \int_0^{vB} d\lambda A(B, \lambda) \sin \lambda t, \quad B > B^*$$

That is, if we make the system too small, we will not observe an exponential time decay asymptotically for large times; the flux will never fall into an asymptotic form; the transport transients will never disappear.

This is a rather amusing result. It seems to imply that at some magic value of system size corresponding to $B = B^*$, the time behavior of the flux will change dramatically. But this interpretation is not quite true. For only the mathematical representation of the flux changes. The pole $s_0 = -\lambda_0$ is still there if we look hard enough, but it has moved onto another branch of the log function—onto another Riemann sheet.^{61,62} To track it down for $B > B^*$, we must analytically continue the dispersion law onto the next

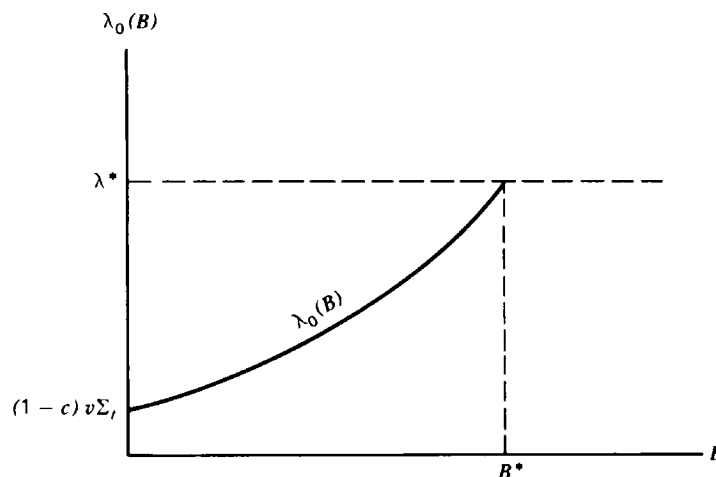


Fig. 2.27 □ Behavior of $\lambda_0(B)$ for increasing B .

Riemann sheet by using as an analytic continuation

$$\begin{aligned}\Lambda(B, s) &= 1 - \frac{c\Sigma_t}{2iB} \int_{-1}^{+1} \frac{d\mu}{\left(\frac{v\Sigma_t + s}{iBv}\right) + \mu} \\ &\rightarrow 1 - \frac{c\Sigma_t}{2iB} \int_{-1}^{+1} \frac{d\mu}{\left(\frac{v\Sigma_t + s}{iBv}\right) + \mu} - \frac{c\Sigma_t}{2iB} (2\pi i) \equiv \Lambda_{ac}(B, s)\end{aligned}$$

Then we find that as B exceeds B^* , the discrete pole moves across the cut onto the next sheet, where it bifurcates into two complex conjugate poles of the analytically continued dispersion law $\Lambda_{ac}(B, s)$ (see Figure 2.28). We can pick up the contribution from the analytic continuation of the pole by appropriate deformation of the Laplace inversion contour as sketched in Figure 2.29. We then find that the form taken by the time dependent flux for $B > B^*$ is

$$\phi(t) = a_0 \exp[-\operatorname{Re}\{\lambda_0\}t] \sin[\operatorname{Im}\{\lambda_0\}t] + e^{-\lambda^*t} \int_{-\infty}^{\infty} d\lambda A(\lambda) \sin \lambda t$$

For intermediate times, $\phi(t)$ assumes a “quasi-exponential” behavior

$$\phi(t) \sim a_0 \exp[-\operatorname{Re}\{\lambda_0\}t]$$

Only for very long times is the nonexponential behavior of $O(\exp(-\lambda^*t))$ from the tip of the branch cut dominant.

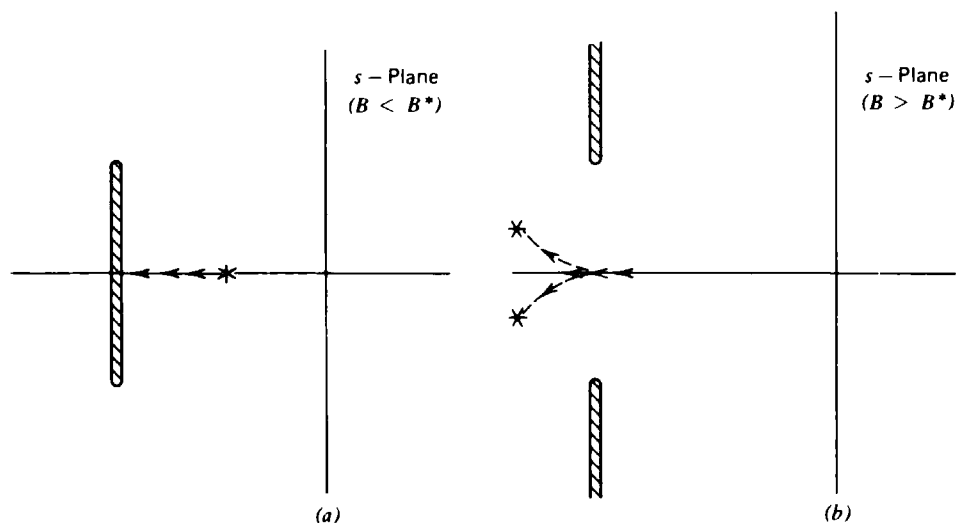


Fig. 2.28 □ Trajectory of pole $\lambda_0(B)$ onto adjacent Riemann sheet for $B > B^*$. (a) Physical sheet for $B < B^*$. (b) Analytical continuation for $B > B^*$.

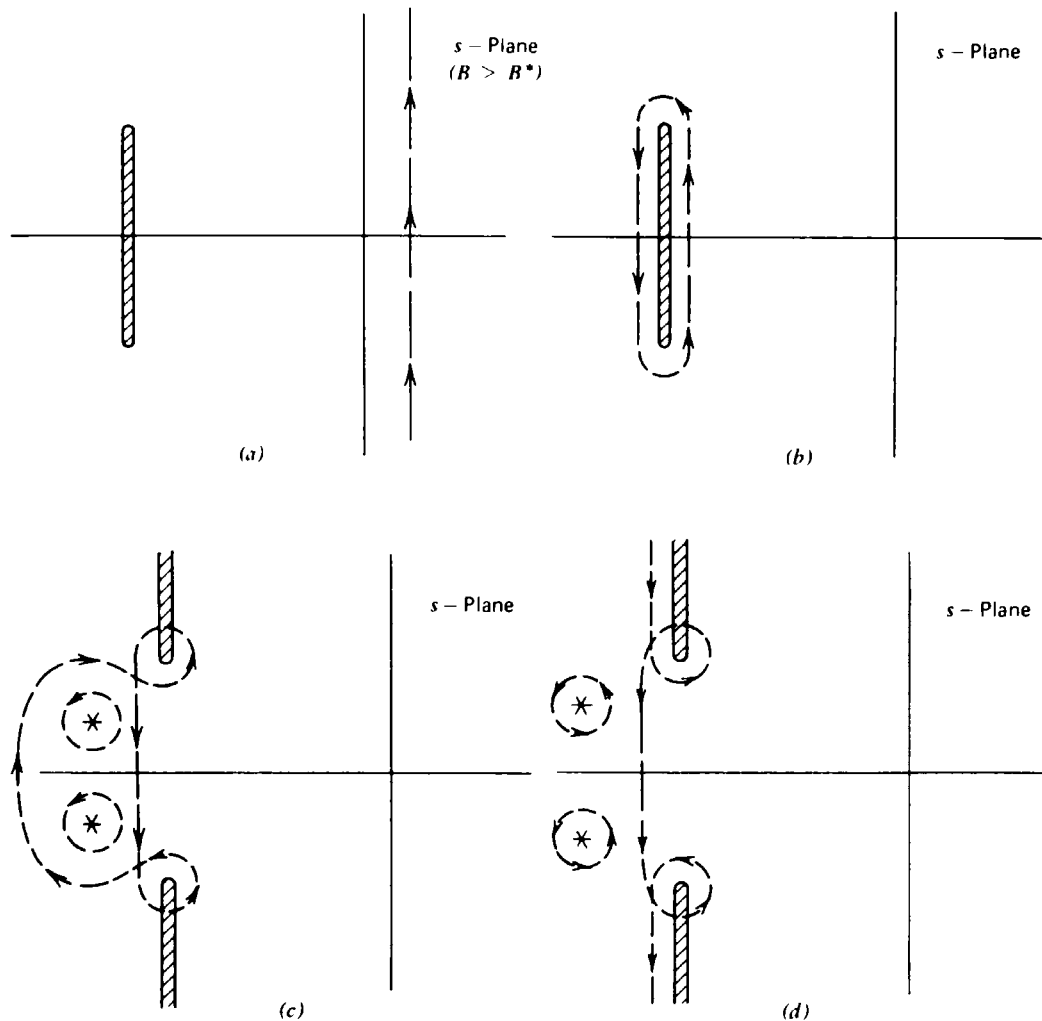


Fig. 2.29 □ Contour deformation to pick up contribution from analytically continued poles for $B > B^*$. (a) Original Bromwich contour. (b) Deformation about branch cut. (c) Deformation onto adjacent Riemann sheet. (d) Contribution from analytical continuation of $\lambda_0(B)$.

As the system size becomes smaller and $B \gg B^*$ becomes larger, the amplitude of the coefficient a_0 becomes smaller and the strength of this quasi-exponential behavior decreases. That is, although there is no sudden change in the nature of the time dependence of the flux for $B > B^*$, the exponential mode will gradually “fade out” if we make B large enough (i.e., the system small enough).

Of course this analysis is based on a very simple model of the spatial dependence of the flux which assumed a constant spatial shape of the form $\exp(iBx)$. However the essential features of this problem remain when a

more accurate treatment of spatial dependence is given, although there are some notable exceptions. For example, in “infinite” geometries such as slabs or infinite cylinders, one finds that there will always be a discrete decay constant λ_0 regardless of the size of the system.^{59,63} By way of contrast, in finite geometries such as spheres or cubes, this discrete decay constant will disappear for sufficiently small systems.⁶⁴ This disappearance of the decay constant also occurs when the one-speed approximation is removed and a more rigorous treatment of the particle energy dependence is included, as Chapter 5 demonstrates.

It should also be noted that the disappearance of decay constants—that is, roots of the dispersion law—for certain limiting values of parameters, arises in other situations as well. For example, if we investigate the response of the angular flux to an oscillating source of the form $S_0 \exp(-i\omega t)$ by seeking solutions to the transport equation of the form

$$\varphi(x, \mu, t) \sim \varphi(\mu) e^{i(kx - \omega t)}$$

it is apparent that the spatial relaxation parameters that govern the asymptotic decay of the flux far away from the source will be determined by a dispersion law of the form

$$\Lambda(k, \omega) = 1 - \frac{c \Sigma_t}{2ik} \int_{-1}^{+1} \frac{d\mu}{ik\mu + \Sigma_t - i\omega/v} = 0$$

But once again we find that the asymptotic relaxation constant $k_0(\omega)$ depends on a parameter, this time the source frequency ω . And once again it can be shown that for sufficiently large frequencies, this root “runs into a branch cut” and disappears.⁶⁵⁻⁶⁷ Then it must be tracked down, using analytic continuation, as we illustrated for the time relaxation problem.

We consider such asymptotic relaxation phenomena in much greater detail in Chapter 5, noting that the relaxation parameters (λ_0 or k_0) can be identified as the fundamental eigenvalues of the appropriate form of the transport operator. In this sense, they play an extremely important role in transport theory.

2.4 □ SOME FINAL COMMENTS ON METHODS FOR SOLVING THE ONE-SPEED TRANSPORT EQUATION □

It should be apparent that there are very few instances in which an analytical solution of the transport equation can be obtained. Even under the most drastic modeling assumptions (e.g., one-speed, isotropic scattering, and one-dimensional symmetry), the direct solution of boundary value problems in transport theory is extremely cumbersome. It is not surprising that the difficulty in

solving even the simplest transport problems, and the hideous complexity of the solutions that have been obtained, have effectively limited the usefulness of these results in the analysis of the more realistic problems that arise in practical studies of transport processes. Indeed, one is quite justified in questioning the rationale behind generating incredibly complicated closed-form solutions to oversimplified problems in preference to far more direct (and transparent) numerical solutions.

Thus the discipline of “analytical” transport theory (i.e., attempts to obtain analytical solutions to drastically simplified or modeled problems) has become effectively divorced from the “real world” of transport phenomena and has turned inward, evolving into essentially a branch of applied mathematics.⁶⁸ Of particular concern has been the subdiscipline of “rigorous transport theory” in which efforts are made to provide the mathematical foundation and justification for such ad hoc approaches as the singular eigenfunction method. And there has always been the underlying hope that such fundamental mathematical studies would lead to the development of methods capable of solving new types of boundary value problem in transport theory.

An excellent case in point is the resolvent integration technique developed by Larsen and Habetler.⁶⁹ By adapting this well-known method⁷⁰ from the theory of boundary value problems in partial differential equations, it has been possible to derive the singular eigenfunction expansion directly. To be more specific, consider our old friend, the one-speed transport equation, under the usual assumptions (and in the usual notation):

$$\mu \frac{\partial \varphi}{\partial x} + \varphi(x, \mu) = \frac{c}{2} \int_{-1}^{+1} d\mu' \varphi(x, \mu') + s(x, \mu)$$

First, let us manipulate this into a “separation of variables”-like form

$$\frac{\partial \varphi}{\partial x} + \frac{1}{\mu} \varphi - \frac{c}{2\mu} \int_{-1}^{+1} d\mu' \varphi(x, \mu') = \frac{s(x, \mu)}{\mu}$$

We denote the angular operator by K^{-1}

$$K^{-1} \varphi \equiv \frac{1}{\mu} \varphi - \frac{c}{2\mu} \int_{-1}^{+1} d\mu' \varphi(x, \mu')$$

One can easily construct the inverse K as

$$K\varphi = \mu\varphi + \frac{c}{2(1-c)} \int_{-1}^{+1} d\mu' \mu' \varphi(\mu')$$

Since K is a bounded integral operator, we can apply well-known results from functional analysis to study the eigenvalue spectrum of K . (Here we must use concepts developed more fully in Chapter 5 and Appendix E.) To this end, we explicitly construct the resolvent operator corresponding to K

$$(zI - K)^{-1}\varphi(\mu) = \frac{1}{z - \mu} \left\{ \varphi(\mu) - \frac{c}{2\Lambda(z)} \int_{-1}^{+1} d\mu' \frac{\mu' \varphi(\mu')}{\mu' - z} \right\}$$

From the known behavior of $\Lambda(z)$, we can identify the eigenvalue spectrum of K as follows:

Point spectrum $\sigma_p(K)$: $+\nu_0, -\nu_0$ [$\Lambda(\pm\nu_0)=0$]

Continuous spectrum $\sigma_c(K)$: $\nu \in [-1, +1]$

Residual spectrum $\sigma_r(K)$: $\emptyset$

With this knowledge, we can construct the spectral representation (i.e., the eigenfunction expansion) of an arbitrary function $\varphi(\mu)$ by using the identity

$$\varphi(\mu) = \frac{1}{2\pi i} \oint_C (zI - K)^{-1} \varphi(\mu) dz$$

where the contour C encloses the spectrum of K (see Figure 2.30).

One can deform the contour to explicitly evaluate the integral and find

$$\varphi(\mu) = a_{0+} \psi_{0+}(\mu) + a_{0-} \psi_{0-}(\mu) + \int_{-1}^{+1} d\nu A(\nu) \psi_\nu(\mu)$$

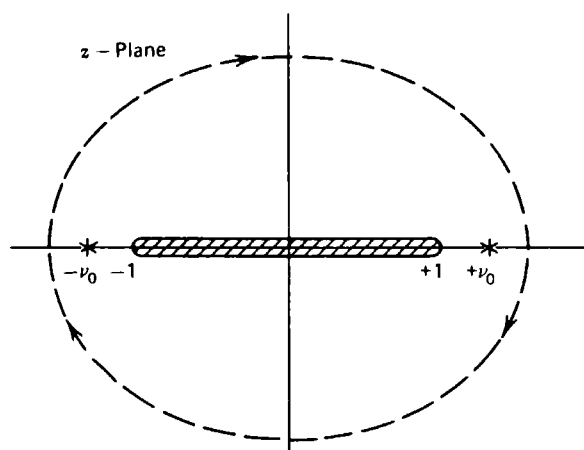


Fig. 2.30 □ Integration contour for resolvent operator.

where $\{\psi_{0\pm}, \psi_\nu\}$ are the usual singular eigenfunctions and $a_{0\pm}, A(\nu)$ are the appropriate (full-range) expansion coefficients.

In this manner Larsen and Habetler have been able to use standard tools from functional analysis to justify the more ad hoc approach taken by Case. A similar analysis can be given for half-range boundary value problems.

By providing the bridge between the singular eigenfunction method and the more familiar (and rigorous) methods of functional analysis, Larsen and Habetler⁶⁹ stimulated a flurry of activity aimed at “rigorizing” the mathematical methods used to solve transport problems.⁷¹ But more significantly, since the resolvent integration approach actually constructs the spectral representation for the boundary value problem of interest, there was great hope that this method could be used to solve more general problems such as the energy-dependent (more specifically, the multigroup) transport equation.⁷² We discuss these developments in Chapter 5.

The study of the mathematical foundations of the transport equation has continued with the work of Hangelbroek.⁷³ By viewing the transport equation as a first-order linear differential equation in the spatial variable x , Hangelbroek was able to transform this equation into a new form using the theory of holomorphic semigroups of operators. He identified Case’s singular eigenfunctions as corresponding to certain functionals on subspaces of the Hilbert space of square-integrable functions of μ . This particular approach is considerably more formal than the resolvent integration method of Larsen and Habetler (and it is steeped in far more abstract mathematics). It has seen only limited application to date, by those seeking actual solutions to boundary value problems in transport theory (as opposed to those interested in studying the properties of the transport equation itself).

The redirection of the mathematical study of transport theory from the solution of specific boundary value problems (no matter how simplified) to more rigorous studies of the mathematical foundations of the transport equation, is certainly understandable. Even the development of newer methods such as the singular eigenfunction approach has not appreciably enlarged the class of solvable problems in transport theory beyond those that were (or could be) solved using the more classical integral transform methods. Furthermore, the development of powerful numerical methods for solving the transport equation for problems of more practical interest has largely eliminated the need for such analytical methods for all but pedagogical purposes. Therefore it is natural that the subject of mathematical transport theory has drifted away from the study of the physics of transport phenomena and has attempted to establish itself as a distinct discipline in applied mathematics.

□ PROBLEMS □

2.1 An isotropic point source is emitting S_0 monoenergetic particles per second in an infinite medium. Assume that the medium is characterized by an absorption cross section Σ_a but only by negligible scattering. Determine the rate at which particle absorptions occur per unit volume at any point in the medium.

2.2 Consider a sphere of radius a in a vacuum. On the surface of the sphere the angular flux is isotropic and constant [i.e., $\varphi(r=a, \mu) = C$]. Determine the angle-integrated flux $\phi(r)$ and examine its behavior for large $|r|/a$. (For simplicity, assume that the interior of the sphere is a “black” absorber so that no particles can penetrate through the sphere.)

2.3 Determine the flux $\phi(r)$ at any position within a spherical shell of radius R if the angular density on the surface of the shell is given by $\varphi(R, \mu) = \phi_0(1 + a\mu)$. In particular, comment on your answer for $a < 0$, $a = 0$, and $a > 0$. Assume that the interior of the shell is a vacuum.

2.4 Consider an isotropic source distributed uniformly throughout a half-space that is purely absorbing. Determine the angular flux and current at the surface of the medium.

2.5 In a laser-induced thermonuclear fusion reaction, a tiny pellet is imploded to superhigh densities such that it ignites in a thermonuclear burn. In such a reaction some 10^{17} 14 MeV neutrons will be emitted essentially instantaneously (within 10^{-11} sec). Compute the neutron flux at a distance of one meter from the reaction as a function of time (assume that the chamber in which the reaction occurs is evacuated).

2.6 Explicitly take the $t \rightarrow \infty$ limit of the general solution to the time-dependent transport equation in purely absorbing media and demonstrate its equivalence to the steady-state result.

2.7 Derive the first-flight kernel for an isotropic line source.

2.8 Demonstrate that the average chord length characterizing a nonreentrant geometry is given by $\langle R \rangle = 4V/S$. (The reader might find it useful to refer to References 2, 5, or 7.)

2.9 Demonstrate that the first-flight escape probability for a nonreentrant volume can be written in the form given by Eq. 2.28. Use this expression to demonstrate that the first-flight escape probability characterizing a large lump is given by $P_0 = S/4V\Sigma_t$.

2.10 Derive the relation between point source and plane source solutions to the transport equation given on page 83.

2.11 Determine the escape probability P_0 for a slab of thickness L using the Dirac chord method.

2.12 Demonstrate that the one-speed, time-independent transport equation in plane geometry takes the form given in Table 2.2 even for space-dependent cross sections, $\Sigma_t = \Sigma_t(x)$, if one introduces the variable transformation to the optical depth, $\tau(x) = \int_0^x dx \Sigma_t(x)$.

2.13 Verify the bound $\|K\| \leq (c\Sigma_t/l)$ for the integral transport operator K defined in Eq. 2.37.

2.14 Weinberg and Wigner⁷⁴ state that there is no closed-form expression for the spatial relaxation constant $\nu_0 \equiv \kappa_0^{-1}$ of the one-speed transport equation. However McInerney⁷⁵ has derived just such an expression. To provide a review in complex variable theory, it is a useful exercise to derive this expression for ν_0 as follows:

- i Define a function

$$\Lambda(z) = 1 - \frac{cz}{2} \ln\left(\frac{z+1}{z-1}\right)$$

which is analytic in the z -plane cut from $[-1, +1]$. Determine the limiting values as z approaches a value ν on the cut from above and below for $\nu \in [-1, +1]$.

- ii Use Cauchy's theorem to show that

$$[\Lambda(z)]^{-1} = -\frac{c}{2} \int_{-1}^{+1} d\nu \frac{\nu g(c, \nu)}{\nu - z} + \frac{1}{1-c} - \frac{2\nu_0}{K(z^2 - \nu_0^2)}$$

$$g(c, \nu) \equiv \left[(1 - c\nu \tanh^{-1} \nu)^2 + \frac{c^2 \pi^2 \nu^2}{4} \right]^{-1}$$

$$K \equiv \frac{\nu_0^2(1-c) - 1}{\nu_0(\nu_0^2 - 1)}$$

- iii Find a similar formula for $z^2/\Lambda(z)$.

- iv Use these results to find

$$\nu_0^2 = \left[\frac{1}{3(1-c)} - (1-c) \int_0^1 d\nu \nu^2 g(c, \nu) \right] \left[1 - (1-c) \int_0^1 d\nu g(c, \nu) \right]^{-1}$$

2.15 Prove that $\Lambda(z) = 1 - (cz/2) \ln(z+1)/(z-1)$ has two zeros, $\pm \nu_0$. *Hint.* Apply the principle of the argument⁷⁴ to $\Lambda(z)$ using the contour indicated in Figure 2.31.

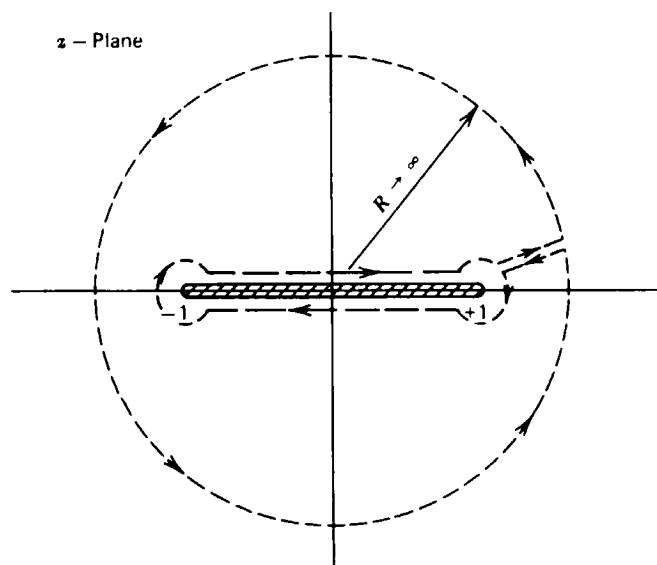


Fig. 2.31 □ Integration contour for application of the principle of the argument to $\Lambda(z)$.

2.16 Obtain an expansion for κ_0 for the case of $(1 - c) \ll 1$.

2.17 State the identity theorem for analytic functions and indicate how it can be used to analytically continue the definition of the Fourier transform off of the real k -axis and into the complex k -plane. (See Knopp⁶¹ or Copson.²⁰)

2.18 Solve the one-speed transport equation for the flux $\phi(\mathbf{r})$ resulting from an isotropic point source at the origin of an infinite medium. (Essentially, imitate the Fourier transform analysis of the plane source problem.)

2.19 Calculate the limits of the point source and plane source solutions as $c \rightarrow 1$. (The plane source limit is somewhat tricky.)

2.20 Consider a directed beam of particles in an isotropically scattering and absorbing infinite medium. Determine the total flux by first computing the distribution of first collisions, then treating each of these as an isotropic point source.

2.21 Modify the usual convolution theorem from the theory of integral transforms to find

$$\mathfrak{F} \left\{ \int_0^\infty dy K(x-y) \varphi(y) \right\} = \tilde{K}(k) \tilde{\varphi}_+(k)$$

where $\mathfrak{F}$ denotes the Fourier transform, $\tilde{K} \equiv \mathfrak{F}\{K\}$, and $\tilde{\varphi}_+$ is the positive “one-sided” Fourier transform.

2.22 Use the integral transport equation to demonstrate that $\phi(x) \sim 0(\exp(\Sigma_t x))$ as $x \rightarrow -\infty$ in the Milne problem.

2.23 Solve the Fredholm integral equation

$$\varphi(x) = \lambda \int_0^\infty dy e^{-|x-y|} \varphi(y)$$

for λ real. Consider only solutions for which $|\varphi(x)| \leq A e^{mx}$ for $x > 0$, for some $A > 0$, $m < 1$.

2.24 Discuss in a general fashion the construction of solutions to integral equations of the following types:

$$\text{i} \quad g(x) = \int_0^\infty dy k(x-y) \varphi(y), \quad x > 0$$

(Fredholm equation of the first kind)

$$\text{ii} \quad \varphi(x) = g(x) + \int_0^\infty dy k(x-y) \varphi(y), \quad x > 0$$

(Fredholm equation of the second kind)

where $g(x)$ and $k(x)$ are given for $x > 0$ and $-\infty < x < \infty$, respectively, and $\varphi(y)$ is unknown.

2.25 Demonstrate that the one-speed transport equation characterizing a uniform medium is invariant under spatial translation.

2.26 Compare the definition of the Hölder condition with the more familiar Lipschitz condition encountered in differential calculus.

2.27 Derive the normalization $N(\nu)$ for the singular eigenfunctions. You will need to employ the Poincaré-Bertrand formula:⁴²

$$\int_L dt_1 \int_L dt \frac{\varphi(t, t_1)}{(t-t_0)(t_1-t)} = \pi^2 \varphi(t_0, t_0) + \int_L dt \frac{1}{(t-t_0)} \int_L dt_1 \frac{\varphi(t, t_1)}{(t_1-t)}$$

2.28 Prove that

$$P \int_C dz \frac{1}{z-\nu} = \pi i, \quad \nu \in C$$

where C is any closed contour of “sufficient” smoothness in the z -plane (see Figure 2.32).

2.29 Using the explicit forms given for $a_{0\pm}$, $A(\nu)$, and $\psi_\nu(\mu)$ for the problem of a plane source at the origin of an infinite medium, demonstrate that the solution obtained by the singular eigenfunction method is identical to that obtained using Fourier transform techniques.

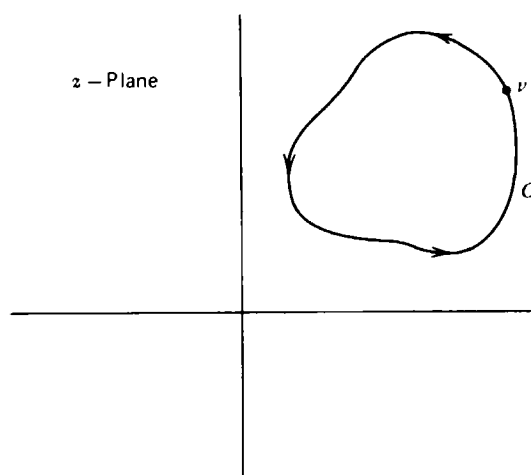


Fig. 2.32 □ A closed contour C characterizing the integral in Problem 2.28.

2.30 To prove the completeness property of the singular eigenfunctions, we explicitly demonstrated the existence (by construction) of the solution to the singular integral equation that arose for the expansion coefficient $A(\nu)$. But how can we assure ourselves that the form we derived for $A(\nu)$ is unique?

2.31 Suggest the form that a “closure” relation for the singular eigenfunctions might take. Sketch how you might go about proving this relation. (Refer to the work of Kuščer and Shure⁴³ if necessary.)

2.32 Determine the flux resulting from an isotropic source located at the interface between two adjacent dissimilar materials of infinite extent (the “two adjacent half-space problem”). Refer to Case and Zweifel²⁸ for the appropriate half-range orthogonality relations.

2.33 Sketch how you would apply the methods of Muskhelishvili⁴² to solve the singular integral equation that results from the Laplace transform approach to the Milne problem.

2.34 Determine the Green’s function for an isotropic source at a position x_0 in a semi-infinite medium.

2.35 Calculate the emerging angular distribution for the case of a uniform source in a semi-infinite medium.

2.36 Prove that $\Lambda_{ac}(z)$ is indeed the analytic continuation of $\Lambda(z)$ onto the adjacent Riemann sheet of $\Lambda(z)$.

2.37 Demonstrate that the analytic continuation of $\lambda_0(B)$ for $B > B^*$ cannot be real.

2.38 Consider the “forced wave propagation” problem in which one studies the angular flux $\varphi(x, \mu, t)$ established by an oscillating plane source

of the form $S_0 e^{-i\omega t}$ located at the origin of an infinite medium. Demonstrate that above some critical source frequency, ω^* , plane wave solutions of the form $\varphi(x, \mu, t) \sim \varphi(\mu) e^{i(kx - \omega t)}$ will not propagate [i.e., prove that the dispersion law $\Lambda(k, \omega)$ has no zeros for $\omega > \omega^*$].

2.39 Derive the form given for the operator K in the resolvent integration method.

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□ 3 □

Collision Phenomena in Particle Transport

In our preliminary discussion of Chapter 1, we indicated that the transport equation describing the particle phase space density $n(\mathbf{r}, \mathbf{v}, t)$ could be written in the general form

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial n}{\partial \mathbf{v}} = \left(\frac{\partial n}{\partial t} \right)_{\text{coll}} \quad (3.1)$$

where $(\partial n / \partial t)_{\text{coll}}$ represents the change in $n(\mathbf{r}, \mathbf{v}, t)$ due to collision or interaction processes. The specific form taken by the collision term depends sensitively on the type of particle transport of interest. We have already provided examples of the form taken by this term for several important processes including neutron, photon, and charged particle transport, and gas and plasma dynamics. We now turn to a more detailed study of the mathematical description of collision events characterizing various transport processes.

First, note that the form of Eq. 3.1 is quite general and exact—provided, of course, that the particles under investigation can be described as distinct point particles and do not exhibit wave properties. The streaming term $\partial n / \partial t + \mathbf{v} \cdot (\partial n / \partial \mathbf{r}) + (\mathbf{F} / m) \cdot (\partial n / \partial \mathbf{v})$ can be derived easily from the microscopic equations of motion for the particles (e.g., Hamilton's equations or the Liouville equation). However one is usually forced to introduce approximations in the treatment of collision processes to arrive at an explicit form for the collision term $(\partial n / \partial t)_{\text{coll}}$ that is amenable to mathematical treatment.

To the extent that transport theory is concerned with the mathematical study of transport equations, it would be appropriate to merely assume that the detailed form of the collision term is *given* to us as a result of the considerable labor of the physicist concerned with microscopic collision processes. In this sense then, transport theory would be concerned with the mathematical study of particle transport phenomena involving multiple collision events in which the result of a single collision event is assumed to be known.¹ However as subsequent chapters reveal, the mathematical tools appropriate for the study of particle transport depend sensitively on the form taken by $(\partial n / \partial t)_{\text{coll}}$; therefore it is necessary to summarize at least the

properties of this term for various types of particle transport.

We will find it useful to distinguish between two different classes of transport process: random walk or self-diffusion processes, and collective or cooperative processes. In *random walk* or *self-diffusion* processes the particles of interest diffuse through a host or background medium, interacting randomly by way of collisions with the microscopic structure of the medium. Examples include the diffusion of neutrons through matter, in which the neutrons interact with the nuclear composition of the host material; the penetration of light through an atmosphere, which involves the interaction of photons with gas atoms or molecules; the transmission of gamma radiation through a shield; and the diffusion of a low density gas through a higher density background gas. A conceptually somewhat different (but mathematically identical) problem concerns the diffusion of a tagged or "test" particle through a medium of identical particles—for example, self-diffusion in gases or plasmas (see Figure 3.1).^{2,3}

Such random walk processes are generally described by linear collision terms; therefore they can be studied readily using the techniques of classical linear mathematical analysis. The assumption of linearity can occasionally become invalid, however. For example, if the density of the test particles becomes too high (e.g., comparable to that of the host), one must also consider interactions among the test particles, and the process becomes a collective phenomenon that must be described by a nonlinear transport equation. This situation is rarely of concern in most of the processes we characterize by linear transport equations. For example, in a nuclear reactor, the typical neutron and nuclei densities are 10^{10} and 10^{22} cm^{-3} , respectively.

A somewhat more significant source of nonlinearity arises if the diffusing particles can perturb the host material and thereby influence the probability of an interaction event. In this case the cross sections become functionals of the phase space density $n(\mathbf{r}, \mathbf{v}, t)$. One example is the temperature changes due to fission heat as neutrons diffuse through a multiplying medium. Another is the deposition of photon energy in a stellar atmosphere.

By way of contrast, in *collective phenomena* the particles of interest diffuse and interact among themselves. Examples here include molecular gas dynamics⁴ and plasma dynamics.⁵ Since the interaction rate clearly depends on the probability that two (or several) particles will find themselves within the interaction force range, it is not surprising that such collective processes usually must be described by collision terms that are nonlinear in the phase space density $n(\mathbf{r}, \mathbf{v}, t)$.

We distinguish in our mathematical studies between such self-diffusion and collective interaction processes. It is convenient to ignore the effects of

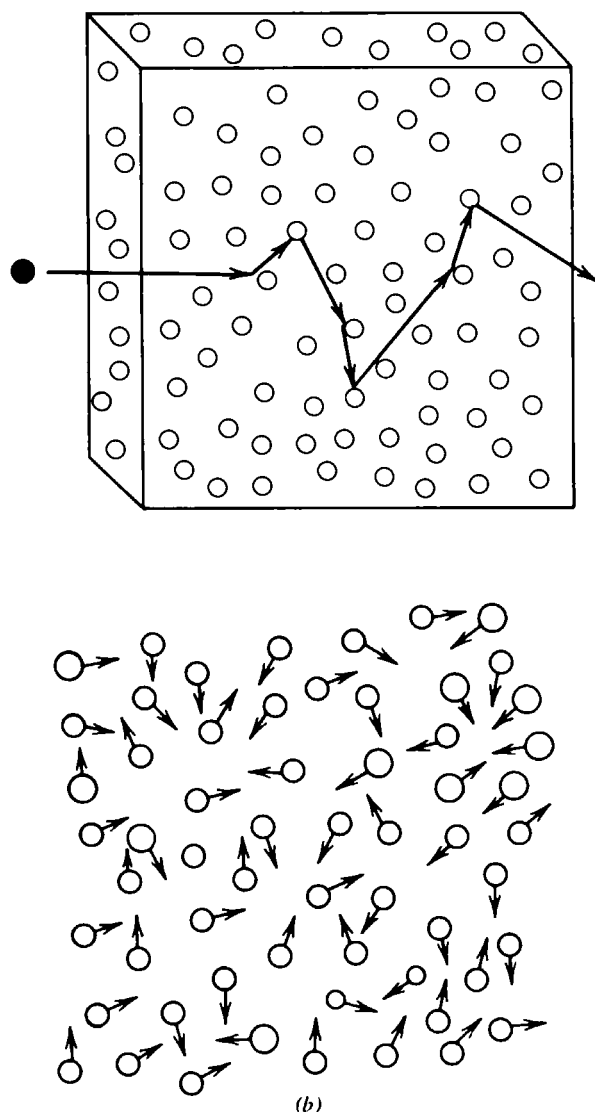


Fig. 3.1 □ Random walk (self-diffusion) processes (a) versus collective transport processes (b).

the diffusing particles on the host medium, permitting us to describe self-diffusion as a linear transport process. In general, collective processes must be described by nonlinear transport equations—although in the specific instance of small disturbances from thermodynamic equilibrium we can approximately linearize these equations.

There are other more subtle differences between self-diffusion and collective processes. Since the transport equation describing self-diffusion does not explicitly describe the effect of the test particle on the host

Table 3.1 □ Characteristics of Self-Diffusion Versus Collective Transport Processes.

	Self-Diffusion	Collective
Examples	Neutron, photon, electron transport	Gas dynamics, plasma dynamics
Mathematical character	Linear	Nonlinear
Continuum limit	Diffusion equation	Hydrodynamics equations
Continuum process	Particle diffusion	Sound propagation, heat conduction, convection plasma waves

medium (e.g., recoil effects), it will only conserve particle number in general, not the test particle momentum or energy. On the other hand, the more complete picture of collision events provided in descriptions of collective phenomena will lead to conservation of the macroscopic counterpart of any microscopic parameter that is a constant of the motion in a collision event (e.g., mass, momentum, or energy). This distinction between the conserved variables in each type of process will lead to dramatically different continuum descriptions of the particle transport. For example, the transport equation characterizing self-diffusion processes reduces in the continuum limit to the well-known diffusion equation (e.g., the neutron transport equation can be approximated by the neutron diffusion equation). Yet transport equations describing collective motions lead in the continuum limit to the equations of hydrodynamics—which are macroscopic manifestations of the conservation laws applying to an individual collision process. These distinctions between self-diffusion and collective processes are summarized in Table 3.1. This chapter sketches the derivation and presents the properties of the collision terms corresponding to both types of transport process.

3.1 □ LINEAR COLLISION OPERATORS □ We first examine linear collision operators that characterize random walk or self-diffusion processes in which the interaction mean free path or macroscopic cross section is independent of the phase space density. Transport equations characterizing such processes are sometimes referred to as equations of the *Lorentz-Boltzmann* type^{2,3} and include the neutron, electron, and photon transport equations as well as test particle equations in gas or plasma dynamics.

3.1.1 □ Neutron Transport □ We have previously developed the collision term in the neutron transport equation essentially by definition. That is, we defined the concept of macroscopic cross sections that characterize the probability of occurrence of a given type of neutron interaction. These allow us to write

$$\left(\frac{\partial n}{\partial t}\right)_{\text{coll}} = -v\Sigma_t(\mathbf{r}, \mathbf{v})n(\mathbf{r}, \mathbf{v}, t) + \int d^3v' v' \Sigma_s(\mathbf{r}, \mathbf{v}' \rightarrow \mathbf{v})n(\mathbf{r}, \mathbf{v}', t)$$

Essentially, we assume that these cross sections are given to us by the nuclear, solid, or liquid state physicist, and concern ourselves more directly with the solution of the neutron transport equation. Nevertheless it is useful to review briefly the principal ingredients of the theory of neutron cross sections to identify the general mathematical properties that are relevant to transport theory.

Of course all macroscopic cross sections can be written in terms of microscopic cross sections, which characterize individual neutron-nuclear encounters:

$$\Sigma(\mathbf{r}, \mathbf{v}) = N(\mathbf{r})\sigma(\mathbf{v})$$

(Here σ may occasionally be interpreted as a microscopic cross section that has been averaged over a distribution of nuclear speeds.) The behavior of these cross sections depends quite sensitively on the neutron kinetic energy. It is convenient to divide the neutron energy range into three different energy regions (see Figure 3.2), each of which is characterized by

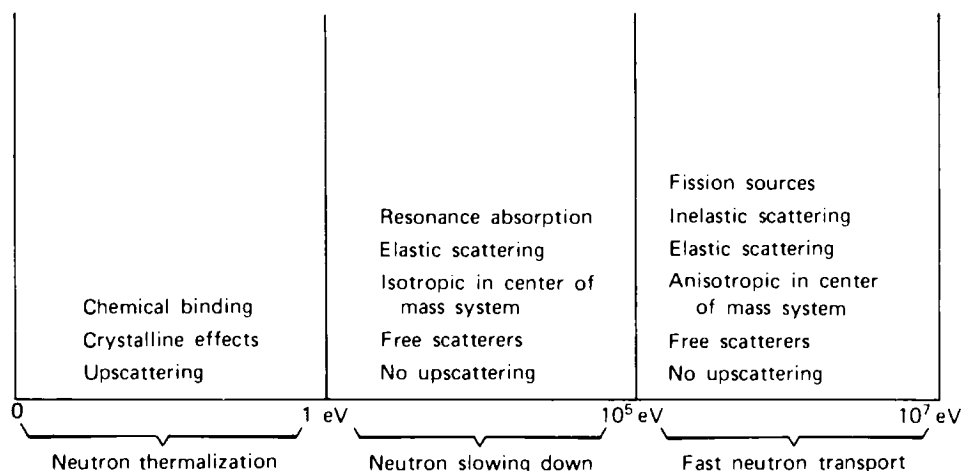


Fig. 3.2 □ The energy regions characterizing neutron transport.

a collision term with somewhat different mathematical properties. For neutron energies far in excess of the thermal energies of the nuclei in the host material, one can essentially treat the nuclei as if they were initially at rest and free to recoil (and ignore upscattering and chemical binding effects). The determination of the corresponding macroscopic cross sections becomes a simple problem in two-body kinematics if one assumes that the microscopic cross sections characterizing interactions with a single nucleus are known. Of course, the detailed interaction dynamics between a neutron and a nucleus can be quite complicated and gives rise to a variety of nuclear reactions including simple scattering (potential scattering), resonance scattering (both elastic and inelastic), radiative capture, and nuclear fission. Since the probability of a given reaction occurring will increase significantly if the incident neutron kinetic energy happens to “match” one of the energy levels of the target nucleus (or more precisely, the compound nucleus formed by absorption of the neutron), the cross sections characterizing neutron-nuclear interactions will exhibit a very complicated resonance behavior as a function of incident neutron kinetic energy.

For lower neutron energies, both nuclear motion and chemical binding effects must be included. Since these “thermal” neutron cross sections contain fast neutron cross sections as a limiting case for large neutron energies, we briefly summarize the theory and properties of thermal neutron cross sections.

Thermal Neutron Cross Sections □ To analyze the transport of low energy ($E < 1 \text{ eV}$) neutrons, we require information concerning both the scattering kernel $\Sigma_s(\mathbf{v}' \rightarrow \mathbf{v})$ and the total macroscopic cross section $\Sigma_t(\mathbf{v}) = \Sigma_a(\mathbf{v}) + \Sigma_s(\mathbf{v})$. There is a vast literature⁶⁻¹² available on the calculation and measurement of thermal neutron cross sections, since they play a central role in the interpretation of neutron spectroscopic data by allowing investigators to infer information about the microscopic structure and dynamics of matter (inelastic neutron scattering and neutron diffraction studies). Within the context of the Born approximation and the Fermi pseudopotential model, Van Hove¹² has shown that the thermal neutron scattering kernel can be written as the sum of two components

$$\Sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) = N_0 [\sigma_{\text{coh}}(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) + \sigma_{\text{inc}}(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega})]$$

where

$$\sigma_{\text{coh}}(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) = a_{\text{coh}}^2 \left(\frac{E}{E'} \right)^{1/2} (2\pi\hbar)^{-1} \int d^3r \int dt e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)} G(\mathbf{r}, t)$$

$$\sigma_{\text{inc}}(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) = a_{\text{inc}}^2 \left(\frac{E}{E'} \right)^{1/2} (2\pi\hbar)^{-1} \int d^3r \int dt e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)} G_s(\mathbf{r}, t)$$

Here a_{coh} and a_{inc} are the coherent and incoherent nuclear scattering lengths, $\kappa = (\mathbf{p}' - \mathbf{p})/\hbar$ is the neutron momentum change or transfer, and $\hbar\omega = (E' - E)$ is the neutron kinetic energy change in the collision. The time correlation functions $G(\mathbf{r}, t)$ and $G_s(\mathbf{r}, t)$ are defined by:

$$G(\mathbf{r}, t) = N_0^{-1} \sum_i \sum_j \langle \delta(\mathbf{x} - \mathbf{x}_i(0)) \delta(\mathbf{x} - \mathbf{x}_j(t)) \rangle, \quad \mathbf{r} \equiv \mathbf{x} - \mathbf{x}'$$

$$G_s(\mathbf{r}, t) = N_0^{-1} \sum_i \langle \delta(\mathbf{x} - \mathbf{x}_i(0)) \delta(\mathbf{x} - \mathbf{x}_i(t)) \rangle$$

Several comments are appropriate here. First, these expressions indicate that a thermal neutron scatters from an aggregate of nuclei, not just individual scatterers. Hence the concept of a microscopic cross section characterizing an interaction event with a single nucleus is no longer strictly relevant. Furthermore the cross section Σ_s depends on the product of two factors: nuclear force laws times motion of scattering nuclei. This separation is a consequence of the use of the Fermi pseudopotential model. The calculation of the nuclear scattering lengths a_{coh} and a_{inc} is left to the nuclear physicist. The calculation of the dynamics of the scattering nuclei is a very fascinating problem in nonequilibrium statistical mechanics.

The Van Hove time correlation functions $G(\mathbf{r}, t)$ and $G_s(\mathbf{r}, t)$ have an extremely interesting classical interpretation:

$G_s(\mathbf{r}, t) d^3r$ = probability that if a nucleus is at the origin at $t=0$, then the *same* nucleus is found at position $\mathbf{r}$ in d^3r at time t

$G(\mathbf{r}, t) d^3r$ = probability that if a nucleus is at the origin at $t=0$, then *any* nucleus is found at position $\mathbf{r}$ in d^3r at time t

This interpretation is the basis for using neutron inelastic scattering as a tool to study the microscopic dynamics of materials.

The cross section is divided into coherent and incoherent parts, which correspond to scattering of the neutron wave function from individual scattering centers with or without interference (see Figure 3.3). There is yet another subdivision of the cross section into elastic or inelastic scattering, depending on whether the neutron energy transfer is zero or nonzero. At first this nomenclature may seem to be in sharp conflict with the more customary concepts of elastic collision processes in physics as corresponding to events in which the kinetic energy of the colliding particles is conserved, not to events in which there is no energy transfer. However if

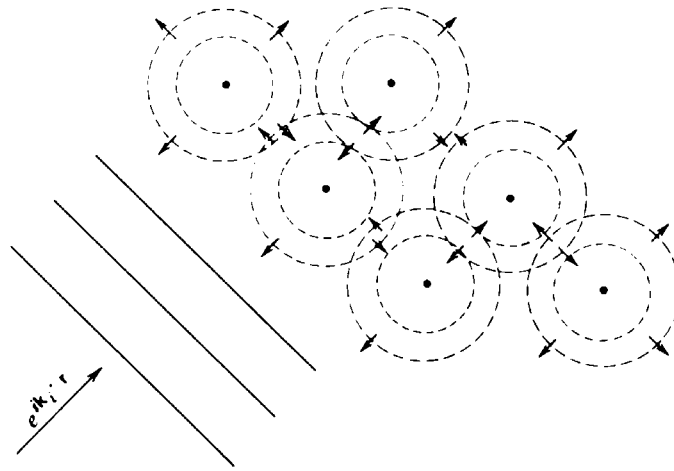


Fig. 3.3 □ Diffraction of the neutron wave function by an ordered lattice of scattering centers.

we remember that a thermal neutron scatters from the entire aggregate of nuclei whose total mass is effectively infinite in comparison to the neutron mass, we see that elastic scattering implies no neutron energy change. In summary, then, we can classify neutron scattering as follows:

- i Elastic, incoherent scattering (e.g., from a free gas).
- ii Inelastic, incoherent scattering (excites energy states of the scattering system—e.g., atom or molecule or lattice).
- iii Elastic, coherent (Bragg diffraction).
- iv Inelastic, coherent.

Each of these components of the scattering cross section is characterized by somewhat different mathematical properties.

We can catalog a variety of useful mathematical properties of thermal neutron cross sections:

- i $\Sigma_s(\mathbf{v})$ and $\Sigma_s(\mathbf{v}' \rightarrow \mathbf{v})$ are nonnegative functions of $\mathbf{v}$ (since they can be interpreted as probability distributions).
- ii For isotropic materials, the scattering cross sections are independent of the incident neutron direction and dependent only on the relative scattering angle in a scattering collision

$$\Sigma_s(\mathbf{v}) = \Sigma_s(v), \quad \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) = \Sigma_s(v' \rightarrow v, \hat{\Omega}' \cdot \hat{\Omega})$$

(This property would be violated in a crystal or in an ordered polycrystalline material.) In general we can then write the angular dependence of the

scattering kernel as an expansion in Legendre polynomials:

$$\Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) = \sum_{l=0}^{\infty} \left(\frac{2l+1}{4\pi} \right) \Sigma_l(v' \rightarrow v) P_l(\hat{\Omega}' \cdot \hat{\Omega}) \quad (3.2)$$

It is frequently a good approximation to retain only the first term in this expansion, that is, to assume isotropic scattering in the lab system, because of the randomizing effects of thermal motion and the increased effective mass of the scatterer (again, this does not hold up if diffraction effects are important). More generally, one retains several terms in the expansion (3.2).

iii The scattering kernel must obey the property of *detailed balance*:

$$vM(\mathbf{v})\Sigma_s(\mathbf{v} \rightarrow \mathbf{v}') = v'M(\mathbf{v}')\Sigma_s(-\mathbf{v}' \rightarrow -\mathbf{v})$$

This is a necessary and sufficient condition for the neutrons to eventually come into thermal equilibrium with the moderator in the absence of leakage, absorption, or sources. On a microscopic level, detailed balance is intimately connected with time reversal symmetry.^{13,14} On a macroscopic level, detailed balance plays an important role in the irreversible relaxation of the neutron gas toward thermal equilibrium.

iv At high v or v' the cross sections must approach those of a free gas, since the neutron energy is much greater than the binding energy of the atoms. They eventually assume the slowing down form in which the motions of the nuclei are neglected entirely. This will occur for energies $E \gg E_{th} \sim 0.025$ eV. Then if we note that over a considerable energy range neutron scattering from nuclei is isotropic in the center of mass system (s -wave scattering), we can calculate the large energy form of the scattering kernel as

$$\begin{aligned} \Sigma_s(E' \rightarrow E, \mu_0) &= \frac{\Sigma_s(E')}{2\pi(1-\alpha)E'} \delta(\mu_0 - \mu_s), \quad E \leq E' \leq \frac{E}{\alpha} \\ &= 0, \quad \text{otherwise} \end{aligned}$$

where

$$\mu_s \equiv \frac{1}{2} \left[(A+1) \left(\frac{E}{E'} \right)^{1/2} - (A-1) \left(\frac{E'}{E} \right)^{1/2} \right], \quad \mu_0 \equiv \hat{\Omega}' \cdot \hat{\Omega}$$

v For incoherent scattering, we find smooth, monotonically decreasing total cross sections that approach the free atom cross section Σ_{fr} for large v . In contrast, the cross sections characterizing coherent scattering behave

very irregularly and exhibit peaks corresponding to Bragg diffraction effects (see Figure 3.4). In both cases, however, the cross sections assume the limiting forms

$$\Sigma_i(v) \sim \Sigma_{ir} = \text{constant} \quad \text{for large } v \gg \left(\frac{kT}{m}\right)^{1/2}$$

$$\Sigma_i(v) \sim \frac{\Sigma_i^0}{v} \quad \text{for small } v \rightarrow 0$$

vi For incoherent inelastic scattering, the scattering kernel $\Sigma_s(\mathbf{v}' \rightarrow \mathbf{v})$ is smooth and well-behaved (actually, we later indicate that the kernel is usually square integrable). For coherent or elastic scattering the kernel becomes quite singular as a consequence of diffraction effects.

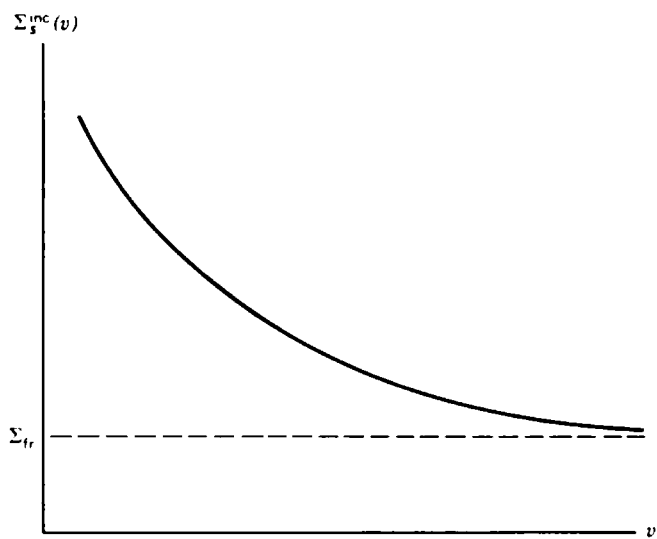
vii A characteristic feature of neutron transport in fissile materials is the presence of nuclear fission reactions that produce additional neutrons. If $\Sigma_f(v)$ is the macroscopic cross section characterizing fission events, $\nu(v)$ is the average number of neutrons emitted per fission event, and $\chi(v)$ is the probability distribution characterizing fission neutron energies (assumed to be emitted isotropically), we can identify the fission source term in the transport equation as

$$s_f(\mathbf{r}, \mathbf{v}, t) \equiv \frac{\chi(v)}{4\pi} \int d^3v' \nu(v') v' \Sigma_f(v') n(\mathbf{r}, \mathbf{v}', t)$$

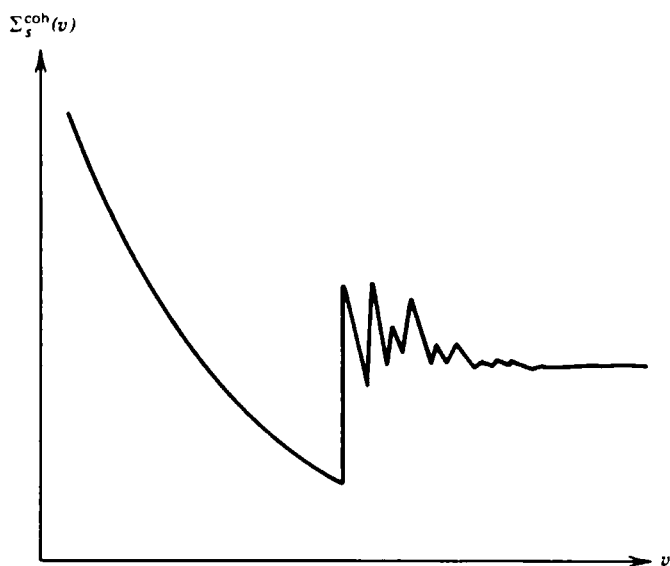
Actually, this term corresponds only to the “prompt” fission neutrons that appear instantaneously with the fission event. There are also neutrons that appear after an appreciable time delay as the decay products of radioactive fission fragments. Appropriate source terms for these delayed neutrons can be written in terms of the nuclei precursor concentrations $C_i(\mathbf{r}, t)$ and their respective radioactive decay constants λ_i as

$$s_f^{\text{delayed}}(\mathbf{r}, \mathbf{v}, t) = \sum_i \frac{\chi_i(v)}{4\pi} \lambda_i C_i(\mathbf{r}, t)$$

The key ingredient in all studies of neutron transport is a knowledge of the various relevant neutron-nuclear cross sections. The complicated dependence of such cross sections on neutron energy and angle of incidence, combined with the large number of isotopes involved in nuclear systems analysis, implies that neutron cross section data can become quite massive.¹⁵ Such data have been accumulated over the past few decades by both experimental measurements and theoretical calculations. Indeed, these



(a)



(b)

Fig. 3.4 □ Neutron scattering cross section behavior for incoherent (a) and coherent (b) scattering.

data have become so voluminous that they are now most conveniently stored on magnetic tapes and manipulated by computer.

To standardize the format and treatment of neutron cross section data, the Evaluated Nuclear Data File (ENDF)¹⁶ was established to consolidate, organize, and present these data in a form convenient for nuclear applications. The ENDF system contains both neutron and photon cross section data, along with data processing computer programs that can manipulate them into the most convenient form for the user. Of most interest is the ENDF/B data set, which contains complete, evaluated sets of nuclear data for approximately 80 isotopes for all significant neutron-induced reactions in the energy range 10^{-5} eV to 20 MeV. In particular, this file provides cross section data for the reactions (n, γ) , $(n, \text{fission})$, (n, p) , (n, α) , (n, n) , (n, n') , $(n, 2p)$, and $(n, 2n)$, as well as for the differential scattering cross sections. ENDF/B is regarded as the standard source of nuclear data for use in nuclear systems analysis in the United States (there are comparable data sets in Europe and in the Soviet Union). The ENDF/B data set is continually being reevaluated and updated as new cross section measurements become available. Revised versions of the data set are issued at one or two year intervals.

Modeled Neutron Cross Sections □ In general, neutron cross sections are rather complicated functions of velocity. Hence it is customary to make one of several standard approximations or models to allow analytical investigations of thermal neutron transport:

i *Isotropic scattering in the lab system:*

$$\Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) = (4\pi)^{-1} \Sigma_s(v' \rightarrow v)$$

ii *Separable or synthetic kernels (also called “amnesia” kernels):*¹⁷

$$\Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) = \left(\frac{\beta}{4\pi} \right) \Sigma_s(v') v M(v) \Sigma_s(v), \quad \beta^{-1} \equiv \int_0^\infty dv v M(v) \Sigma_s(v)$$

This particularly simple model of the scattering kernel satisfies detailed balance and gives the correct total cross section. It represents an “instant thermalization” process in which one collision is sufficient to throw a neutron into thermal equilibrium with the moderator. Synthetic kernels are frequently used as the first level of attack on a given problem in thermal neutron transport, since they usually allow an exact analytical solution.

iii *Modified synthetic kernel:*¹⁸

$$\Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) = \left(\frac{\beta}{4\pi} \right) \Sigma_{in}(v') v M(v) \Sigma_{in}(v) + \left(\frac{1}{4\pi} \right) \Sigma_e(v) \delta(v - v')$$

The $\delta(v' - v)$ term in this model mocks the elastic scattering contribution so that the kernel is useful for the study of transport in polycrystalline materials.

iv *N-term degenerate kernels*:^{19,20}

$$\Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) = vM(v) \sum_{i=1}^N \sum_{j=1}^N a_{ij} g_i(\mathbf{v}) f_j(\mathbf{v}')$$

Various prescriptions can be used to determine the functions $g_i(\mathbf{v})$ and $f_j(\mathbf{v}')$ in this model (e.g., variational or least squares methods), and by allowing N to become large, this model can describe the true scattering kernel to a high degree of accuracy (see Section 7.3.5).

v *Continuous slowing down models*. To describe collision events experienced by neutrons with speeds considerably in excess of those characterizing the thermal motion of the host nuclei, it is common to ignore “up-scattering” events and assume that the interaction rate $\Sigma_s(E)\phi(E)$ is a slowly varying function of energy so that a low order Taylor series expansion

$$\Sigma_s(E')\phi(E') \sim \Sigma_s(E)\phi(E) + (E - E') \frac{\partial}{\partial E} [\Sigma_s(E)\phi(E)] + \dots$$

can be introduced into the collision integral to write

$$\begin{aligned} \int_0^\infty dE' \Sigma_s(E' \rightarrow E)\phi(E') &\sim \Sigma_s(E)\phi(E) \\ &+ \frac{\partial}{\partial E} \left[\left(\int_0^\infty dE' f(E' \rightarrow E)(E' - E) \right) \Sigma_s(E)\phi(E) \right] \end{aligned}$$

Then the collision term $(\partial n / \partial t)_{\text{coll}}$ takes the form of a differential operator

$$\left(\frac{\partial n}{\partial t} \right)_{\text{coll}} \cong -\Sigma_a(E)\phi(E) + \frac{\partial}{\partial E} [\xi(E)\Sigma_s(E)\phi(E)]$$

Such continuous slowing down models (so-called because truncating the Taylor series expansion is tantamount to assuming only an infinitesimal energy loss in each collision) have played an important role in both the understanding of neutron slowing down (Fermi age theory)²¹ as well as in forming a basis for practical computational tools.^{22,23}

Problems Encountered in Neutron Transport Theory □ The problems arising in neutron transport theory can be grouped into three classes:

- i Determination of the neutron distribution established by a steady-state source in a subcritical medium.
- ii Determination of the geometric size or composition of a multiplying medium that will yield a stable fission chain reaction (i.e., the criticality problem).
- iii Various types of time-dependent problem.

Neutron transport problems are somewhat unique because of the enormous range of neutron kinetic energies (some 10^8 kT) that appear in fission chain reacting systems. Since most neutron diffusion problems involve energetic fission neutrons slowing down into thermal equilibrium with the host material, there arises a nonsymmetric mathematical structure quite different from that encountered in many other areas of transport theory. Since neutrons can easily penetrate materials and cannot be held in by surfaces, the boundary conditions characterizing neutron transport problems are usually very simple, and standard techniques from applied mathematics (e.g., integral transforms or separation of variables) can be utilized to solve the neutron transport equation in many cases.

The subject of neutron transport theory has also benefited from its central role in the development of atomic energy. This attracted at an early stage the interest of eminent physicists such as Fermi, Wick, Peierls, Placzek, Wigner, Bethe, Marshak, and many others. This level of intense activity has continued to be stimulated by the demands of the nuclear power industry, and over the past decade some 1200 papers have been published on the subject of neutron transport theory.²⁴

3.1.2 □ The Transport of Charged Particles □

The Transport of High Energy Electrons □ We might expect that the transport of any high energy particle through matter could be described by a transport equation of the form

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \nabla n + v \Sigma_i n = \int d^3v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) n(\mathbf{r}, \mathbf{v}', t) + s \quad (3.3)$$

where $n(\mathbf{r}, \mathbf{v}, t)$ is the phase space density for the particle of interest, and Σ_i is the interaction cross section. Of course, implicit in this equation are the assumptions of essentially random scattering centers and the neglect of quantum effects such as coherent scattering. (Even these effects can be included, provided we calculate the cross sections properly. We can evidence the inclusion of coherent scattering in neutron transport.)

We would now like to apply this equation to the study of the transport of high energy electrons. Several comments concerning this transport

process are necessary. First, the electrons can experience a variety of interactions including elastic scattering by atomic nuclei, inelastic scattering by atomic electrons, the production of secondary electrons, and bremsstrahlung. Because of the high energy of the electrons, we can essentially neglect upscattering. This makes electron transport very similar to the neutron slowing down process (see Figure 3.5).

Perhaps the primary difference from neutron transport is due to the inelastic scattering from atomic electrons. The charged particle suffers large numbers of such encounters because of the long range of the Coulomb interaction. This results in an effectively continuous interaction with the scattering material. Each of these collisions results in only a very small deflection and energy change because of the small mass of the atomic electrons. Whereas only several neutron-nucleus collisions were sufficient to reduce the neutron energy to a fraction of its original value, a similar reduction in charged particle energy would typically require about 10^4 interactions.

In addition to these frequent small angle deflections, there also occur infrequent catastrophic encounters with nuclei in which the electron suffers a large deflection in angle. This latter collision mechanism is more reminiscent of neutron-nuclei interactions.

The presence of the small angle Coulomb scattering is the principal complication arising in fast charged particle transport, and it is one of the reasons that most studies of such phenomena go directly to computer calculations (e.g., using Monte Carlo²⁵ or moments methods²⁶). A variety of analytical methods have been used to simplify the treatment of small angle scattering within such computer studies.²⁵⁻²⁸

To illustrate, let us rewrite Eq. 3.3 in such a way as to separate the contributions from weak interactions (primarily inelastic) with atomic

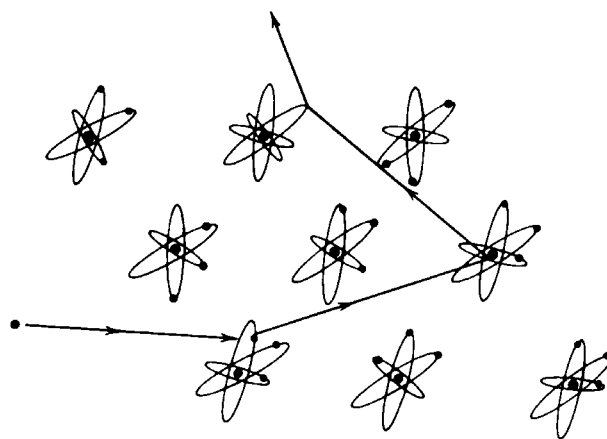


Fig. 3.5 □ Electron scattering from atomic electrons and nuclei.

electrons that are frequent, but cause small angle deflection from infrequent strong interactions (primarily elastic) with nuclei, which are characterized by large angle scattering and little energy loss. To decouple the angular scattering from the energy loss interactions, we first treat large angle scattering as a monoenergetic process

$$\int d^3v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) n(\mathbf{r}, \mathbf{v}', t) - v \Sigma_s(v) n(\mathbf{r}, \mathbf{v}, t) \\ \rightarrow \int d\hat{\Omega}' v \Sigma_s(\hat{\Omega}' \cdot \hat{\Omega}) [n(\mathbf{r}, \hat{\Omega}', t) - n(\mathbf{r}, \hat{\Omega}, t)]$$

and then use continuous slowing down theory to describe the electron energy loss. That is, we assume the differential energy loss per path length s is given by the Bethe formula²⁵

$$\frac{dE}{ds} = - \frac{2\pi\rho N r_0^2 m c^2}{(v/c)^2} \frac{Z}{A} \ln \left[\frac{E^2(E + 2mc^2)}{2mc^2 \bar{E}^2} \right]$$

Now if we note

$$\frac{1}{v} \frac{\partial}{\partial t} = \frac{\partial}{\partial s}$$

we can eliminate t in terms of the path length s (hence the energy E). If we normalize s to the electron range R_E by defining $t = s/R_E$, we can rewrite the electron transport equation as

$$\frac{\partial \varphi}{\partial t} + \hat{\Omega} \cdot \frac{\partial \varphi}{\partial \mathbf{r}} = \int d\hat{\Omega}' \Sigma_s(\hat{\Omega}' \cdot \hat{\Omega}) [\varphi(\mathbf{r}, \hat{\Omega}', t) - \varphi(\mathbf{r}, \hat{\Omega}, t)] + s \quad (3.4)$$

A variety of techniques have been applied to solve this equation. For example, it is possible to go one step further and model the scattering as an “angular dispersion” process (after Bethe²⁹)

$$\mu \frac{\partial \varphi}{\partial x} = \alpha \frac{\partial}{\partial \mu} \left[(1 - \mu^2) \frac{\partial \varphi}{\partial \mu} \right]$$

An alternative method is to attack Eq. 3.4 directly by seeking a relation among the spatial moments of the angular flux (Spencer²⁶). Most frequently in modern calculations, it is customary to use Monte Carlo methods that include an approximate treatment of the small angle scattering events.²⁸

Electron Conduction in Solids □ The motion of electrons in the conduction band of a solid is yet another problem that can be described by

transport theory.³⁰ Of course the actual electrons must be described by quantum mechanics. Provided the external field applied to the solid is sufficiently weak, however, the motion of the electrons can be represented by that of a fictitious classical particle with momentum $\hbar k$ (the “effective mass theorem”). That is, we describe a collection of such particles by a distribution function

$$f(\mathbf{r}, \mathbf{k}, t) d^3r d^3k = \text{average occupancy of an electron state in } d^3k \text{ about } \mathbf{k}, d^3r \text{ about } \mathbf{r}, \text{ at time } t$$

Since the electrons are Fermi particles, a state can hold either zero or one electron. Hence we use the concept of the average occupancy of a state rather than the more customary concept of particle density.

The equation describing the time evolution of $f(\mathbf{r}, \mathbf{k}, t)$ is now the classical transport equation

$$\frac{\partial f}{\partial t} + \dot{\mathbf{r}} \cdot \frac{\partial f}{\partial \mathbf{r}} + \dot{\mathbf{k}} \cdot \frac{\partial f}{\partial \mathbf{k}} = \left(\frac{\partial f}{\partial t} \right)_{\text{coll}}$$

where

$$\dot{\mathbf{r}} \equiv \frac{1}{\hbar} \frac{\partial}{\partial \mathbf{k}} E(k), \quad \hbar \dot{\mathbf{k}} \equiv q(\mathbf{E} + \dot{\mathbf{r}} \times \mathbf{B})$$

Here, $(\partial f / \partial t)_{\text{coll}}$ is the change in $f(\mathbf{r}, \mathbf{k}, t)$ due to the scattering of an electron of $\mathbf{k}'$ into $\mathbf{k}$ caused by interaction with an irregularity in the crystal lattice. The probability for such a transition can be calculated from quantum mechanics. There are several sources of such interactions: scattering by lattice vibrations (energy change), impurity scattering (no energy change), electron-electron scattering, and other mechanisms attributable to vacancies, grain boundaries, or dislocations. If we characterize the scattering by a conditional probability $W(\mathbf{k}', \mathbf{k})$ that gives the probability for scattering from $\mathbf{k}'$ to $\mathbf{k}$, the corresponding scattering rate is

$$\begin{array}{c} \text{(probability state } \mathbf{k}' \\ \text{contains electron)} \end{array} \times W(\mathbf{k}', \mathbf{k}) \times \begin{array}{c} \text{(probability state } \mathbf{k} \\ \text{contains no electron)} \end{array}$$

Hence we find

$$\left(\frac{\partial f}{\partial t} \right)_{\text{coll}} = \int_{\text{BZ}} d^3k' \{ f(\mathbf{k}') W(\mathbf{k}, \mathbf{k}') [1 - f(\mathbf{k})] - f(\mathbf{k}) W(\mathbf{k}, \mathbf{k}') [1 - f(\mathbf{k}')] \}$$

where BZ means that we are to integrate over a Brillouin zone in $\mathbf{k}$ -space. Notice here that the equilibrium distribution is not the Maxwellian $M(\mathbf{v})$

but rather the Fermi-Dirac distribution

$$f_0(\mathbf{k}) = \left[\exp\left(\frac{E_k}{k_B T}\right) + 1 \right]^{-1}$$

This equation can be solved using many of the same ideas that prove to be useful for neutron transport or gas dynamics. Since the transport equation is nonlinear, the first step is linearization. Then various standard approximations can be introduced to allow an analytical study of the transport equation.

3.1.3 □ Photon Transport □ The subject of photon transport can be conveniently separated into two distinct topics: the transfer of thermal energy by low energy photons (“radiative transfer”), and the transport of high energy photons through matter (e.g., gamma or hard X-ray transport). The second process is usually analyzed under the assumption that the photon fluxes are so low that their energy deposition in matter does not significantly perturb the background medium. Therefore this transport process is quite similar to such other linear transport phenomena as neutron or charged particle transport and can be analyzed accordingly.

In sharp contrast, radiative transfer processes usually involve the transport of significant quantities of energy by relatively low energy photons (e.g., in the visible, UV, or soft X-ray spectrum) of atomic origin, and this radiant energy transport can significantly affect the background medium by changing its temperature or optical properties. The theory of radiative transfer is also similar, in certain cases, to that of neutron transport and therefore is susceptible to many of the mathematical methods we discussed in Chapter 2. In fact, we have already noted that several of these techniques actually originated in the theory of radiative transfer (e.g., the Wiener-Hopf method).³¹

Radiative Transfer □ Although the transport equation characterizing radiative transfer is quite similar in form to that describing neutron transport, there are some rather significant differences between the physics of these two processes.

- i The optical properties (i.e., the cross sections) of a medium depend strongly on the radiation field itself. Hence we usually have to contend with a highly nonlinear transport problem.
- ii The macroscopic cross sections characterizing photon interactions are continuous functions of position because of variations in the material

- density. (Neutron cross sections are usually constant, at least piecewise, in position.)
- iii The photon mean free path varies strongly with wavelength over the entire frequency spectrum (line absorption). (This is analogous to the resonance behavior in neutron cross sections.)
 - iv In radiative transfer we are frequently interested in the inverse problem, that of determining the source and material from the measured radiation field. (In neutron transport calculations we only encounter the direct problem of determining the neutron distribution given the source and material.)

In a broad sense radiative transfer encompasses all phenomena involving the propagation of electromagnetic radiation and its interaction with matter—at least to the extent that such phenomena can be described by a transport equation. Hence the applications are quite varied. For example, radiative transfer problems arise in astrophysics, meteorology, photometry, high speed gas dynamics (radiation hydrodynamics), the use of optical measurements to study materials (e.g., plasmas), and many other areas.

The Radiation Field □ In analyzing photon transport we emphasize the particle aspect of electromagnetic radiation by considering the radiation field to be composed of a “photon gas”.^{32–38} Rather than use the photon phase space density $n(\mathbf{r}, \mathbf{v}, t)$, it is customary in radiative transfer to define the *radiation specific intensity*

$$I_\nu(\mathbf{r}, \hat{\Omega}, t) \equiv h\nu c n(\mathbf{r}, \hat{\Omega}, \nu, t)$$

where the frequency ν has replaced energy $E = h\nu$ as an independent variable. If we recall that photons always move with a speed c (if we can ignore refraction effects) and are characterized by an energy $E = h\nu$, we can see that

$$I_\nu(\mathbf{r}, \hat{\Omega}, t) = \frac{\text{energy}}{\text{photon}} \times \text{photon speed} \times \text{angular density}$$

and therefore can interpret $I_\nu(\mathbf{r}, \hat{\Omega}, t)$ as the “energy angular flux.” Of related interest is the angle-integrated or *average intensity* $J_\nu(\mathbf{r}, t)$

$$J_\nu(\mathbf{r}, t) \equiv \left(\frac{1}{4\pi} \right) \int d\hat{\Omega} I_\nu(\mathbf{r}, \hat{\Omega}, t) \quad (3.5)$$

We also define the *radiant energy density* at frequency ν by

$$u_\nu(\mathbf{r}, t) \equiv \left(\frac{1}{c} \right) \int d\hat{\Omega} I_\nu(\mathbf{r}, \hat{\Omega}, t) \quad (3.6)$$

and the *total radiant energy density* is given by

$$u(\mathbf{r}, t) \equiv \left(\frac{1}{c} \right) \int_0^\infty d\nu \int d\hat{\Omega} I_\nu(\mathbf{r}, \hat{\Omega}, t) \quad (3.7)$$

The *radiant heat flux vector* is defined by

$$\mathbf{q}(\mathbf{r}, t) \equiv \int_0^\infty d\nu \int d\hat{\Omega} \hat{\Omega} I_\nu(\mathbf{r}, \hat{\Omega}, t) \quad (3.8)$$

and corresponds in neutron transport to what we would call the current density $\mathbf{J}(\mathbf{r}, t)$, except that it now describes energy flow rather than particle flow. Finally, we can define the *radiation pressure tensor*

$$\mathbf{P}(\mathbf{r}, t) \equiv \left(\frac{1}{c} \right) \int_0^\infty d\nu \int d\hat{\Omega} \hat{\Omega} \hat{\Omega} I_\nu(\mathbf{r}, \hat{\Omega}, t) \quad (3.9)$$

As an example, note that when the radiation field is isotropic,

$$P_{ij} = \left(\frac{4\pi}{3c} \right) \delta_{ij} \int_0^\infty d\nu I_\nu = \left(\frac{1}{3} \right) u \delta_{ij}$$

The Equation of Radiative Transfer □ Using the foregoing concepts, we can derive an equation of radiative transfer in a manner very similar to that used for neutron transport, by equating

$$\begin{aligned} \frac{1}{c} \frac{\partial I_\nu}{\partial t} + \hat{\Omega} \cdot \nabla I_\nu &= \text{change in } I_\nu \text{ due to sources and sinks} \\ &= j_\nu(\mathbf{r}, \hat{\Omega}, t) - k_\nu(\mathbf{r}, t) I_\nu(\mathbf{r}, \hat{\Omega}, t) \end{aligned}$$

where we have denoted the photon emission and absorption terms by j_ν and $k_\nu I_\nu$ (and explicitly noted that the absorption rate will be linearly proportional to the radiative intensity I_ν). These terms are more commonly expressed in terms of the photon *mass emission coefficient* ϵ_ν defined by

$$j_\nu \equiv \rho \epsilon_\nu = \text{rate of radiant energy emitted per unit phase space volume}$$

and *mass attenuation coefficient* κ_ν

$$k_\nu I_\nu \equiv \rho \kappa_\nu I_\nu = \text{rate of radiant energy absorption per unit phase space volume}$$

where $\rho = \rho(\mathbf{r}, t)$ is the mass density of the host material. Photon scattering processes are customarily included in the definitions of ϵ_ν and κ_ν (since a

scattering event corresponds to the absorption followed by the reemission of a photon).

The equation of radiative transfer can be written then as

$$\frac{1}{c} \frac{\partial I_\nu}{\partial t} + \hat{\Omega} \cdot \nabla I_\nu = \rho(\mathbf{r}, t) [-\kappa_\nu(\mathbf{r}, t) I_\nu(\mathbf{r}, \hat{\Omega}, t) + \epsilon_\nu(\mathbf{r}, t)] \quad (3.10)$$

In writing this equation, we have also neglected polarization and dispersion (dependence of the refractive index on ν) and collective effects (correlations), and we have assumed an isotropic medium, permitting us to regard photon interactions as independent, successive isolated events. Coherent phenomena such as reflection of light are also omitted from this description.

Radiative Processes □ If we note that $\rho\kappa_\nu/N$ has the units of area, we can identify this quantity as just the microscopic cross section for photon absorption. To calculate the absorption and emission coefficients κ_ν and ϵ_ν , we must consider the possible interaction mechanisms for a low energy photon propagating through a material.³⁹ Such processes are associated with transitions between the energy levels of the atoms or molecules comprising the host medium. The change in the internal energy will be equal to the radiant energy absorbed or emitted. A variety of different processes may be involved, as noted in Table 3.2. All these mechanisms contribute to the absorption coefficient κ_ν . The emission coefficient represents the effective photon source term. Every capture process that appears in κ_ν has an inverse that contributes to ϵ_ν . These inverse processes may be

Table 3.2 □ Radiative Processes in Photon Transport

Elastic scattering
Rayleigh scattering by atoms and molecules
Thomson scattering by free electrons
Inelastic scattering
Compton scattering from electrons accompanied by photon frequency change
Raman scattering by atoms and molecules, with the photon energy loss going into internal degrees of freedom
Capture (and emission)
Line absorption (bound-bound)
Photoionization (bound-free)
Inverse bremsstrahlung (free-free)
Photodissociation of molecules

stimulated by a preceding absorption, or they may occur spontaneously. In an isotropic medium, the stimulated emission propagates in the same direction (in phase) as the incident radiation; therefore it is customary to subtract out this component by defining

$$\kappa'_\nu = \text{capture} - \text{stimulated emission} + \text{scattering}$$

$$\epsilon'_\nu = \text{spontaneous emission} + \text{scattering}$$

To be more specific, let us briefly consider the photon interaction processes of most concern in radiative transfer: photoexcitation and photoionization (and their inverses).

i *Photoexcitation and radiative transitions (bound-bound)*. The three types of photon interaction involving an atomic transition between states E_i and E_j are indicated schematically in Figure 3.6, along with their corresponding reaction rates. Here we have introduced the Einstein coefficients characterizing transitions between states E_i and E_j . We recall that these coefficients are related by

$$A_{ij} = \frac{2h\nu_{ij}^3 B_{ij}}{c^2}$$

Since photons appearing in stimulated emission are “in phase” with the incident photon, it is customary to combine the absorption and stimulated emission terms to write an effective absorption coefficient as

$$\kappa'_\nu \equiv \frac{(N_i - N_j) B_{ij}}{\rho}$$

Notice here that if $N_j > N_i$ —that is, if we have a state “population inversion”—then κ'_ν will be negative corresponding to an exponential growth in intensity—that is, a laser.

ii *Photoionization and radiative recombination (bound-free)*. Of similar importance are bound-free processes in which a photon ionizes an atom (or is emitted in an ion-electron recombination event)

$$h\nu + N_Z \rightarrow N_{Z+1} + e \quad (\text{rate} = N_Z \beta I_\nu)$$

$$e + N_{Z+1} \rightarrow N_Z + h\nu \quad (\text{rate} = N_{Z+1} n_e \alpha)$$

iii *Photon scattering*. There are also interactions in which a photon is scattered by an atom. The most common scattering event involves elastic or coherent scattering in which the incident photon energy is unchanged (therefore is a “one-speed process”). Scattering may be a very important

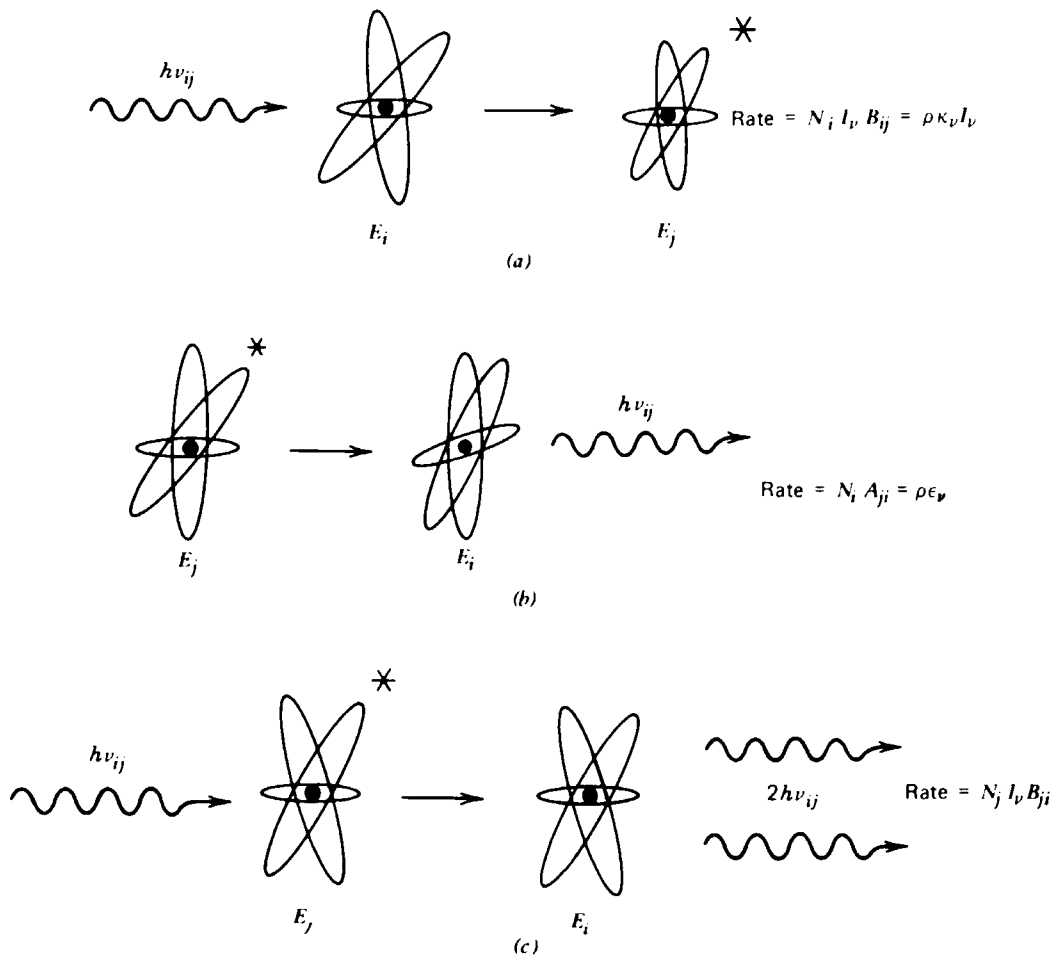


Fig. 3.6 □ Photon interactions with a two-state atom. (a) Absorption. (b) Spontaneous emission. (c) Stimulated emission.

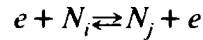
process in dilute media such as planetary atmospheres in which atomic collision processes are relatively infrequent. It also appears in a somewhat different guise in line self-absorption or radiation trapping in optically thick media in which a photon may be emitted, absorbed, reemitted, and so on, many times before leaving the medium or being destroyed in a nonradiative event.

The determination of photon interaction rates depends directly on the state populations of the various atomic energy levels. Hence any consideration of photon transport must involve the rate equations for these population densities, which take the form

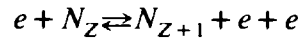
$$\frac{\partial N_i}{\partial t} + \nabla \cdot (N_i \mathbf{u}) = \sum_{j=1}^n W_{ij} N_j, \quad i = 1, \dots, n$$

Of course, the rate coefficients W_{ij} in these equations involve a variety of processes in addition to photon interactions. Of most importance are electron impact processes:

iv *Excitation and de-excitation by free electrons:*



v *Electron impact ionization and three-body ionization:*



Needless to say, the subject of photon interactions in radiative transfer processes can become very complicated indeed. Fortunately, in many cases one can considerably simplify this analysis by assuming that the medium is in thermodynamic equilibrium (or at least partial equilibrium).

Equilibrium Models □ Although the general nonlinear form of the equation of radiative transport presents a formidable computational challenge in most applications,³⁵ one solution can be obtained rather easily—that characterizing the equilibrium between the radiation field and its surroundings:

$$I_\nu^0 = \frac{2h\nu^3/c^2}{\exp(h\nu/kT) - 1} \equiv B_\nu(T)$$

Here $B_\nu(T)$ is known as the *Planck distribution function*. If we insert this form for the specific intensity into our definitions Eqs. 3.5 to 3.9, we find the equilibrium or “black body” values

$$u_\nu^0 = \left(\frac{4\pi}{c} \right) B_\nu(T)$$

$$u^0 = \left(\frac{4}{c} \right) \sigma T^4$$

$$q_i^0 = 0$$

$$P_{ij} = \left(\frac{4}{3c} \right) \sigma T^4 \delta_{ij}$$

where $\sigma = 2\pi^5 k^4 / 15h^3 c^2$ is known as the Stefan-Boltzmann constant.

A far less restrictive model assumes that the material (but *not* the radiation field) is in *local thermodynamic equilibrium* (LTE), which is maintained by electron collisions. That is, the radiation field is assumed to

be sufficiently dilute that electron excitation and ionization exceed photon-induced processes to yield an equilibrium condition in which the state populations are related by the Boltzmann factor

$$\frac{N_j}{N_i} \rightarrow \frac{g_j}{g_i} \exp\left(\frac{-h\nu_{ij}}{kT}\right)$$

Then the photon emission processes are essentially independent of the radiation field and are given by

$$S_\nu \equiv \frac{\epsilon'_\nu}{\kappa'_\nu} = B_\nu(T) \quad (3.11)$$

in which it is noted that the Planck function $B_\nu(T)$ depends *only* on the local temperature of the material. Equation 3.11 is known as *Kirchhoff's law*.

The assumption of LTE results in an enormous simplification, and it is customarily made in radiative transfer problems. It is not necessarily a good assumption (it certainly does not hold in stellar atmospheres in which the particle density is quite low). However the equations describing radiative transfer are so horrible without this assumption, that LTE is assumed simply for mathematical convenience in many cases.

A somewhat different model takes the opposite extreme by assuming that both the free electron density and the radiation field are dilute enough to permit excited atoms to emit spontaneously and ionized atoms to recombine by photorecombination. In this *corona equilibrium* model there is no collisional excitation or de-excitation; therefore to achieve equilibrium, the electron impact ionization and photorecombination processes are balanced.

In many instances these quasi-equilibrium models are inadequate and one is forced to a fully non-LTE calculation in which coupled rate equations for state population densities must be solved simultaneously with the equation of radiative transfer (and perhaps also with the hydrodynamics equations characterizing the motion of the host medium). For example, in many problems of plasma dynamics, energy is added to the plasma at a rate sufficient to produce a non-LTE state (e.g., laser heating of plasmas). Needless to say, the complexities of such calculations quickly oblige one to resort to brute force numerical solutions of the equations of non-LTE "radiation hydrodynamics."

To include elastic scattering processes, we can define $\gamma_\nu \equiv \sigma_a/\sigma_t$ so that the photon source function becomes

$$S_\nu \rightarrow \gamma_\nu B_\nu + (1 - \gamma_\nu) \int \frac{d\hat{\Omega}}{4\pi} I_\nu(\mathbf{r}, \hat{\Omega}, t)$$

Customarily, the LTE model used in astrophysics assumes that $\gamma_\nu = 1$. That is, if the density is high enough for LTE to be valid, scattering processes usually can be ignored. In the study of photon transport in atmospheres, one frequently assumes the low density limit in which $\gamma_\nu = 0$, and only scattering interactions are considered.

Some Representative Problems in Radiative Transfer □ The classical model of a stellar atmosphere in radiative equilibrium is based on the LTE assumption. The problem of determining the emergent intensity I_ν from the surface of a star is just the Milne problem. To simplify this calculation, one frequently makes the rather drastic assumption that κ'_ν and γ_ν are constant or that they can be replaced by appropriate averages over frequency ν . Then Eq. 3.10 becomes linear and frequency independent

$$\hat{\Omega} \cdot \nabla I + \kappa' I(\mathbf{r}, \hat{\Omega}) = (1 - \gamma) \kappa' \int d\hat{\Omega}' f(\hat{\Omega}' \rightarrow \hat{\Omega}) I(\mathbf{r}, \hat{\Omega}')$$

where $I \equiv \int_0^\infty d\nu I_\nu$. This model is known as the *grey approximation* and corresponds to the one-speed approximation in neutron transport theory. The model can be simplified even further by using the equilibrium condition

$$\int_0^\infty d\nu \kappa'_\nu J_\nu = \int_0^\infty d\nu \kappa'_\nu B_\nu$$

to relate temperature to the average intensity J . Then if κ_ν is not dependent on frequency ν , we can integrate to find

$$\left(\frac{\sigma}{\pi}\right) T^4 = \int_0^\infty d\nu B_\nu(T)$$

which implies that in radiative equilibrium

$$J = \sigma T^4$$

Thus we find that T^4 obeys the one-speed transport equation of the form

$$T^4(z) = \frac{1}{2} \int_0^\infty dz' E_1(\kappa|z - z'|) T^4(z')$$

A slightly more general model is the so-called uniform picket fence model in which one divides up the frequency range and assumes that κ'_ν

and γ_ν are independent of ν in each range to arrive at

$$\hat{\Omega} \cdot \nabla I_i + \kappa_i I_i = \left[2 \sum_{j=1}^N \kappa_j \nu_j \right]^{-1} \kappa_i \nu_i \sum_{j=1}^N \kappa_j \int d\hat{\Omega}' I_j(\mathbf{r}, \hat{\Omega}')$$

where

$$I_i(\mathbf{r}, \hat{\Omega}) = \int_{\Delta\nu_i} d\nu I_\nu(\mathbf{r}, \hat{\Omega}), \quad \nu_i \equiv \left(\frac{\pi}{\sigma T^4} \right) \int_{\Delta\nu_i} d\nu B_\nu(T)$$

This is obviously just the analogy to multigroup transport theory.

Other representative problems in radiative transfer include the following:

- i Visible and infrared radiation transport in a planetary atmosphere (the analogue to the albedo problem in neutron transport).
- ii Trapping of resonance radiation in a gas (the analogue to the slab criticality problem).
- iii Sunlight at large depths in the ocean (analogue to calculation of the asymptotic flux in an infinite medium).
- iv Radiative shock wave structure (analogue of the two adjacent half-space problem).

For more details and a bibliography on these problems, the interested reader should refer to the review by Stewart³² and the monograph of Pomraning.³⁵

High Energy Photon Transport □ Thus far our attention has been directed toward radiant energy transfer by photons of low energy. Of major concern in the analysis of nuclear systems, however, is the transport of high energy photons such as gamma or hard X-radiation. In one sense the latter transport processes are complicated somewhat by the possibility of new types of photon interaction such as Compton scattering, pair production, and photonuclear reactions.

However the transport of high energy photons is greatly simplified by the recognition that the photon fluxes of interest are invariably low enough that photon energy deposition does not significantly perturb the background medium. Thus, in sharp contrast to radiative transfer problems, gamma or hard X-ray transport is essentially a linear transport process, similar in many respects to neutron transport. Indeed, this similarity is so strong that the notation and methods used to analyze neutron transport

can be taken over directly to high energy photon transport with only a change in the relevant interaction cross sections.⁴⁰

The dominant physical process in such transport phenomena is usually Compton scattering, in which the photon scatters from a free electron, suffering a change in direction and frequency (energy). The differential scattering cross section for this process is given by the Klein-Nishina formula. One can include appropriate correction factors to account for atomic electrons. For lower photon energies one must also account for coherent scattering from atomic electrons (although in this case no photon energy change occurs).

Photon absorption processes include the photoelectric effect (photoionization or excitation usually followed by subsequent photon emission as the excited atom decays) and pair production (photon decay into an electron-positron pair, followed by the annihilation of the positron accompanied by the emission of two photons of energy 0.511 MeV). The cross sections for all these processes have been measured or calculated and are available in extensive evaluated nuclear data files similar to those compiled for neutron interactions.

3.2 □ THE BOLTZMANN COLLISION TERM □ Many of the mathematical concepts used to describe particle transport processes can be traced back to developments in the kinetic theory of gases. In fact it was more than a century ago that Boltzmann derived the original “transport equation” that bears his name to describe the particle distribution function of a rarefied gas.

Yet there is one very important difference between Boltzmann’s equation for a rarefied gas and the transport equations characterizing random walk processes such as neutron, electron, or photon transport we have been studying to this point. In the latter instances we could justifiably neglect all collisions among the transporting particles (e.g., neutron-neutron or photon-photon interactions) and consider only interactions in which the nuclei or atoms comprise the host medium. This assumption led us to a *linear* transport equation.

However in a gas composed of a single type of particle, the only collisions are those of the gas particles with one another. Hence the neglect of particle-particle collisions would result in a trivial description of the gas (“free molecular flow” or the ideal gas model). Thus we must consider such collisions, and as we might expect, this makes it necessary to use a *nonlinear* transport equation, the Boltzmann equation, to describe the gas.^{41–50}

3.2.1 □ Derivation of the Boltzmann Equation □ Boltzmann's original derivation of the transport equation for a gas was based on physical arguments. A variety of attempts have been made to provide a more "rigorous" derivation of Boltzmann's equation directly from particle mechanics (i.e., Newton's laws). Even today this subject is a very lively one, as a glance at the literature of nonequilibrium statistical mechanics will indicate.⁵¹⁻⁵⁶ Section 3.4 reviews some of the more exotic questions concerning the foundation of kinetic theory in general and Boltzmann's equation in particular. For the present we simply note that such studies have indicated that the usual form of the Boltzmann equation is valid under the assumptions of (i) short-range initial correlations among the gas particles, (ii) low densities (sufficiently low that only binary collisions occur) and times long compared with the duration of a collision, and (iii) density gradients small over the range of the interparticle potential.

We adopt a more heuristic and conventional approach to the derivation of the Boltzmann equation here by implementing the following assumptions:⁴¹⁻⁴⁵ (i) considering only binary collisions (e.g., a dilute gas), (ii) ignoring the presence of external forces, and (iii) assuming that the velocity of the gas molecule is uncorrelated with its position. The third assumption is known as the "stosszahl ansatz" or "molecular chaos" assumption. It implies that the probability of finding two particles simultaneously in d^3r is given simply by the product $n(\mathbf{r}, \mathbf{v}, t) n(\mathbf{r}, \mathbf{v}', t) d^3r$. This is only of limited validity if the particles are interacting, of course, since the presence of one particle will influence the orbit of the second particle, hence its distribution function. We apply this assumption to determine the changes in $n(\mathbf{r}, \mathbf{v}, t)$ due to binary collision events. First note that the rate of decrease in $n(\mathbf{r}, \mathbf{v}, t)$ due to collisions of the type $(\mathbf{v}_1, \mathbf{v}) \rightarrow (\mathbf{v}', \mathbf{v}')$ is (see Figure 3.7):

$$|\mathbf{v}_1 - \mathbf{v}| n(\mathbf{r}, \mathbf{v}, t) n(\mathbf{r}, \mathbf{v}_1, t) \sigma(|\mathbf{v} - \mathbf{v}_1|, \theta) d\hat{\Omega} d^3v_1$$

where $\sigma(|\mathbf{v}_1 - \mathbf{v}|, \theta)$ is the differential cross section for scattering through an angle θ . If we now integrate over $\mathbf{v}_1$ and $\hat{\Omega}$, we find the loss term due to collisions as

$$n(\mathbf{r}, \mathbf{v}, t) \int d^3v_1 \int d\hat{\Omega} \sigma(|\mathbf{v}_1 - \mathbf{v}|, \theta) |\mathbf{v}_1 - \mathbf{v}| n(\mathbf{r}, \mathbf{v}_1, t) \quad (3.12)$$

Next, we calculate the gain term due to collisions by first noting in analogy to Eq. 3.12 that the rate of collision transfer from $(\mathbf{v}', \mathbf{v}') \rightarrow (\mathbf{v}_1, \mathbf{v})$ is just

$$\int d^3v'_1 \int d\hat{\Omega} \sigma'(|\mathbf{v}'_1 - \mathbf{v}'|, \theta) |\mathbf{v}'_1 - \mathbf{v}'| n(\mathbf{r}, \mathbf{v}', t) n(\mathbf{r}, \mathbf{v}'_1, t)$$

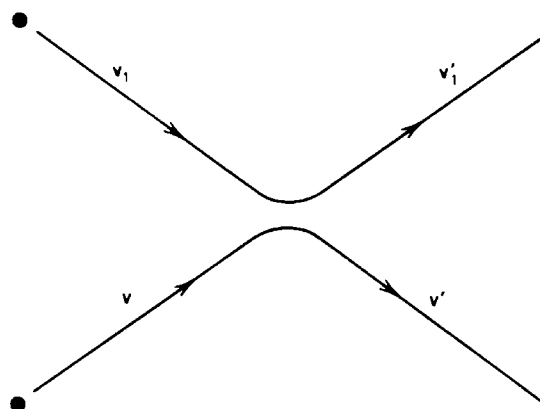


Fig. 3.7 □ Coordinates characterizing a binary collision event.

where $\sigma'(|\mathbf{v}'_1 - \mathbf{v}'|, \theta)$ is the differential cross section for scattering from $(\mathbf{v}'_1, \mathbf{v}') \rightarrow (\mathbf{v}_1, \mathbf{v})$. But since these scattering processes are the inverse of the $(\mathbf{v}_1, \mathbf{v}) \rightarrow (\mathbf{v}'_1, \mathbf{v}')$ collisions, we know

$$\sigma'(|\mathbf{v}'_1 - \mathbf{v}'|, \theta) = \sigma(|\mathbf{v}_1 - \mathbf{v}|, \theta)$$

Furthermore, conservation of momentum in a collision event implies

$$|\mathbf{v}_1 - \mathbf{v}| = |\mathbf{v}'_1 - \mathbf{v}'|$$

while

$$d^3v d^3v_1 = d^3v' d^3v'_1$$

Hence the gain term can be rewritten in terms of the precollision coordinates $(\mathbf{v}_1, \mathbf{v})$ as

$$\int d^3v_1 \int d\hat{\Omega} |\mathbf{v}_1 - \mathbf{v}| \sigma(|\mathbf{v}_1 - \mathbf{v}|, \theta) n(\mathbf{r}, \mathbf{v}', t) n(\mathbf{r}, \mathbf{v}'_1, t)$$

Note here that the final velocities $\mathbf{v}'$ and $\mathbf{v}'_1$ can be determined as functions of the initial velocities $\mathbf{v}$ and $\mathbf{v}_1$ by solving the kinematics equations characterizing the two-body collision event. If we now combine this with the loss term, we find the usual Boltzmann collision term

$$\left(\frac{\partial n}{\partial t} \right)_{\text{coll}} = \int d^3v_1 \int d\hat{\Omega} |\mathbf{v} - \mathbf{v}_1| \sigma(|\mathbf{v} - \mathbf{v}_1|, \theta) \times [n(\mathbf{r}, \mathbf{v}', t) n(\mathbf{r}, \mathbf{v}'_1, t) - n(\mathbf{r}, \mathbf{v}, t) n(\mathbf{r}, \mathbf{v}_1, t)] \quad (3.13)$$

or in the conventional (and obvious) notation

$$\left(\frac{\partial n}{\partial t}\right)_{\text{coll}} = \int d^3v_1 \int d\hat{\Omega} |\mathbf{v} - \mathbf{v}_1| \sigma(n' n'_1 - n n_1) \equiv J(n, n)$$

The Boltzmann equation itself can then be written as

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} = \int d^3v_1 \int d\hat{\Omega} |\mathbf{v} - \mathbf{v}_1| \sigma(|\mathbf{v} - \mathbf{v}_1|, \theta) (n' n'_1 - n n_1) \quad (3.14)$$

Here we should note that the assumption of molecular chaos leads directly to the quadratic dependence on the phase space density, $(n' n'_1 - n n_1)$. Actually, using this assumption we could have immediately written the collision term as⁵⁷

$$\left(\frac{\partial n}{\partial t}\right)_{\text{coll}} = \int d^3v_1 \int d^3g' g \sigma(\mathbf{g}' \rightarrow \mathbf{g}) (n' n'_1 - n n_1) \quad (3.15)$$

where $\mathbf{g} = \mathbf{v} - \mathbf{v}_1$ is the relative velocity between the colliding particles. But conservation of energy demands $|\mathbf{g}| = |\mathbf{g}'|$, hence implying that $\sigma(\mathbf{g}' \rightarrow \mathbf{g})$ must contain a factor $\delta(\mathbf{g}' - \mathbf{g})$. Consequently the six-fold integral in Eq. 3.15 reduces to the five-fold integral in Eq. 3.13 over the variables $\mathbf{v}_1$ and $\hat{\Omega} \equiv \mathbf{g}/|\mathbf{g}|$.

To proceed further we must choose a specific two-body interaction potential, then solve the two-body problem for the particle orbits to arrive at a more explicit form for the collision integral. Fortunately we only require the relationship between the asymptotic precollisional states $\mathbf{v}, \mathbf{v}_1$ and the postcollisional states $\mathbf{v}', \mathbf{v}'_1$, and this considerably simplifies a rather cumbersome calculation. We avoid even this analysis, since most of the features of the Boltzmann collision term we wish to utilize in our subsequent studies hold for general central force laws.^{46,49}

3.2.2 □ Properties of the Boltzmann Collision Term $J(n, n)$ □ The Boltzmann equation is *nonlinear*. Therefore its solution is an extremely difficult task in all but the most trivial situations. However there is one nontrivial solution of some importance. Suppose $n(\mathbf{r}, \mathbf{v}, t)$ is independent of $\mathbf{r}$ and t . Then in the absence of external forces, Eq. 3.14 implies

$$J(n, n) = \int d^3v_1 \int d\hat{\Omega} |\mathbf{v} - \mathbf{v}_1| \sigma(|\mathbf{v} - \mathbf{v}_1|, \theta) (n' n'_1 - n n_1) = 0 \quad (3.16)$$

Certainly a sufficient condition on $n(\mathbf{v})$ is that

$$n(\mathbf{v}') n(\mathbf{v}'_1) - n(\mathbf{v}) n(\mathbf{v}_1) = 0$$

One can demonstrate^{41,44} that the most general solution consistent with energy and momentum conservation is

$$n_0(\mathbf{v}) = c \exp[-A(\mathbf{v} - \mathbf{u}_0)^2]$$

where c , A , and $\mathbf{u}_0$ are arbitrary constants.

If we introduce the usual concept of temperature and normalize, we find that the equilibrium distribution takes the form

$$n_0(\mathbf{v}) = n_0 M(\mathbf{v}) \equiv n_0 \left(\frac{m}{2\pi kT} \right)^{3/2} \exp \left[-\frac{m(\mathbf{v} - \mathbf{u})^2}{2kT} \right]$$

This is the usual Maxwell-Boltzmann distribution. For future use, note here that since Eq. 3.16 involves only the $\mathbf{v}$ dependence of $n_0(\mathbf{v})$, we could allow n_0 , T , and $\mathbf{u}$ to be functions of $\mathbf{r}$ and t and still preserve the property that $J(n_0, n_0) = 0$.

We can extend this result to include an external force field that is derivable from a potential, $\mathbf{F} = -\partial\Phi/\partial\mathbf{r}$. Then a simple calculation indicates that the more general form of the equilibrium distribution function is

$$n_0(\mathbf{r}, \mathbf{v}) = n_0 \left(\frac{m}{2\pi kT} \right)^{3/2} \exp \left[-\frac{m(\mathbf{v} - \mathbf{u})^2/2 + \Phi}{kT} \right]$$

where $\mathbf{u}$ is normal to $\nabla\Phi$. Notice that the equilibrium number density is now spatially dependent

$$n_0(\mathbf{r}) = \int d^3v n_0(\mathbf{r}, \mathbf{v}) = n_0 \exp \left[-\frac{\Phi(\mathbf{r})}{kT} \right]$$

Hence we find that the Maxwell-Boltzmann distribution $n_0(\mathbf{v})$ is an equilibrium solution of the Boltzmann equation. But will any solution of Eq. 3.14 tend to approach $n_0(\mathbf{v})$ for long times? This is answered by the famous *H-theorem* of kinetic theory.⁵⁸

Boltzmann's *H*-Theorem. Define the quantity

$$H(t) \equiv \int d^3r \int d^3v n(\mathbf{r}, \mathbf{v}, t) \ln[n(\mathbf{r}, \mathbf{v}, t)]$$

where $n(\mathbf{r}, \mathbf{v}, t)$ satisfies the Boltzmann equation 3.14. Then

$$\frac{dH}{dt} \leq 0$$

Proof. To simplify, we restrict ourselves to the case in which there are no external forces present and the gas is assumed to be in a homogeneous

state so that the Boltzmann equation becomes

$$\frac{\partial n}{\partial t} = J(n, n)$$

Now we explicitly compute

$$\begin{aligned} \frac{dH}{dt} &= \int d^3v_1 \frac{\partial n_1}{\partial t} [1 + \ln n(\mathbf{v}_1, t)] \\ &= \int d^3v_1 \int d^3v_2 \int d\hat{\Omega} \sigma(\hat{\Omega}) |\mathbf{v}_1 - \mathbf{v}_2| (n'_2 n'_1 - n_2 n_1) (1 + \ln n_1) \end{aligned}$$

Next we note that since this expression is invariant under the interchange $\mathbf{v}_1 \leftrightarrow \mathbf{v}_2$, we can write

$$\frac{dH}{dt} = \frac{1}{2} \int d^3v_1 \int d^3v_2 \int d\hat{\Omega} \sigma(\hat{\Omega}) |\mathbf{v}_1 - \mathbf{v}_2| (n'_2 n'_1 - n_2 n_1) (2 + \ln n_1 n_2) \quad (3.17)$$

or

$$\frac{dH}{dt} = \frac{1}{2} \int d^3v'_1 \int d^3v'_2 \int d\hat{\Omega} \sigma'(\hat{\Omega}) |\mathbf{v}'_1 - \mathbf{v}'_2| (n_2 n_1 - n'_2 n'_1) (2 + \ln n'_1 n'_2) \quad (3.18)$$

where we have noted the invariance under the interchange $(\mathbf{v}_1, \mathbf{v}_2) \leftrightarrow (\mathbf{v}'_1, \mathbf{v}'_2)$. But $d^3v'_1 d^3v'_2 = d^3v_1 d^3v_2$, $|\mathbf{v}'_2 - \mathbf{v}'_1| = |\mathbf{v}_2 - \mathbf{v}_1|$, and $\sigma'(\hat{\Omega}) = \sigma(\hat{\Omega})$. Thus we can take half the sum of Eqs. 3.17 and 3.18 to find

$$\frac{dH}{dt} = \frac{1}{4} \int d^3v_1 \int d^3v_2 \int d\hat{\Omega} \sigma(\hat{\Omega}) |\mathbf{v}_1 - \mathbf{v}_2| \underbrace{(n'_2 n'_1 - n_2 n_1) [\ln(n_1 n_2) - \ln(n'_1 n'_2)]}_{\leq 0}$$

But the integrand of this expression can never be positive. Thus we conclude that $dH/dt \leq 0$, and our proof is complete. (For the extension to a spatially nonuniform system, refer to Chapman and Cowling.⁴¹)

Notice furthermore that $dH/dt = 0$ only when the integrand vanishes, that is, only when

$$n(\mathbf{v}'_2) n(\mathbf{v}'_1) - n(\mathbf{v}_2) n(\mathbf{v}_1) = 0$$

But this is just the condition that gave us the equilibrium distribution $n_0(\mathbf{v})$. Thus we conclude that any initial distribution function $n(\mathbf{r}, \mathbf{v}, t)$ will approach the equilibrium distribution $n_0(\mathbf{v})$ for long times, a comforting though not unexpected result.

We also define a *collisional invariant* or *summational invariant* $\psi(\mathbf{r}, \mathbf{v})$ as any quantity associated with a particle at $\mathbf{r}$ of velocity $\mathbf{v}$ that is conserved in a collision event $(\mathbf{v}', \mathbf{v}_1) \rightarrow (\mathbf{v}, \mathbf{v}_1)$ such that

$$\psi' + \psi_1 = \psi + \psi_1$$

Examples of such collisional invariants include $\psi = m, m\mathbf{v}, m\mathbf{v}^2/2$ (corresponding to particle mass, momentum, and kinetic energy, respectively).

We can now easily demonstrate a very important property of the Boltzmann collision term:

$$\int d^3v \psi(\mathbf{v}) J(n, n) = 0$$

where $n(\mathbf{r}, \mathbf{v}, t)$ is any solution of the Boltzmann equation. To do so, we first write

$$\int d^3v_2 \psi(\mathbf{v}_2) J(n, n) = \int d^3v_1 \int d^3v_2 \int d\hat{\Omega} \sigma(\hat{\Omega}) |\mathbf{v}_2 - \mathbf{v}_1| \psi(\mathbf{v}_2) (n'_1 n'_2 - n_1 n_2) \quad (3.19)$$

Now we proceed in a manner similar to the proof of the H -theorem by making the indicated variable exchanges and adding terms together:

$$\frac{1}{4} [(\text{Eq. 3.19}) + (\mathbf{v}_1 \leftrightarrow \mathbf{v}_2) + (\mathbf{v}_1, \mathbf{v}_2) \leftrightarrow (\mathbf{v}'_1, \mathbf{v}'_2) + (\mathbf{v}_1, \mathbf{v}_2) \leftrightarrow (\mathbf{v}'_2, \mathbf{v}'_1)]$$

to find

$$\begin{aligned} \int d^3v_2 \psi(\mathbf{v}_2) J(n, n) &= \frac{1}{4} \int d^3v_2 \int d^3v_1 \int d\hat{\Omega} \sigma(\hat{\Omega}) |\mathbf{v}_2 - \mathbf{v}_1| (n'_2 n'_1 - n_2 n_1) \\ &\quad \times (\psi_1 + \psi_2 - \psi'_1 - \psi'_2) = 0 \end{aligned}$$

by the definition of a collisional invariant. We use this important result later in Chapter 4 in deriving the equations of hydrodynamics.

3.2.3 □ The Linearized Boltzmann Equation □ We next consider the situations in which a rarefied gas is perturbed only slightly from equilibrium. That is, we assume that these disturbances can be described as perturbations from the equilibrium distribution $n_0(\mathbf{v})$

$$n(\mathbf{r}, \mathbf{v}, t) = n_0(\mathbf{v}) [1 + \varphi(\mathbf{r}, \mathbf{v}, t)], \quad \|\varphi\| \ll 1$$

where the norm $\|\varphi\|$ is usually chosen as

$$\|\varphi\| \equiv \left[\int d^3r \int d^3v n_0(\mathbf{v}) |\varphi(\mathbf{r}, \mathbf{v}, t)|^2 \right]^{1/2}$$

If we now substitute this into the Boltzmann equation and neglect second order quantities, we encounter terms such as

$$n(\mathbf{r}, \mathbf{v}', t) n(\mathbf{r}, \mathbf{v}_1', t) \sim n_0(\mathbf{v}') n_0(\mathbf{v}_1') [1 + \varphi(\mathbf{r}, \mathbf{v}', t) + \varphi(\mathbf{r}, \mathbf{v}_1', t)]$$

But notice that

$$n_0(\mathbf{v}') n_0(\mathbf{v}_1') = n_0^2 \left(\frac{m}{2\pi kT} \right)^3 \exp \left[-\frac{m(\mathbf{v}'^2 + \mathbf{v}_1'^2)}{2kT} \right] = n_0(\mathbf{v}) n_0(\mathbf{v}_1)$$

since by conservation of energy

$$\mathbf{v}_1'^2 + \mathbf{v}'^2 = \mathbf{v}_1^2 + \mathbf{v}^2$$

Hence we are led to the *linearized Boltzmann equation* of the form

$$\begin{aligned} \frac{\partial \varphi}{\partial t} + \mathbf{v} \cdot \frac{\partial \varphi}{\partial \mathbf{r}} &= \int d^3v_1 \int d\hat{\Omega} |\mathbf{v} - \mathbf{v}_1| \sigma(|\mathbf{v} - \mathbf{v}_1|, \hat{\Omega}) n_0(\mathbf{v}_1) [\varphi' + \varphi_1' - \varphi - \varphi_1] \\ &\equiv L[\varphi] \end{aligned} \quad (3.20)$$

This equation is now very similar in form to the neutron transport equation, except for the form of the collision operator L . In fact, the equations would be identical if we could write

$$L[\varphi] = -\nu(v)\varphi(\mathbf{r}, \mathbf{v}, t) + \int d^3v' K(\mathbf{v}' \rightarrow \mathbf{v}) \varphi(\mathbf{r}, \mathbf{v}', t) \quad (3.21)$$

where the collision frequency ν is defined as

$$\nu(v) = \int d^3v_1 \int d\hat{\Omega} |\mathbf{v} - \mathbf{v}_1| \sigma(|\mathbf{v} - \mathbf{v}_1|, \hat{\Omega}) n_0(\mathbf{v}_1)$$

(and corresponds to $v\Sigma_s(v)$ in neutron transport theory). Unfortunately, for repulsive power law potentials of the form $V(r) = V_0/r^{s-1}$, we find that $\nu(v) = \infty$. That is, we cannot perform such a separation as Eq. 3.21 for infinite range potentials. To circumvent this difficulty, it is usually argued that the quantum mechanical calculation of $V(r)$ will always have a cutoff in the effective range and will allow us to define a finite collision frequency

$\nu(v)$. (Of course the value of ν is now dependent on the type of cutoff one introduces; hence this assumption leaves much to be desired.) For such finite-range or “truncated” potentials, one finds the following behavior of the collision frequency:⁴²

“hard potentials” $s > 5 \quad \Rightarrow \quad \nu(v)$ monotonically increasing

“Maxwell potentials” $s = 5 \quad \Rightarrow \quad \nu(v) = \nu_0 = \text{constant}$

“soft potentials” $s < 5 \quad \Rightarrow \quad \nu(v)$ monotonically decreasing

Moreover, for these power law potentials we can also write

$$|\mathbf{v} - \mathbf{v}_1| \sigma(|\mathbf{v} - \mathbf{v}_1|, \theta) = |\mathbf{v} - \mathbf{v}_1|^\gamma \beta(\theta)$$

where $\gamma = (s - 5)/(s - 1)$.

Therefore for cutoff range potentials, the linearized Boltzmann equation (3.20) can be written as follows:

$$\frac{\partial \varphi}{\partial t} + \mathbf{v} \cdot \frac{\partial \varphi}{\partial \mathbf{r}} + \nu(v) \varphi(\mathbf{r}, \mathbf{v}, t) = \int d^3 v' K(\mathbf{v}' \rightarrow \mathbf{v}) \varphi(\mathbf{r}, \mathbf{v}', t)$$

which is mathematically almost identical to the neutron transport equation. We can crank up all our neutron transport machinery to solve this equation. However one very important difference in the scattering kernels characterizing neutron transport and linearized gas dynamics must be kept in mind. To illustrate this most clearly,⁵⁰ suppose we use a slightly different form of the phase space density to linearize the Boltzmann equation

$$n(\mathbf{r}, \mathbf{v}, t) = n_0(\mathbf{v}) + N(\mathbf{r}, \mathbf{v}, t), \quad \|N\| \ll \|n_0\|$$

Then the linearized Boltzmann equation can be written as follows:

$$\frac{\partial N}{\partial t} + \mathbf{v} \cdot \frac{\partial N}{\partial \mathbf{r}} = \int d^3 v_1 \int d^3 g' g \sigma(\mathbf{g}' \rightarrow \mathbf{g}) [N' n'_{01} + N'_1 n'_0 - N_1 n_0 - N n_{01}]$$

If we distinguish between the fraction of gas atoms in equilibrium (n_0) and the disturbance (N), we can interpret each term in the collision integral as follows:

- $N' n'_{01}$ Atoms in disturbance scattered to $\mathbf{v}$.
- $N'_1 n'_0$ Atoms in equilibrium scattered to $\mathbf{v}$.
- $N_1 n_0$ Atoms in equilibrium scattered away from $\mathbf{v}$.
- $N n_{01}$ Atoms in disturbance scattered away from $\mathbf{v}$.

Notice that the first two terms are identical. Next we define

$$v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) \equiv \int d^3 g' g \sigma(\mathbf{g}' \rightarrow \mathbf{g}) n_0(\mathbf{v}')$$

$$v' \Sigma_K(\mathbf{v}' \rightarrow \mathbf{v}) \equiv n_0(\mathbf{v}) \int d^3 g' g \sigma(\mathbf{g}' \rightarrow \mathbf{g})$$

and, if individual terms give convergent integrals (i.e., for cutoff potentials)

$$\begin{aligned} v \Sigma(v) &= \int d^3 v_1 n_0(\mathbf{v}_1) \int d^3 g' g \sigma(\mathbf{g}' \rightarrow \mathbf{g}) \\ &= \int d^3 v' v \Sigma_s(\mathbf{v} \rightarrow \mathbf{v}') = \int d^3 v' v \Sigma_K(\mathbf{v} \rightarrow \mathbf{v}') \end{aligned}$$

Therefore we can write the linearized Boltzmann equation for gases as

$$\frac{\partial N}{\partial t} + \mathbf{v} \cdot \frac{\partial N}{\partial \mathbf{r}} + v \Sigma(v) N(\mathbf{r}, \mathbf{v}, t) = \int d^3 v' [2v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) - v' \Sigma_K(\mathbf{v}' \rightarrow \mathbf{v})] N(\mathbf{r}, \mathbf{v}', t)$$

Within the framework of kinetic theory, neutron transport is actually just the “foreign” gas problem in which the second and third terms are absent:

$$\frac{\partial N}{\partial t} + \mathbf{v} \cdot \frac{\partial N}{\partial \mathbf{r}} + v \Sigma(v) N(\mathbf{r}, \mathbf{v}, t) = \int d^3 v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) N(\mathbf{r}, \mathbf{v}', t)$$

We can now see rather clearly the similarities as well as the differences between the linearized gas dynamics and neutron transport problem by noting

$$\underbrace{\Sigma_s(\mathbf{v}' \rightarrow \mathbf{v})}_{\text{neutrons}} \longrightarrow \underbrace{2\Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) - \Sigma_K(\mathbf{v}' \rightarrow \mathbf{v})}_{\text{gas dynamics}} \equiv \Sigma(\mathbf{v}' \rightarrow \mathbf{v})$$

The physical difference, of course, is that in the gas dynamics problem the disturbance atoms can kick equilibrium atoms away from $\mathbf{v}$, thereby contributing to a *negative* disturbance. Mathematically, this implies that whereas $\Sigma_s(\mathbf{v}' \rightarrow \mathbf{v})$ for neutron transport is everywhere positive, $2\Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) - \Sigma_K(\mathbf{v}' \rightarrow \mathbf{v})$ may, in fact, be negative for some values of $\mathbf{v}'$, $\mathbf{v}$, and this can lead to negative solutions to the linearized Boltzmann equation for a gas. We find in Chapter 5 that this produces some rather subtle differences in the types of solutions possible for the respective transport equations.

3.2.4 □ Boundary Conditions in the Kinetic Theory of Gases □ There is yet another very important difference between neutron transport and gas dynamics problems: the types of boundary condition relevant for each

class of problems. In neutron transport the boundary conditions were rather well established (e.g., no reentrant neutrons on free surfaces). Such is not the case in rarefied gas dynamics, since one can have rather complicated processes occurring when a gas particle collides with a surface (e.g., “specular” reflection in which a particle simply bounces off, or “diffuse” reflection in which the particle is absorbed by the wall and is then reemitted with an isotropic, Maxwellian distribution).

Most of the past effort in the kinetic theory of gases has been directed at “infinite medium” problems such as the calculation of transport coefficients or the study of wave propagation. Only relatively recently has serious attention been focused on boundary value problems that involve gas-surface interactions.⁵⁹ The most general form of the surface boundary condition is usually taken as (see Figure 3.8)

$$|\hat{\mathbf{e}}_s \cdot \mathbf{v}| n_+(\mathbf{R}_s, \mathbf{v}) = \int_{\hat{\mathbf{e}}_s \cdot \mathbf{v}' < 0} d^3v' P(\mathbf{v}' \rightarrow \mathbf{v}) |\hat{\mathbf{e}}_s \cdot \mathbf{v}'| n_-(\mathbf{R}_s, \mathbf{v}') \quad (3.22)$$

where $\hat{\mathbf{e}}_s$ is the unit normal to the surface, and $n_-(\mathbf{v})$ and $n_+(\mathbf{v})$ are the incident and scattered phase space densities, respectively. If one assumes that no gas atoms are lost or gained in a collision with the surface, then the surface interaction kernel must be normalized such that

$$\int_{\hat{\mathbf{e}}_s \cdot \mathbf{v} > 0} d^3v P(\mathbf{v}' \rightarrow \mathbf{v}) = 1$$

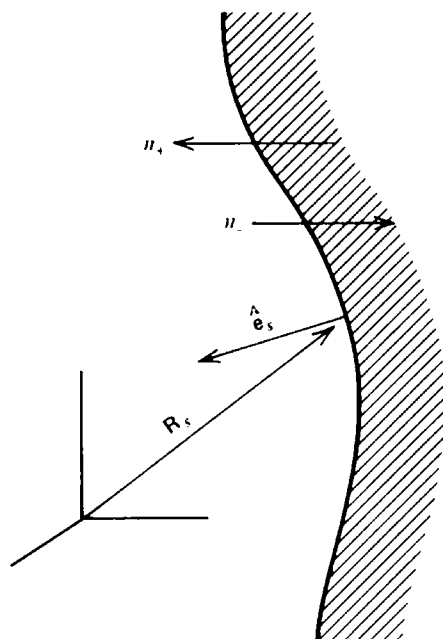


Fig. 3.8 □ Coordinates characterizing gas-surface boundary conditions.

We should also note that the form (3.22) implicitly assumes that the gas-surface interaction is instantaneous and is not dependent on the phase space density—as it might be if there were significant wall heating, for example. Since the surface is usually taken to be in thermal equilibrium at a temperature T , the $P(\mathbf{v}' \rightarrow \mathbf{v})$ must also obey a detailed balance condition

$$|\hat{\mathbf{e}}_s \cdot \mathbf{v}'| M(\mathbf{v}') P(\mathbf{v}' \rightarrow \mathbf{v}) = |\hat{\mathbf{e}}_s \cdot \mathbf{v}| M(\mathbf{v}) P(-\mathbf{v} \rightarrow -\mathbf{v}')$$

Of course, the major difficulty inherent in studying gas-surface interactions involves the determination of the interaction kernel itself. Since the subject of gas-surface physics is exceedingly complex (and still primitively understood), it is customary to model the form of $P(\mathbf{v}' \rightarrow \mathbf{v})$. For example, one of the most popular models was proposed by Maxwell:

$$P(\mathbf{v}' \rightarrow \mathbf{v}) = (1 - \alpha) \delta(\mathbf{v} - \mathbf{v}_r) + \alpha (\hat{\mathbf{e}}_s \cdot \mathbf{v}) M(\mathbf{v})$$

where $\mathbf{v}_r$ is the mirror reflection of the incident velocity, and α is referred to as the *accommodation coefficient* for the surface. If $\alpha = 0$, we find specular reflection, whereas $\alpha = 1$ corresponds to perfect accommodation or diffuse reflection.

One can implement more sophisticated models of the surface interaction kernel, but these are usually limited by the paucity of data on gas-surface interactions. In certain classes of problem it suffices to express the surface condition in terms of only a few moments of the kernel $P(\mathbf{v}' \rightarrow \mathbf{v})$, which represent generalized accommodation coefficients that must then be calculated or measured experimentally. An excellent review of boundary conditions in gas kinetic theory has recently been given by Kuščer.⁵⁹

3.2.5 □ Alternative Forms of the Boltzmann Collision Term □

Bhatnager-Gross-Krook (BGK) Model □ The complexity of the Boltzmann collision term forces us to seek simpler models of the collision process to facilitate mathematical analysis. Perhaps the most popular such collision model was proposed simultaneously by Bhatnager, Gross, and Krook⁶⁰ and Welander⁶¹ in 1954 and is known as the BGK model:

$$J(n, n) \sim \nu [n_0(\mathbf{v}) - n(\mathbf{r}, \mathbf{v}, t)]$$

Here ν is an adjustable parameter and $n_0(\mathbf{r}, \mathbf{v}, t)$ is the local thermodynamic equilibrium distribution

$$n_0(\mathbf{r}, \mathbf{v}, t) = N(\mathbf{r}, t) \left[\frac{m}{2\pi kT(\mathbf{r}, t)} \right]^{3/2} \exp \left[-\frac{m(\mathbf{v} - \mathbf{u}(\mathbf{r}, t))^2}{2kT(\mathbf{r}, t)} \right]$$

This model is sometimes referred to as the “single relaxation time” approximation, since in the absence of spatial dependence it will imply $n(t) \rightarrow n_0(\mathbf{v})$ exponentially in time as $\exp(-\nu t)$. The relaxation parameter ν can be identified as just the collision frequency and could be calculated from the collision cross section as

$$\nu(v) = \int d^3v_1 \int d\hat{\Omega} |\mathbf{v} - \mathbf{v}_1| \sigma(|\mathbf{v} - \mathbf{v}_1|, \theta) n_0(\mathbf{v}_1)$$

More frequently, it is regarded as an adjustable constant in the model, independent of the variables $\mathbf{v}$, $N(\mathbf{r}, t)$, $T(\mathbf{r}, t)$, or $\mathbf{u}(\mathbf{r}, t)$.

This model preserves several of the important properties of the more general Boltzmann collision term. For example, it satisfies an H -theorem and preserves the conservation laws governing mass, momentum, and kinetic energy (thereby preserving the structure of the hydrodynamics equations). It does not yield the correct values for the transport coefficients, however, and most particularly, it yields the incorrect Prandtl number μ/κ .⁴⁴

It should be noted that the model is highly nonlinear, since $N(\mathbf{r}, t)$, $\mathbf{u}(\mathbf{r}, t)$, and $T(\mathbf{r}, t)$ are in fact moments of the phase space density $n(\mathbf{r}, \mathbf{v}, t)$. Nevertheless, the BGK model allows one to reduce the Boltzmann equation characterizing steady flow problems to a set of nonlinear integral equations for the hydrodynamic variables $N(\mathbf{r}, t)$, $T(\mathbf{r}, t)$, and $\mathbf{u}(\mathbf{r}, t)$, which can then be solved using straightforward numerical methods. One can also linearize the BGK model to describe small disturbances from equilibrium. Then the scattering kernel $K(\mathbf{v}' \rightarrow \mathbf{v})$ assumes the form of a degenerate kernel

$$K(\mathbf{v}' \rightarrow \mathbf{v}) = \nu n_0(\mathbf{v}) n_0(\mathbf{v}') \left\{ 1 + \frac{m(\mathbf{v} - \mathbf{u}_0)}{kT_0} \cdot \frac{m(\mathbf{v}' - \mathbf{u}_0)}{kT_0} + \left[\frac{m(\mathbf{v} - \mathbf{u}_0)^2}{2kT_0} - \frac{3}{2} \right] \left[\frac{m(\mathbf{v}' - \mathbf{u}_0)^2}{2kT_0} - \frac{3}{2} \right] \right\} \quad (3.23)$$

Generalized BGK Models (Gross-Jackson Models)^{63–65} □ One can easily generalize the linearized BGK model by simply adding on more terms to the degenerate kernel representation (3.23)

$$K(\mathbf{v}' \rightarrow \mathbf{v}) = \nu(v) n_0(\mathbf{v}) n_0(\mathbf{v}') \sum_{i=1}^N \alpha_{ij} \psi_i(\mathbf{v}) \psi_j(\mathbf{v}')$$

One popular approach is to choose the expansion functions as the eigenfunctions ψ_i of the linearized Boltzmann operator L . This yields in effect a “multiple relaxation time” collision model. Typically, the eigenfunctions are calculated for a simple modeled potential such as the Maxwell potential, in which case the ψ_i are identified as Sonine polynomials.

Application to Gas Mixtures □ The Boltzmann equation can be easily extended to the description of gas mixtures by writing down a collision term for each type of interaction that can occur.^{66,67} The general form of the Boltzmann equation for a species “ i ” can then be written as follows:

$$\frac{\partial n_i}{\partial t} + \mathbf{v} \cdot \frac{\partial n_i}{\partial \mathbf{r}} = \sum_{j=1}^N \int d^3v_1 \int d\hat{\Omega} |\mathbf{v} - \mathbf{v}_1| \sigma_{ij}(|\mathbf{v} - \mathbf{v}_1|, \theta) [n_i(\mathbf{v}') n_j(\mathbf{v}_1') - n_i(\mathbf{v}) n_j(\mathbf{v}_1)]$$

For the special case of binary mixtures, A and B, this yields a set of coupled transport equations

$$\frac{\partial n_A}{\partial t} + \mathbf{v} \cdot \frac{\partial n_A}{\partial \mathbf{r}} = J_{AA}(n_A, n_A) + J_{AB}(n_A, n_B)$$

$$\frac{\partial n_B}{\partial t} + \mathbf{v} \cdot \frac{\partial n_B}{\partial \mathbf{r}} = J_{BA}(n_B, n_A) + J_{BB}(n_B, n_B)$$

The study of gas mixtures can be simplified by the introduction of linearization or modeled collision operators. For example, the BGK model characteristic of a binary gas mixture would be

$$\frac{\partial n_A}{\partial t} + \mathbf{v} \cdot \frac{\partial n_A}{\partial \mathbf{r}} = \nu_{AA}(n_{0A} - n_A) + \nu_{AB}(n_{0AB} - n_B)$$

$$\frac{\partial n_B}{\partial t} + \mathbf{v} \cdot \frac{\partial n_B}{\partial \mathbf{r}} = \nu_{BA}(n_{0BA} - n_A) + \nu_{BB}(n_{0B} - n_B)$$

It should be noted that this model contains three adjustable parameters, ν_{AA} , ν_{BB} , and $\nu_{AB} = (n_B/n_A)\nu_{BA}$, as well as the parameters T_{AB} , T_{BA} , $\mathbf{u}_{AB}$, and $\mathbf{u}_{BA}$, which must be determined. A variety of prescriptions have been proposed for determining these parameters, usually by demanding that the corresponding hydrodynamic equations satisfy certain constraints.^{68,69}

The Enskog-Boltzmann Equation for Dense Gases □ Enskog⁷⁰ proposed a modification of the Boltzmann collision term to account for the fact that since gas molecules have a finite size, they cannot be located at precisely the same point in space in a collision event. This would be a significant effect in the description of dense gases.

If we assume the gas molecules to be rigid spheres of radius R , the Enskog modification takes the form

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} = \int d^3v_1 \int d\hat{\Omega} (\mathbf{v}_1 - \mathbf{v}) \cdot \hat{\Omega} R^2 \left[\chi \left(\mathbf{r} + \frac{1}{2} R \hat{\Omega} \right) n'(\mathbf{r}) n'_1(\mathbf{r} + R \hat{\Omega}) - \chi \left(\mathbf{r} - \frac{1}{2} R \hat{\Omega} \right) n(\mathbf{r}) n_1(\mathbf{r} - R \hat{\Omega}) \right]$$

where χ is a factor that accounts for the increase in the probability of a collision event as the free volume of a gas is reduced at high densities. If we define

$$b\rho = \left(\frac{4}{3} \pi R^3 \right) n_0$$

a useful expression for χ is given by

$$\chi = 1 + 0.6250b\rho + 0.2869(b\rho)^2 + 0.115(b\rho)^3 + \dots$$

The Enskog equation has been applied to calculate transport coefficients (e.g., viscosity or thermal conductivity) in dense gases.^{71,72}

A variety of other generalizations of the Boltzmann collision term can be developed. For example, the collision term can be extended to the description of inelastic collisions or even chemical reactions.⁷³⁻⁷⁵ Furthermore, the gas molecules can be allowed to possess structure so that internal degrees of freedom are allowed (e.g., rotational or vibrational). However we refer the interested reader to several review articles on these more specialized extensions of the Boltzmann equation.

3.2.6 □ Sample Problems in Rarefied Gas Dynamics □ Despite the fundamental difference in boundary conditions, there are some similarities between many of the standard problems in rarefied gas dynamics and problems familiar from neutron transport.

i *Calculation of transport coefficients.* Perhaps the easiest (and most popular) problem in the kinetic theory of gases involves the calculation of transport coefficients such as viscosity or thermal conductivity from the Boltzmann equation.⁷⁶ This is analogous to deriving neutron diffusion theory from the neutron transport equation, thereby obtaining a microscopic definition of the diffusion coefficient. We consider this subject in detail in the next chapter.

ii *Shear flow⁷⁷ (Milne problem).* Here one studies flow past a flat plate and calculates the “slip coefficient” (similar to the extrapolated endpoint in neutron transport theory).

- iii *Couette flow*⁷⁸ (*slab problem*). Flow between two moving plates.
- iv *Free sound propagation*^{79,80} (*pulsed neutron problem assuming an asymptotic $\exp(i\mathbf{B}\cdot\mathbf{r})$ spatial dependence*). Solution of the initial value problem for the linearized Boltzmann equation assuming an $\exp(i\mathbf{k}\cdot\mathbf{r})$ spatial dependence.
- v *Forced sound propagation*^{80,81} (*neutron wave propagation*). Determine the response to an oscillating source of the form $\exp(i\omega t)$.

There is a very remarkable parallel between mathematical developments in neutron transport theory and the linearized kinetic theory of gases. Unfortunately until rather recently these fields have been developed independently. Investigators such as Cercignani,⁴⁷ Kuščer,⁵⁰ Williams,⁴⁸ and Ferziger⁴⁶ have opened up lines of communication between the two disciplines, and the cross-fertilization that has resulted has been quite beneficial.

3.3 □ THE FOKKER-PLANCK (LANDAU) EQUATION □

3.3.1 □ Derivation □ The Boltzmann equation is extremely successful in the description of dilute gases characterized by short-range intermolecular interactions, as proved by more than a century of applications. However the binary collision approximation is certainly invalid in systems such as ionized gases or plasmas, which have long-range interactions. No longer can one assume that binary collisions dominate—rather, large numbers of particles will interact simultaneously. Transport processes in such fluids are most conveniently described by separating off the long-range, many particle interactions using a self-consistent field term (the Vlasov term), then treating the relatively weak short-range Coulomb collisions using a stochastic model borrowed from the theory of random processes (the Fokker-Planck collision term).^{82,83}

One very convenient scheme for obtaining the latter model is to assume that the interaction forces are weak, then to expand the Boltzmann collision term to lowest order in the interaction potential.⁸⁴ To be more precise, let us consider a single species charged fluid. Of course, any ionized gas will contain free electrons as well as ions to yield macroscopic charge neutrality, but since the extension of our results to several species is straightforward, we carry through the analysis for this model.

We begin by noting that the differential scattering cross section for Coulomb interactions (Rutherford scattering) is just

$$\sigma_{ij}(|\mathbf{v}_i - \mathbf{v}_j|, \theta) = \frac{e_i^2 e_j^2}{4|\mathbf{v}_i - \mathbf{v}_j|^4 \mu_{ij}^2} \frac{1}{\sin^4 \theta / 2}$$

where $\mu_{ij} = m_i m_j / (m_i + m_j)$ is the reduced mass. Since the Coulomb interaction is weak, apparently the change in velocity $\Delta \mathbf{v} = \mathbf{v}' - \mathbf{v}$ experienced by a colliding particle will be small. With this in mind, let us expand the phase space density $n(\mathbf{r}, \mathbf{v}', t)$ appearing in the Boltzmann collision term about $\mathbf{v}$ and retain only terms to order $\Delta \mathbf{v} \Delta \mathbf{v}$ (in a manner very similar to the continuous slowing down approximation we introduced in studying neutron transport):

$$\begin{aligned} \left(\frac{\partial n}{\partial t} \right)_{\text{coll}} \cong & \int d^3 v_1 \int d\hat{\Omega} |\mathbf{v} - \mathbf{v}_1| \sigma(|\mathbf{v} - \mathbf{v}_1|, \theta) \left[-\Delta \mathbf{v} \cdot \mathbf{n} \frac{\partial n_1}{\partial \mathbf{v}} + \Delta \mathbf{v} \cdot \mathbf{n}_1 \frac{\partial n}{\partial \mathbf{v}} \right. \\ & \left. + \frac{1}{2} \Delta \mathbf{v} \Delta \mathbf{v} : \mathbf{n} \frac{\partial^2 n_1}{\partial \mathbf{v} \partial \mathbf{v}} - \Delta \mathbf{v} \Delta \mathbf{v} : \frac{\partial n_1}{\partial \mathbf{v}} \frac{\partial n}{\partial \mathbf{v}} + \frac{1}{2} \Delta \mathbf{v} \Delta \mathbf{v} : \mathbf{n}_1 \frac{\partial^2 n}{\partial \mathbf{v} \partial \mathbf{v}} \right] \end{aligned}$$

We can perform the integrations by transforming to center of mass coordinates. The details, although straightforward, are sufficiently cumbersome to avoid in our cursory discussion (see, e.g., Montgomery and Tidman⁸⁴). Instead we merely note that performing the angular integration yields

$$\begin{aligned} \left(\frac{\partial n}{\partial t} \right)_{\text{coll}} = & \int d^3 v_1 \left[\frac{1}{2} \langle \Delta \mathbf{g} \rangle \cdot \left(\mathbf{n}_1 \frac{\partial n}{\partial \mathbf{v}} - \mathbf{n} \frac{\partial n_1}{\partial \mathbf{v}} \right) \right. \\ & \left. + \langle \Delta \mathbf{g} \Delta \mathbf{g} \rangle : \left(\frac{1}{4} \mathbf{n} \frac{\partial^2 n_1}{\partial \mathbf{v} \partial \mathbf{v}} - \frac{1}{2} \frac{\partial n}{\partial \mathbf{v}} \frac{\partial n_1}{\partial \mathbf{v}} + \frac{1}{4} \mathbf{n}_1 \frac{\partial^2 n}{\partial \mathbf{v} \partial \mathbf{v}} \right) \right] \end{aligned}$$

where $\mathbf{g} = \mathbf{v}_1 - \mathbf{v}$ and

$$\begin{aligned} \langle \Delta \mathbf{g} \rangle & \equiv \int d\hat{\Omega} g \sigma_{ij} \Delta \mathbf{g} = \frac{4\pi e_i^2 e_j^2}{m_{ij}^2 g^2} \ln \left(\frac{\sin \theta_{\min}}{2} \right) \left(\frac{\mathbf{g}}{g} \right) \\ \langle \Delta \mathbf{g} \Delta \mathbf{g} \rangle & \equiv \int d\hat{\Omega} g \sigma_{ij} \Delta \mathbf{g} \Delta \mathbf{g} = -\frac{4\pi e_i^2 e_j^2}{m_{ij}^2} \ln \left(\frac{\sin \theta_{\min}}{2} \right) g^{-3} (\mathbf{I} g - \mathbf{g} \mathbf{g}) \end{aligned}$$

Note here that when evaluating $\langle \Delta \mathbf{g} \rangle$ and $\langle \Delta \mathbf{g} \Delta \mathbf{g} \rangle$ for a Coulomb potential, one encounters the familiar logarithmic divergence. In this case, we have handled it by truncating the integration at some minimum scattering angle, $\theta_{\min}$. If we now perform the integration over $\mathbf{v}_1$, we arrive at the usual form of the Fokker-Planck collision term first derived by Landau⁸⁵ and later by a somewhat different route by Rosenbluth, MacDonald, and Judd.⁸⁶

$$\left(\frac{\partial n}{\partial t} \right)_{\text{coll}} = -\Gamma_i \left[\frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{n}_i \frac{\partial H_i}{\partial \mathbf{v}} + \frac{1}{2} \frac{\partial^2}{\partial \mathbf{v} \partial \mathbf{v}} : \left(\mathbf{n}_i \frac{\partial^2 G_i}{\partial \mathbf{v} \partial \mathbf{v}} \right) \right] \quad (3.24)$$

where

$$H_i \equiv \sum_j n_{0j} \left(\frac{e_j}{e_i} \right)^2 \frac{(m_i + m_j)}{m_j} \int d^3v g^{-1} n_j$$

$$G_i \equiv \sum_j n_{0j} \left(\frac{e_j}{e_i} \right)^2 \int d^3v g n_j$$

$$\Gamma_i \equiv - \frac{4\pi e_i^4}{m_i^2} \ln \left(\frac{\sin \theta_{\min}}{2} \right) = \frac{4\pi e_i^2}{m_i^2} \ln \Lambda$$

$$\Lambda \equiv 24\pi n_0 \lambda_D^3$$

This collision term can be written in an alternative form due to Landau:

$$\left(\frac{\partial n}{\partial t} \right)_{\text{coll}} = \frac{\partial}{\partial \mathbf{v}} \cdot \int d^3v' \mathbf{Q}(\mathbf{v}, \mathbf{v}') \cdot \left[\frac{\partial n}{\partial \mathbf{v}} n(\mathbf{v}') - n(\mathbf{v}) \frac{\partial n}{\partial \mathbf{v}'} \right] \equiv J_{\text{FP}}(n, n) \quad (3.25)$$

where

$$\mathbf{Q} \equiv - \frac{\pi e^4}{m^2} \ln \left[\frac{(kT)^3}{4\pi n_0 e^6} \right] \left(\frac{g^2 \mathbf{I} - \mathbf{g}\mathbf{g}}{g^3} \right)$$

The nonlinearity of the Fokker-Planck collision term is most clearly revealed in this form.

An alternative derivation that is independent of the Boltzmann equation (which is extremely suspect for a plasma in any event) can be borrowed from the theory of random Markov processes.⁸⁷ If we assume that collision events are indeed a Markov process, the phase space density at a time t , $n(\mathbf{r}, \mathbf{v}, t)$, can be written in terms of n at earlier times as

$$n(\mathbf{r}, \mathbf{v}, t) = \int d(\Delta \mathbf{v}) \psi(\mathbf{v} - \Delta \mathbf{v}, \Delta \mathbf{v}) n(\mathbf{r}, \mathbf{v} - \Delta \mathbf{v}, t - \Delta t) \quad (3.26)$$

where $\psi(\mathbf{v}, \Delta \mathbf{v})$ is the probability that in time Δt , a particle is scattered from $\mathbf{v}$ to $\mathbf{v} + \Delta \mathbf{v}$. We can then identify

$$\left(\frac{\partial n}{\partial t} \right)_{\text{coll}} = \lim_{\Delta t \rightarrow 0} \frac{n(\mathbf{r}, \mathbf{v}, t) - n(\mathbf{r}, \mathbf{v}, t - \Delta t)}{\Delta t}$$

For small Δt , we can use a Taylor expansion to find

$$\begin{aligned} n(\mathbf{r}, \mathbf{v}, t) = \int d(\Delta \mathbf{v}) & \left[n(\mathbf{r}, \mathbf{v}, t) \psi(\mathbf{v}, \Delta \mathbf{v}) - \Delta t \psi \frac{\partial n}{\partial t} - \Delta \mathbf{v} \left(\frac{\partial n}{\partial \mathbf{v}} \psi + n \frac{\partial \psi}{\partial \mathbf{v}} \right) \right. \\ & \left. + \frac{1}{2} \Delta \mathbf{v} \Delta \mathbf{v} : \left(\psi \frac{\partial^2 n}{\partial \mathbf{v} \partial \mathbf{v}} + 2 \frac{\partial n}{\partial \mathbf{v}} \frac{\partial \psi}{\partial \mathbf{v}} + n \frac{\partial^2 \psi}{\partial \mathbf{v} \partial \mathbf{v}} \right) + \dots \right] \end{aligned}$$

If we now use this in Eq. 3.26, we find

$$\left(\frac{\partial n}{\partial t}\right)_{\text{coll}} = -\frac{\partial}{\partial \mathbf{v}} \cdot [\langle \Delta \mathbf{v} \rangle n] + \frac{1}{2} \frac{\partial}{\partial \mathbf{v}} \frac{\partial}{\partial \mathbf{v}} : [\langle \Delta \mathbf{v} \Delta \mathbf{v} \rangle n]$$

where we define

$$\langle \Delta \mathbf{v} \rangle \equiv \int d(\Delta \mathbf{v}) \psi(\mathbf{v}, \Delta \mathbf{v}) \Delta \mathbf{v}$$

$$\langle \Delta \mathbf{v} \Delta \mathbf{v} \rangle \equiv \int d(\Delta \mathbf{v}) \psi(\mathbf{v}, \Delta \mathbf{v}) \Delta \mathbf{v} \Delta \mathbf{v}$$

In terms of our earlier notation, we can explicitly write

$$\langle \Delta \mathbf{v} \rangle = \int d^3 v_1 \int d\hat{\Omega} |\mathbf{v} - \mathbf{v}_1| \sigma(|\mathbf{v} - \mathbf{v}_1|, \theta) n(\mathbf{v}_1) \Delta \mathbf{v}$$

$$\langle \Delta \mathbf{v} \Delta \mathbf{v} \rangle = \int d^3 v_1 \int d\hat{\Omega} |\mathbf{v} - \mathbf{v}_1| \sigma(|\mathbf{v} - \mathbf{v}_1|, \theta) n(\mathbf{v}_1) \Delta \mathbf{v} \Delta \mathbf{v}$$

As a side remark at this point, although it is customary to refer to equations of the form (3.24) or (3.25) as Fokker-Planck equations, they are in fact quite different from the Fokker-Planck equation familiar from the theory of Brownian motion⁸⁷ (see Section 3.6), which is a *linear* equation for the distribution function.⁸⁸ A more appropriate terminology would be to refer to Eq. 3.24 or 3.25 as equations of the *Landau* type.

3.3.2 □ The Balescu-Lenard Equation □ In plasma physics it is occasionally important to take into account the effects of plasma waves on short-range collisions (i.e., “wave-particle” interactions). This can be accomplished to a degree by using a generalized Fokker-Planck collision model first derived using statistical mechanics arguments by Balescu⁸⁹ and Lenard:⁹⁰

$$\left(\frac{\partial n}{\partial t}\right)_{\text{coll}} = -\frac{\partial}{\partial \mathbf{v}} \cdot \int d^3 v' \mathbf{Q}_{\text{BL}}(\mathbf{v}, \mathbf{v}') \cdot \left[\frac{\partial n}{\partial \mathbf{v}} n(\mathbf{v}') - n(\mathbf{v}) \frac{\partial n}{\partial \mathbf{v}'} \right] \equiv J_{\text{BL}}(n, n)$$

where now

$$\mathbf{Q}_{\text{BL}}(\mathbf{v}, \mathbf{v}') \equiv -\int d^3 k \frac{\mathbf{k} \mathbf{k}}{k} \delta(\hat{\mathbf{k}} \cdot \mathbf{v} - \hat{\mathbf{k}} \cdot \mathbf{v}') \frac{(2\pi)^3 n_0 \tilde{V}(k) \pi^2 / m^2}{|D^+(-k, i\mathbf{k} \cdot \mathbf{v})|}$$

$\tilde{V}(k)$ is the Fourier transform of the interaction potential [in the case of Coulomb interactions, $\tilde{V}(k) = e^2/k^2$], and where $D^+(-k, i\mathbf{k} \cdot \mathbf{v})$ is the limit as $z \rightarrow i\mathbf{k} \cdot \mathbf{v}$ of the plasma dielectric function

$$D(k, z) \equiv 1 - \omega_p^2 \frac{i}{k} \int_{-\infty}^{\infty} du \frac{\partial n_0 / \partial u}{z + iku}$$

The Balescu-Lenard collision term can be shown to be the first order correction to the Vlasov equation in an expansion in the plasma parameter, $\epsilon = 1/n\lambda_D^3$.⁸⁹ It no longer contains the characteristic Coulomb logarithmic divergence at small k , but unfortunately this is replaced by a new divergence at large k . This divergence can be patched up by taking somewhat more care in the short-range treatment of the Coulomb interactions, and this leads to a three-component collision term containing the Balescu-Lenard, Boltzmann, and Fokker-Planck forms. But this more complex kinetic equation has been only of formal interest to date.^{91,92}

3.3.3 □ Properties □ Both the Fokker-Planck-Landau and Balescu-Lenard collision terms are nonlinear. Nevertheless a few general properties of these collision operators can be demonstrated.⁸⁴ For convenience, we write both terms in the form

$$\left(\frac{\partial n}{\partial t} \right)_{\text{coll}} = - \frac{\partial}{\partial \mathbf{v}} \cdot \int d^3 v' \mathbf{Q}(\mathbf{v}, \mathbf{v}') \cdot \left(\frac{\partial n}{\partial \mathbf{v}} n' - n \frac{\partial n'}{\partial \mathbf{v}'} \right) \equiv - \frac{\partial}{\partial \mathbf{v}} \cdot \mathcal{G}(n)$$

and consider only the homogeneous problem for which the transport equation reduces to the form

$$\frac{\partial n}{\partial t} = - \frac{\partial}{\partial \mathbf{v}} \cdot \mathcal{G}(n)$$

First we note that both the Fokker-Planck-Landau and Balescu-Lenard collision terms exhibit the property that

$$\int d^3 v \psi_i(\mathbf{v}) \left(\frac{\partial n}{\partial t} \right)_{\text{coll}} = - \int d^3 v \psi_i(\mathbf{v}) \frac{\partial}{\partial \mathbf{v}} \cdot \mathcal{G}(n) = 0 \quad (3.27)$$

where ψ_i are the collision invariants: m , $m\mathbf{v}$, and $m\mathbf{v}^2/2$. To demonstrate each of these, note first

$$\int d^3 v \frac{\partial}{\partial \mathbf{v}} \cdot \mathcal{G}(n) = 0$$

Next, we calculate

$$-\int d^3v \mathbf{v} \frac{\partial}{\partial \mathbf{v}} \cdot \mathcal{F}(n) = \int d^3v \mathcal{F}(n) = \int d^3v \int d^3v' \mathbf{Q}(\mathbf{v}, \mathbf{v}') \cdot \left(\frac{\partial n}{\partial \mathbf{v}} n' - n \frac{\partial n'}{\partial \mathbf{v}'} \right)$$

but since $\mathbf{Q}(\mathbf{v}, \mathbf{v}') = \mathbf{Q}(\mathbf{v}', \mathbf{v})$, this also vanishes. Finally

$$\begin{aligned} -\int d^3v \frac{v^2}{2} \frac{\partial}{\partial \mathbf{v}} \cdot \mathcal{F}(n) &= \int d^3v \int d^3v' \mathbf{v} \cdot \mathbf{Q}(\mathbf{v}, \mathbf{v}') \cdot \left(\frac{\partial n}{\partial \mathbf{v}} n' - n \frac{\partial n'}{\partial \mathbf{v}'} \right) \\ &= \frac{1}{2} \int d^3v \int d^3v' (\mathbf{v} - \mathbf{v}') \cdot \mathbf{Q}(\mathbf{v}, \mathbf{v}') \cdot \left(\frac{\partial n}{\partial \mathbf{v}} n' - n \frac{\partial n'}{\partial \mathbf{v}'} \right) \end{aligned}$$

But from the form of $\mathbf{Q}(\mathbf{v}, \mathbf{v}')$ it is evident that $\mathbf{v} \cdot \mathbf{Q}(\mathbf{v}, \mathbf{v}') = \mathbf{v}' \cdot \mathbf{Q}(\mathbf{v}, \mathbf{v}')$ so that this term vanishes as well. The property (3.27) is particularly important because it implies that the moments of the Fokker-Planck-Landau or Balescu-Lenard equations will yield the correct hydrodynamics equations consistent with conservation of mass, momentum, and kinetic energy.

Next one can demonstrate that both these collision terms exhibit an H -theorem property, $dH/dt \leq 0$, where we recall

$$H(t) \equiv \int d^3r \int d^3v n(\mathbf{r}, \mathbf{v}, t) \ln n(\mathbf{r}, \mathbf{v}, t)$$

(For a detailed demonstration of this property, see, e.g., Montgomery and Tidman.⁸⁴) Finally, one can demonstrate that $dH/dt = 0$ if and only if $n(\mathbf{v})$ is the Maxwell-Boltzmann distribution, so that both collision terms yield the proper equilibrium behavior.

The Fokker-Planck-Landau equation has come to play a very important role in a variety of plasma physics calculations. It is routinely used to calculate transport coefficients characterizing collision processes in plasmas. It is even implemented in computer codes that calculate the plasma phase space density in plasma devices (e.g., controlled fusion systems).

In sharp contrast, there has been little application of the Balescu-Lenard equation, and in fact in the applications that have been attempted, it is usually found that the Fokker-Planck-Landau equation gives comparable results. Certainly the theory of the Balescu-Lenard equation, in either its nonlinear or linearized form, is in a very primitive stage compared to that of the Fokker-Planck-Landau equation.

3.4 □ COLLISIONLESS TRANSPORT WITH SELF-CONSISTENT FIELDS: THE VLASOV EQUATION □ A wealth of various types of transport phenomena arise in plasma physics. Most studies of such processes ignore short-range Coulomb encounters entirely⁸² and include

only the long-range interactions among large numbers of particles by using a self-consistent treatment of the force term in

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial n}{\partial \mathbf{v}} = 0$$

To be more precise, we restrict our attention to uniform, field-free plasmas that can be described by the Vlasov-Maxwell equations in the electrostatic approximation

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} + \frac{q}{m} \mathbf{E} \cdot \frac{\partial n}{\partial \mathbf{v}} = 0$$

$$\frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{E} = 4\pi q \int d^3v [n(\mathbf{r}, \mathbf{v}, t) - n_0(\mathbf{v})]$$

If we denote the interaction potential between particles as $V(r)$, we can combine these two equations to write an alternative form of the Vlasov equation as follows:

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} - \frac{1}{m} \int d^3r' \int d^3v' \frac{\partial}{\partial \mathbf{r}} V(|\mathbf{r} - \mathbf{r}'|) n(\mathbf{r}', \mathbf{v}', t) \cdot \frac{\partial}{\partial \mathbf{v}} n(\mathbf{r}, \mathbf{v}, t) = 0$$

The Vlasov equation is deceptively simple looking. Its nonlinear structure gives rise to many enormously complex solutions. Indeed, most theoretical research in plasma physics utilizes the Vlasov equation as the accepted model of the plasma state.

The Vlasov equation is time reversible (invariant under the transformation $\mathbf{v} \rightarrow -\mathbf{v}$, $\mathbf{r} \rightarrow \mathbf{r}$, $t \rightarrow -t$). It does not contain dissipative terms such as the collision term, which will force solutions asymptotically to the equilibrium distribution $n_0(\mathbf{v})$ for long times, as with the Boltzmann or Fokker-Planck equations, for example.

As with other types of nonlinear transport processes, we can linearize the Vlasov equation by assuming small disturbances from some known solution.⁹³ In this case we first note that any solution $n_0(\mathbf{v})$ that is independent of space and time is an equilibrium solution of the Vlasov equation. Hence we linearize about an arbitrary uniform distribution that also has the property that it does not yield a zeroth order electric field:

$$n(\mathbf{r}, \mathbf{v}, t) = n_0(\mathbf{v}) + n_1(\mathbf{r}, \mathbf{v}, t), \quad \|n_1\| \ll \|n_0\|$$

If we now substitute this into the Vlasov-Maxwell equation and note

$E_0 = 0$, we find

$$\frac{\partial n_1}{\partial t} + \mathbf{v} \cdot \frac{\partial n_1}{\partial \mathbf{r}} + \frac{q}{m} \mathbf{E}_1 \cdot \frac{\partial n_0}{\partial \mathbf{v}} = - \frac{q}{m} \mathbf{E}_1 \cdot \frac{\partial n_1}{\partial \mathbf{v}}$$

$$\frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{E}_1 = 4\pi q \int d^3v n_1(\mathbf{v})$$

We linearize this equation by neglecting the second order term on the right-hand side to arrive at the linearized Vlasov equation

$$\frac{\partial n_1}{\partial t} + \mathbf{v} \cdot \frac{\partial n_1}{\partial \mathbf{r}} + \frac{q}{m} \mathbf{E}_1 \cdot \frac{\partial n_0}{\partial \mathbf{v}} = 0, \quad \frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{E}_1 = 4\pi q \int d^3v n_1(\mathbf{v})$$

Chapter 5 develops in some detail the application of this equation to the study of wave propagation in plasmas. We also study schemes that can be utilized to attack the more general nonlinear form of the Vlasov equation.

3.5 □ MODERN DEVELOPMENTS IN THE DERIVATION OF TRANSPORT EQUATIONS □

Thus far we have confined our attention to the collision terms of the more familiar types, used to describe particle transport processes. However the field of nonequilibrium statistical mechanics has recently experienced a flurry of activity concerned with the derivation of new forms of transport or kinetic equations that possess the capability of describing dense many body systems (such as liquids or plasmas) or systems that exhibit highly nonequilibrium behavior (e.g., turbulence). Such modern developments have provided a far better understanding of the range of validity of the more traditional transport equations such as the Boltzmann or Fokker-Planck equation. Therefore it seems appropriate to include in a treatise on transport theory some discussion of modern developments in kinetic theory that are leading to new forms of the transport equation.

As noted in Chapter 1, there are almost as many approaches to the derivation of transport or kinetic equations as there are investigators in this field of nonequilibrium statistical mechanics. All such approaches eventually converge when they introduce approximations by performing a perturbation expansion (possibly to infinite order by way of renormalization methods) in a suitable parameter such as density or interaction strength. We therefore exercise a personal preference and approach this topic using the very powerful and versatile theory of generalized Brownian motion developed by Mori,⁹⁴ Zwanzig,⁹⁵ Kawasaki,⁹⁶ and others.⁹⁷

In this theory the projection operator methods of Zwanzig are used to recast exact microscopic equations of motion characterizing a many body

system into a form very similar to that of the classical Langevin equation familiar from the theory of Brownian motion. Since this “generalized Langevin equation” is merely an identity with the equations of motion, it is still quite exact and contains all the information (and complexity) of the microscopic particle dynamics. Hence this equation appears at first to be a curiosity of formal interest only. However the generalized Langevin equation has proved itself to be a very useful framework on which to base approximate theories of many body systems.

This section briefly surveys the foundations and several typical applications of the generalized Langevin method to the study of linear transport processes and equilibrium time correlation functions. Then we turn our attention to recent attempts to extend the method to the description of nonlinear processes and highly nonequilibrium states. This survey is not intended to be complete, but rather to illustrate how modern methods in statistical mechanics can be utilized to develop generalized forms of transport or kinetic equations. It will also serve to introduce the reader to the generalized forms of the more familiar transport equations (e.g., Boltzmann, Fokker-Planck, or Balescu-Lenard equations).

3.5.1 □ General Derivation □ Certainly one of the most familiar problems in statistical mechanics involves the fluctuating motion of a Brownian particle in a background medium (a “bath” of background particles).⁹⁸ For example, one might consider the motion of a macroscopic test particle through a molecular fluid, or the motion of a neutron through a crystalline lattice. This problem is usually introduced by postulating that the random fluctuations in the velocity of the test particle $v(t)$ that arise from microscopic collision events with bath particles can be modeled by adding a random force term $R(t)$ to the phenomenological, deterministic equation for $v(t)$ (see Figure 3.9)

$$m \frac{dv}{dt} + m\gamma v(t) = R(t)$$

(We restrict ourselves to one-dimensional motion for the moment, to avoid vector notation.) Here, m is the mass of the Brownian particle, and γ is the friction coefficient characterizing the dissipative frictional forces on the test particle due to the bath. This technique of modeling microscopic phenomena by adding random force terms to the deterministic equation describing a macroscopic process is known as the *Langevin method*. The corresponding equation for the fluctuating variable is then referred to as the *Langevin equation*.

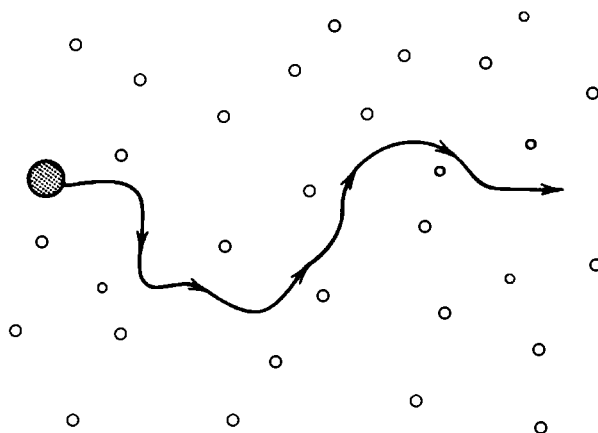


Fig. 3.9 □ Brownian motion of a test particle through a background medium (a “bath”).

In the traditional Langevin approach one restricts the statistical nature of the random force by demanding that it satisfy several constraints:

- i $\langle R(t) \rangle = 0$.
- ii $\langle R(t) v(t') \rangle = 0, \quad t > t' \quad (\text{causality}).$
- iii $\langle R(t) R(t') \rangle \sim \delta(t - t') \quad (\text{Markov behavior}).$

where $\langle \rangle$ denotes an average over the nonequilibrium ensemble of interest. (Note here that conditions i, ii, and iii actually represent restrictions on the natures of both the random force and the ensemble itself.) An additional feature of the classical Langevin equation is a relation between the equilibrium average $\langle \rangle_{\text{eq}}$ of the random force correlation function and the dissipation or transport coefficient γ . Such a relation is known as the *fluctuation-dissipation theorem*, and it can be written either as

$$\langle R(t) R(t') \rangle_{\text{eq}} = 2 \left(\frac{m\gamma}{\beta} \right) \delta(t - t')$$

or

$$\gamma = \left(\frac{\beta}{m} \right) \int_0^\infty dt \langle R(t_0) R(t_0 + t) \rangle_{\text{eq}} \quad (3.28)$$

The success of the Langevin method in statistical physics provided a strong motivation to generalize the theory by developing its microscopic counterpart, working directly from the equations of motion for the Brownian particle and the individual bath particles.⁹⁹ It was recognized

quite early that such a generalized theory of Brownian motion would have to allow for non-Markovian behavior, for example, by allowing the friction coefficient to become time dependent. Although a number of fundamental contributions to this theory have been made (notably the work of Kirkwood¹⁰⁰), we confine our attention to the schemes that proceed by recasting the equations of motion into the form of exact (microscopic) Langevin-like equations.

The first major contribution in this direction was due to Zwanzig,⁹⁵ who utilized projection operator methods to arrive at a generalized Langevin equation that assumed a non-Markovian form

$$m \frac{dv}{dt} + m \int_0^t d\tau \gamma(\tau) v(t-\tau) = R(t) \quad (3.29)$$

[Actually, Zwanzig obtained a very similar exact equation for the time correlation function $\langle v(0)v(t) \rangle_{\text{eq}}$, but we generalize his results a bit for the purposes of this discussion.] Moreover, he provided explicit (albeit formal) microscopic expressions for the generalized transport coefficient $\gamma \rightarrow \gamma(\tau)$ and the random force term $R(t)$.

Zwanzig's projection operator methods have been extended and refined by Mori^{94,101} into a very elegant theory of generalized Brownian motion capable of describing the dynamics of any many body system. Mori's generalized Langevin method represents an *exact, microscopic* counterpart to the original *phenomenological, macroscopic* Langevin method, which has proved so useful in the study of random processes. Mori began by considering the equation of motion for a vector $\mathbf{a}(t)$ whose components $a_j(t)$ are dynamical variables of the coordinates $(\mathbf{x}_1, \dots, \mathbf{x}_N; \mathbf{v}_1, \dots, \mathbf{v}_N)$ of a many particle system (i.e., the "Heisenberg form" of Liouville's equation):

$$\frac{d\mathbf{a}}{dt} = iL\mathbf{a}(t) \quad (3.30)$$

Here, the equilibrium values of the variables have been subtracted for convenience [i.e., $a_j(t) = A_j(t) - \langle A_j \rangle_{\text{eq}}$], so that $a_j(t)$ represents a fluctuation from equilibrium. By using projection operator methods (see Appendix D), Mori was able to transform this equation into a form

$$\frac{d\mathbf{a}}{dt} - i\Omega \cdot \mathbf{a}(t) + \int_0^t d\tau \boldsymbol{\varphi}(\tau) \cdot \mathbf{a}(t-\tau) = \mathbf{f}(t) \quad (3.31)$$

which is somewhat similar in appearance to the Langevin equation familiar from the stochastic theory of Brownian motion. However unlike the Langevin equation, Eq. 3.31 is an exact equation for the dynamical

variable $\mathbf{a}(t)$, hence is equivalent to the equation of motion (3.30) for the many particle system.

The terms in this “generalized Langevin equation” are given explicitly in terms of equilibrium ensemble averages as

$$i\Omega \equiv \langle \dot{\mathbf{a}}\mathbf{a}^* \rangle_{\text{eq}} \cdot \langle \mathbf{a}\mathbf{a}^* \rangle_{\text{eq}}^{-1} \quad \text{“frequency matrix”} \quad (3.32)$$

$$\boldsymbol{\varphi}(t) \equiv \langle \dot{\mathbf{f}}(t)\mathbf{f}^*(0) \rangle_{\text{eq}} \cdot \langle \mathbf{a}\mathbf{a}^* \rangle_{\text{eq}}^{-1} \quad \text{“damping or memory matrix”} \quad (3.33)$$

$$\mathbf{f}(t) \equiv e^{i\mathbf{t}(1-P)L} \mathbf{i}(1-P)L\mathbf{a} \quad \text{“random force”} \quad (3.34)$$

where $\langle \cdots \rangle_{\text{eq}}$ denotes an average over the equilibrium canonical ensemble $\rho_{\text{eq}} = \exp(-\beta H)/Z$, $\beta \equiv 1/kT$; $\mathbf{a} = \mathbf{a}(0)$; $\mathbf{a}^*$ is the row vector adjoint to $\mathbf{a}$; and P is a projection operator defined by its action on an arbitrary dynamical variable vector $\mathbf{G}$ as

$$P\mathbf{G} \equiv \langle \mathbf{G}\mathbf{a}^* \rangle_{\text{eq}} \cdot \langle \mathbf{a}\mathbf{a}^* \rangle_{\text{eq}}^{-1} \cdot \mathbf{a}$$

The matrix $\langle \mathbf{a}\mathbf{a}^* \rangle_{\text{eq}}^{-1}$ is the inverse of the static correlation matrix $\langle \mathbf{a}\mathbf{a}^* \rangle_{\text{eq}} \equiv [\langle a_i a_j^* \rangle_{\text{eq}}]$. Since we later find that the damping matrix $\boldsymbol{\varphi}(t)$ will give rise to dissipative processes, Eq. 3.33 can be regarded as a generalization of the fluctuation-dissipation theorem Eq. 3.28.

Of what use is this rather formidable mass of definitions? Let us proceed to demonstrate how the generalized Langevin equation can be applied rather easily to study equilibrium time correlations among variables in the set $\mathbf{a}$ or to obtain equations of motion (e.g., transport equations) for the nonequilibrium ensemble averaged components of $\mathbf{a}$.

To calculate equilibrium time correlation functions, one begins by noting that

$$\langle \mathbf{f}(t)\mathbf{a}^* \rangle_{\text{eq}} = 0, \quad t \geq 0$$

(i.e., the random force is “orthogonal” to the dynamical variables $\mathbf{a}$). Therefore by multiplying Eq. 3.31 by $\mathbf{a}^* \cdot \langle \mathbf{a}\mathbf{a}^* \rangle_{\text{eq}}^{-1}$ from the right and averaging, we can derive an equation for the correlation matrix

$$\mathbf{C}(t) \equiv \langle \mathbf{a}(t)\mathbf{a}^* \rangle_{\text{eq}} \cdot \langle \mathbf{a}\mathbf{a}^* \rangle_{\text{eq}}^{-1}$$

which takes the form

$$\frac{d}{dt}\mathbf{C}(t) - i\Omega \cdot \mathbf{C}(t) + \int_0^t d\tau \boldsymbol{\varphi}(\tau) \cdot \mathbf{C}(t-\tau) = 0 \quad (3.35)$$

Hence the generalized Langevin method can be used to obtain an exact

equation of motion for equilibrium-averaged time correlation functions. Such time correlation functions are of major importance in the study of many body systems.¹⁰² In particular, most experimental techniques for investigating the microscopic dynamics of dense systems (e.g., neutron¹⁰³ or light scattering¹⁰⁴) measure such time correlation functions directly. Moreover, the transport coefficients related to the linear response of a system to a perturbation can be expressed in terms of such time correlation functions. As we will see, the generalized Langevin equation for $\mathbf{C}(t)$ greatly facilitates the study of equilibrium-time correlation functions and has become an extremely powerful tool in statistical mechanics.

Suppose we wish instead to follow the traditional Langevin approach and average the generalized Langevin equation (3.31) over a non-equilibrium ensemble $\rho(\Gamma, 0)$ characterizing the initial state of the system in an attempt to arrive at a "transport equation" for the average $\langle \mathbf{a}(t) \rangle \equiv \langle \mathbf{a}(t) \rangle_{\rho(0)}$. Here we have for the moment adopted the customary terminology by referring to closed equations for the average motion $\langle \mathbf{a}(t) \rangle$ as *transport equations*. We can also define *transport coefficients* as the coefficients of the linear terms in $\langle \mathbf{a}(t) \rangle$ in such equations (recognizing that in more general situations, transport equations are nonlinear). Then the average of the generalized Langevin equation yields:

$$\frac{d}{dt} \langle \mathbf{a}(t) \rangle - i\Omega \cdot \langle \mathbf{a}(t) \rangle + \int_0^t d\tau \boldsymbol{\varphi}(\tau) \cdot \langle \mathbf{a}(t-\tau) \rangle = \langle \mathbf{f}(t) \rangle \quad (3.36)$$

At this point, however, we notice one very important difference from the phenomenological Langevin theory. In the classical theory, the average of the random force over an arbitrary ensemble is assumed to vanish, $\langle \mathbf{R}(t) \rangle = 0$. However in the microscopic (and exact) generalized Langevin theory, $\langle \mathbf{f}(t) \rangle$ is not zero in general [although because we have chosen to work with fluctuations $\mathbf{a} = \mathbf{A} - \langle \mathbf{A} \rangle_{\text{eq}}$, $\langle \mathbf{f}(t) \rangle_{\text{eq}} = 0$] hence, strictly speaking, Eq. 3.31 is not a true Langevin equation.

Mori⁹⁴ proposed the following scheme for eliminating the random force term: in any experimental situation, we usually are given only the initial values of the macroscopic or averaged variables, $\langle \mathbf{a}(0) \rangle \equiv \mathbf{a}_0$. Since this does not uniquely determine the initial ensemble $\rho(0)$, Mori suggested that we choose $\rho(0)$ to be the equilibrium ensemble, established subject to constraints that yield the correct initial values $\mathbf{a}_0$. Such a constrained ensemble is given by

$$\rho_0 = Z^{-1} \exp[-\beta(H - \mathbf{a}^* \cdot \mathbf{b})]$$

The conjugate parameters $\mathbf{b}$ are then chosen such that the proper initial

conditions on the averages are satisfied:

$$\langle \mathbf{a}(0) \rangle_0 \equiv \int d\Gamma \rho_0(\Gamma) \mathbf{a}(\Gamma) = \mathbf{a}_0$$

(For $t > 0$, one removes the constraints and allows the system to evolve freely in time, of course.) Now suppose that the initial values $\mathbf{a}_0$ are small; that is, the initial state of the system is close to equilibrium. Then $\mathbf{b}$ must be similarly small; hence we can expand ρ_0 and retain only linear terms

$$\rho_0 \cong \rho_{\text{eq}}(1 + \beta \mathbf{a}^* \cdot \mathbf{b})$$

To this order, Mori then notes that

$$\langle \mathbf{f}(t) \rangle_0 \cong \langle \mathbf{f}(t) \rangle_{\text{eq}} + \beta \langle \mathbf{f}(t) \mathbf{a}^* \rangle_{\text{eq}} \cdot \mathbf{b} = 0$$

Hence in the linear approximation of small initial departures from equilibrium, the average of the random force term vanishes, and we arrive at a linearized (but otherwise exact) transport law

$$\frac{d}{dt} \langle \mathbf{a}(t) \rangle_0 - i\Omega \cdot \langle \mathbf{a}(t) \rangle_0 + \int_0^t d\tau \boldsymbol{\varphi}(\tau) \cdot \langle \mathbf{a}(t-\tau) \rangle_0 = 0 \quad (3.37)$$

3.5.2 □ Choice of Dynamical Variable Sets □ Since Eqs. 3.35 and 3.37 are still exact, hence only formal identities with the equations of motion, one must eventually resort to approximation to obtain useful results. The frequency matrix Ω can usually be calculated explicitly in terms of static quantities. However the damping matrix $\boldsymbol{\varphi}(t)$ requires the study of the “modified” propagator $\exp[it(1-P)L]$ which, in turn, would involve solving the many body problem directly. The attractive feature of equations such as Eq. 3.31, which are generated by projection operator techniques, is that the “damping” or “memory” terms are quite susceptible to approximation or modeling. That is, the generalized Langevin equation is of value primarily because it reexpresses the quantities of interest (e.g., time correlation functions) in forms involving damping terms, which can then be easily approximated.

In Mori’s formalism⁹⁴ the choice of the set of dynamical variables $\mathbf{a}$ was essentially arbitrary. Different choices of $\mathbf{a}$ will lead to different, but exact, descriptions of the system under consideration. However a given approximation of the damping term will yield results that may vary considerably, depending on the choice that is made for $\mathbf{a}$. Usually by increasing the number of components in the set $\mathbf{a}$, the description of the system can be improved within the framework of a given approximation.

We can illustrate this by considering three different levels of sets of dynamical variables.

i *Single particle, space-independent variables.* The simplest level of description could be illustrated by choosing $\mathbf{a}$ to be the velocity characterizing a test particle, say $\mathbf{a} = \mathbf{v}_1$. Then the generalized Langevin equation reduces immediately to Zwanzig's⁹⁵ generalization of the Langevin equation characterizing Brownian motions, Eq. 3.29. To improve on this description, one could go to a multicomponent set in which the a_j are chosen as polynomials in velocity of order j .¹⁰⁵

ii *Microscopic densities.* A second choice of dynamical variable $\mathbf{a}$ utilizes microscopic densities in configuration space that are the analogues to the macroscopic hydrodynamic variables. Examples include mass density, $\rho(\mathbf{x}, t) = \sum_{j=1}^N m \delta(\mathbf{x} - \mathbf{x}_j(t))$, momentum density, and energy density. Akcasu and Daniels¹⁰⁶ have used such sets of dynamical variables to develop an exact generalization of the linearized hydrodynamics equations that involve wavelength- and frequency-dependent transport coefficients. This theory has been quite successful in describing time correlation functions in equilibrium liquids.¹⁰⁶⁻¹⁰⁹

iii *Microscopic phase space densities.* On a more detailed level, one can use the generalized Langevin method to develop a kinetic theory capable of describing fluctuations in the microscopic phase space density¹¹⁰

$$g(\mathbf{x}, \mathbf{v}, t) \equiv \sum_{j=1}^N \delta[\mathbf{x} - \mathbf{x}_j(t)] \delta[\mathbf{v} - \mathbf{v}_j(t)]$$

For convenience, we work with the Fourier transform of such variables in configuration space, for example,

$$g(\mathbf{k}, \mathbf{v}, t) = \sum_{j=1}^N e^{i\mathbf{k} \cdot \mathbf{x}_j(t)} \delta[\mathbf{v} - \mathbf{v}_j(t)]$$

There are essentially two ensemble averages involving $g(\mathbf{k}, \mathbf{v}, t)$ that are of interest in the study of many particle systems. Of course, one such quantity would be the one particle distribution function

$$F_1(\mathbf{k}, \mathbf{v}, t) = \langle g(\mathbf{k}, \mathbf{v}, t) \rangle$$

defined as the average of $g(\mathbf{k}, \mathbf{v}, t)$ over some initial nonequilibrium ensemble $\rho(0)$. Of comparable significance, however, is the time correlation function

$$C(\mathbf{k}, \mathbf{v}, \mathbf{v}', t) \equiv \langle g(\mathbf{k}, \mathbf{v}, t) g^*(\mathbf{k}, \mathbf{v}', 0) \rangle = \sum_{j=1}^N \sum_{i=1}^N e^{i\mathbf{k} \cdot [\mathbf{x}_j(t) - \mathbf{x}_i]} \delta[\mathbf{v} - \mathbf{v}_j(t)] \delta[\mathbf{v}' - \mathbf{v}_i]$$

By taking suitable moments in $\mathbf{v}$, one can easily verify that these two quantities can be used to generate any of the hydrodynamic variables or time correlation functions of interest. For example, the Van Hove density correlation function that arises in the analysis of radiation scattering experiments is given quite simply by

$$G(\mathbf{k}, t) = \int d^3v \int d^3v' C(\mathbf{k}, \mathbf{v}, \mathbf{v}', t)$$

To apply the generalized Langevin method to the calculation of these phase space quantities, we choose $\mathbf{a}(t)$ to be a “vector” whose “components” $a_j = a(\mathbf{v}, t)$ are indexed by a continuous parameter $\mathbf{v}$ and are defined by

$$a(\mathbf{v}, t) \equiv \delta g(\mathbf{k}, \mathbf{v}, t) = \sum_{j=1}^N e^{i\mathbf{k} \cdot \mathbf{x}_j(t)} \delta[\mathbf{v} - \mathbf{v}_j(t)] - n\delta(\mathbf{k})M(\mathbf{v})$$

where it has been noted that $\langle g(\mathbf{k}, \mathbf{v}, t) \rangle_{\text{eq}} = n\delta(\mathbf{k})M(\mathbf{v})$, n being the equilibrium number density, and

$$M(\mathbf{v}) = \left(\frac{m\beta}{2\pi} \right)^{3/2} \exp\left(-\frac{\beta v^2}{2} \right)$$

The extension of the generalized Langevin equation to such a continuous representation is straightforward:

$$\frac{\partial a}{\partial t} - i \int d^3v' \Omega(\mathbf{v}, \mathbf{v}') a(\mathbf{v}', t) + \int_0^t d\tau \int d^3v' \varphi(\mathbf{v}, \mathbf{v}', \tau) a(\mathbf{v}', t - \tau) = f(\mathbf{v}, t) \quad (3.38)$$

Here one can calculate

$$\begin{aligned} i\Omega(\mathbf{v}, \mathbf{v}') &= i\mathbf{k} \cdot \mathbf{v} \delta(\mathbf{v} - \mathbf{v}') - i\mathbf{k} \cdot \mathbf{v} M(\mathbf{v}) n c(k) \\ \varphi(\mathbf{v}, \mathbf{v}', \tau) &= [nM(\mathbf{v}')]^{-1} \langle f^*(\mathbf{v}', 0) e^{i\tau(1-P)L} f(\mathbf{v}, 0) \rangle_{\text{eq}} \\ f(\mathbf{v}, 0) &= \sum_{j=1}^N e^{i\mathbf{k} \cdot \mathbf{x}_j} \frac{\mathbf{F}_j}{m} \cdot \frac{\partial}{\partial \mathbf{v}} \delta(\mathbf{v} - \mathbf{v}_j) + i\mathbf{k} \cdot \mathbf{v} M(\mathbf{v}) n c(k) \sum_{j=1}^N e^{i\mathbf{k} \cdot \mathbf{x}_j} \end{aligned}$$

where $c(k) = h(k)/[1 + nh(k)]$, and $h(k)$ is the Fourier transform of $[g(r) - 1]$, $g(r)$ being the static pair correlation function (presumed to be known).

Hence we can now average Eq. 3.38 over the constrained ensemble $\rho(0)$ to find a kinetic equation for $F_1(\mathbf{k}, \mathbf{v}, t)$:

$$\begin{aligned} \frac{\partial F_1}{\partial t} - i\mathbf{k} \cdot \mathbf{v} F_1 + i\mathbf{k} \cdot \mathbf{v} M(\mathbf{v}) nc(k) \int d^3v' F_1(\mathbf{k}, \mathbf{v}', t) \\ + \int_0^t d\tau \int d^3v' \varphi(\mathbf{v}, \mathbf{v}', \tau) F_1(\mathbf{k}, \mathbf{v}', t - \tau) = \langle f(\mathbf{v}, t) \rangle_{\rho(0)} \end{aligned} \quad (3.39)$$

This is still a perfectly exact equation—hence it must be regarded as only a formal identity with the equations of motion. The complexities of the many body problem now appear in the calculation of the damping kernel $\varphi(\mathbf{v}, \mathbf{v}', t)$ and the “random force” $\langle f(\mathbf{v}, t) \rangle_{\rho(0)}$. In the linear approximation of small departures of the constrained initial ensemble from equilibrium (“linear response theory”), we again note that $\langle f(\mathbf{v}, t) \rangle_{\rho(0)}$ vanishes, leaving us with “only” the calculation of $\varphi(\mathbf{v}, \mathbf{v}', t)$. In the more general case of arbitrary departures from equilibrium, $\langle f(\mathbf{v}, t) \rangle_{\rho(0)}$ will introduce nonlinear terms in $F_1(\mathbf{k}, \mathbf{v}, t)$ into the kinetic equation.

In a similar manner, one can obtain a kinetic equation for $C(\mathbf{k}, \mathbf{v}, \mathbf{v}'', t)$ by multiplying by $\delta g^*(\mathbf{k}, \mathbf{v}'', 0)$ and averaging over the equilibrium ensemble

$$\begin{aligned} \frac{\partial C}{\partial t} - i\mathbf{k} \cdot \mathbf{v} C + i\mathbf{k} \cdot \mathbf{v} M(\mathbf{v}) nc(k) \int d^3v' C(\mathbf{k}, \mathbf{v}', \mathbf{v}'', t) \\ + \int_0^t d\tau \int d^3v' \varphi(\mathbf{v}, \mathbf{v}', \tau) C(\mathbf{k}, \mathbf{v}', \mathbf{v}'', t - \tau) = 0 \end{aligned} \quad (3.40)$$

where we have noted $\langle f(\mathbf{v}, t) \delta g^*(\mathbf{k}, \mathbf{v}'', 0) \rangle_{\text{eq}} = 0$. Hence we find that the time correlation function $C(\mathbf{k}, \mathbf{v}, \mathbf{v}', t)$ obeys a kinetic equation identical to the linearized kinetic equation for the single particle distribution function $F_1(\mathbf{k}, \mathbf{v}, t)$.^{111, 112} It should be stressed, however, that Eq. 3.40 is an *exact* equation for $C(\mathbf{k}, \mathbf{v}, \mathbf{v}', t)$ in which no linearization assumption was necessary. Hence Eq. 3.40 is of only formal significance until we introduce approximations sufficient to obtain an explicit and tractable form for the damping kernel $\varphi(\mathbf{v}, \mathbf{v}', t)$.

It is appropriate to make some general comments about these exact kinetic equations: first notice that these kinetic equations contain the characteristic transport or streaming term

$$-i\mathbf{k} \cdot \mathbf{v} F(\mathbf{k}, \mathbf{v}, t) \rightarrow \mathbf{v} \cdot \nabla F(\mathbf{x}, \mathbf{v}, t)$$

Hence we can regard the remaining terms as characterizing collisions or interactions. If we assume that $nc(k) = \beta V_{\text{eff}}(k)$ is an effective potential, the

term

$$i\mathbf{k} \cdot \mathbf{v} M(\mathbf{v}) n c(k) \int d^3 v' F(\mathbf{k}, \mathbf{v}', t)$$

is just the “self-consistent field” term that appears in the linearized Vlasov equation familiar from plasma physics. The damping term also accounts for interactions among the particles. As we see momentarily, under certain approximations it reduces to either the Boltzmann collision term or the Fokker-Planck collision term. However, in its present exact form, the damping term corresponds to a collision operator that is nonlocal in time (“non-Markovian”) and involves spatial gradients (since the damping kernel is k -dependent).

Let us rewrite the exact kinetic equation characterizing the phase space density–time correlation function (after Laplace transforming in time) in a slightly different form:

$$(s - i\mathbf{k} \cdot \mathbf{v}) C(\mathbf{k}, \mathbf{v}, \mathbf{v}', s) - \int d^3 v'' \Sigma(\mathbf{k}, \mathbf{v}, \mathbf{v}'', s) C(\mathbf{k}, \mathbf{v}'', \mathbf{v}', s) = C(\mathbf{k}, \mathbf{v}, \mathbf{v}', 0)$$

where

$$C(\mathbf{k}, \mathbf{v}, \mathbf{v}', 0) = n \delta(\mathbf{v} - \mathbf{v}') M(\mathbf{v}') + n^2 M(\mathbf{v}) M(\mathbf{v}') h(k)$$

is the initial value of $C(\mathbf{k}, \mathbf{v}, \mathbf{v}', t)$, and

$$\Sigma(\mathbf{k}, \mathbf{v}, \mathbf{v}', s) \equiv \Sigma^{(s)}(\mathbf{k}, \mathbf{v}) + \Sigma^{(c)}(\mathbf{k}, \mathbf{v}, \mathbf{v}', s) = -i\mathbf{k} \cdot \mathbf{v} M(\mathbf{v}) n c(k) - \varphi(\mathbf{k}, \mathbf{v}, \mathbf{v}', s)$$

where $\Sigma^{(s)}$ and $\Sigma^{(c)}$ correspond to the static and dynamic components of the “memory” kernel Σ , respectively. This kinetic equation has been obtained in an independent fashion by a number of investigators (including Akcasu and Duderstadt;¹¹⁰ Lebowitz, Percus, and Sykes;¹¹² Forster and Martin;¹¹³ Mazenko;¹¹⁴ Gross;¹¹⁵ and probably many others), using a variety of approaches.

3.5.3 □ Approximation Schemes □ Of course in the generalized Langevin equation formalism, one has merely succeeded in disguising the complexities of the many body problem by deferring them to the calculation of the frequency matrix Ω and damping matrix $\varphi(t)$. Fortunately, since the frequency matrix involves a static equilibrium correlation function, it can usually be readily calculated in terms of equilibrium quantities. For example, it is frequently possible to use symmetries and identities to simplify Ω . One common approach is to use static information [e.g., the

pair correlation function $g(r)$] from molecular dynamics computer simulations to assist in the calculation of this quantity.

The memory or damping matrix $\varphi(t)$ is a far more complicated beast, since it involves the modified time propagator $\exp[it(1-P)L]$ dynamics. It is at this point that one introduces approximations into the theory. Such approximations usually can be classified as one of several types:

- i Simply set $\varphi(t) = 0$. We will see that this is tantamount to a short time approximation.
- ii If $\varphi(t)$ damps out on a time scale much shorter than $\mathbf{a}(t)$, one can replace the memory term by its Markovian limit:

$$\int_0^t d\tau \varphi(\tau) \cdot \mathbf{a}(t-\tau) \rightarrow \left[\int_0^\infty d\tau \varphi(\tau) \right] \mathbf{a}(t) \equiv \gamma \cdot \mathbf{a}(t)$$

- iii Perturbation theory.
- iv Guessing or modeling the form of $\varphi(t)$.

To illustrate each of these approximation schemes, we consider approximations of the memory or generalized collision kernel $\varphi(\mathbf{v}, \mathbf{v}', t)$ [or $\Sigma^{(c)}(\mathbf{k}, \mathbf{v}, \mathbf{v}', t)$], which appears in the exact kinetic equations (3.39) and (3.40). Since in the linear approximation of small initial departures from equilibrium, the kinetic equations for $F_1(\mathbf{k}, \mathbf{v}, t)$ and $C(\mathbf{k}, \mathbf{v}, \mathbf{v}'', t)$ are identical, we consider only the latter equation (3.40) in this discussion.

i *Vlasovlike approximations.* Of course the crudest approximation would be to simply set $\varphi(\mathbf{v}, \mathbf{v}', \tau) = 0$. Interestingly enough, the resulting approximate kinetic equation

$$\frac{\partial C}{\partial t} - i\mathbf{k} \cdot \mathbf{v} C(\mathbf{k}, \mathbf{v}, \mathbf{v}', t) + i\mathbf{k} \cdot \mathbf{v} M(\mathbf{v}) n c(k) \int d^3 v' C(\mathbf{k}, \mathbf{v}'', \mathbf{v}' t) = 0 \quad (3.41)$$

is just the Vlasovlike equation first derived by Zwanzig¹¹⁶ and later applied to the study of neutron scattering in liquids by Nelkin and Ranganathan.¹¹⁷ If one treats static correlations only to lowest order in the interaction potential $V(r)$, then $c(k) \sim \beta V(k)$, and Eq. 3.41 reduces to the standard linearized Vlasov equation familiar from plasma physics. Such Vlasov descriptions are frequently adequate for plasmas in which the number of particles in a Debye sphere, $n\lambda_D^3 \ll 1$ (a limit we comment on further in a moment). However Eq. 3.41 is capable of describing only the very short time (high frequency) behavior of a liquid or dense gas.

ii *Weak coupling approximations.* A somewhat less trivial approximation is obtained by calculating $\varphi(\mathbf{v}, \mathbf{v}', t)$ to lowest order in the interaction

strength $\lambda = 0(V)$. If one notes that

$$\langle f^*(0) e^{it(1-P)L} f(0) \rangle = \langle f^*(0) e^{itL} f(0) \rangle + O(\lambda^3)$$

where

$$L_0 \equiv -i \sum_{j=1}^N \mathbf{v}_j \cdot \frac{\partial}{\partial \mathbf{x}_j}$$

then a straightforward calculation¹¹⁰ yields the kinetic equation (Laplace transformed with respect to time t) to $O(\lambda^3)$ as

$$\begin{aligned} (s - i\mathbf{k} \cdot \mathbf{v}) C + i\mathbf{k} \cdot \mathbf{v} M(\mathbf{v}) n c(k) \int d^3 v' C(\mathbf{k}, \mathbf{v}', \mathbf{v}'', s) = C(\mathbf{k}, \mathbf{v}, \mathbf{v}'', 0) \\ + n \int d^3 v' \int \frac{d^3 \kappa}{(2\pi)^3} \left[V^2(\kappa) S(k) \kappa \cdot \frac{\partial}{\partial \mathbf{v}} \kappa \cdot \frac{\partial}{\partial \mathbf{v}'} \delta(\mathbf{v} - \mathbf{v}') \right. \\ \left. - V(\mathbf{k} - \kappa) V(\kappa) S(\kappa) \kappa \cdot \frac{\partial}{\partial \mathbf{v}} (\mathbf{k} - \kappa) \frac{\partial}{\partial \mathbf{v}'} \right] \frac{M(\mathbf{v}) C(\mathbf{k}, \mathbf{v}', \mathbf{v}'', s)}{s - i(\mathbf{k} - \kappa) \cdot \mathbf{v} - i\kappa \cdot \mathbf{v}'} \quad (3.42) \end{aligned}$$

This equation is still non-Markovian and in fact is still reversible. It was first derived by Akcasu and Duderstadt¹¹⁰ and has been studied in considerable detail by Forster and Martin,¹¹³ who have also applied it to the calculation of transport coefficients.

If we pass to the Markovian limit in which $\lambda \rightarrow 0, t \rightarrow \infty, \mathbf{x} \rightarrow \infty$ in such a way that $\lambda^2 t$ and $\lambda^2 \mathbf{x}$ remain finite, we find that Eq. 3.42 reduces to the more familiar irreversible form

$$\begin{aligned} \frac{\partial C}{\partial t} - i\mathbf{k} \cdot \mathbf{v} C + i\mathbf{k} \cdot \mathbf{v} M(\mathbf{v}) n c(k) \int d^3 v' C(\mathbf{k}, \mathbf{v}', \mathbf{v}'', t) \\ - \int d^3 v' \int \frac{d^3 \kappa}{(2\pi)^3} n S(\kappa) V^2(\kappa) \kappa \cdot \frac{\partial}{\partial \mathbf{v}} \pi \delta[\kappa \cdot (\mathbf{v} - \mathbf{v}')] \kappa \cdot \left(\frac{\partial}{\partial \mathbf{v}} - \frac{\partial}{\partial \mathbf{v}'} \right) \\ [C(\mathbf{k}, \mathbf{v}', \mathbf{v}'', t) M(\mathbf{v}) + C(\mathbf{k}, \mathbf{v}, \mathbf{v}'', t) M(\mathbf{v}')] = 0 \quad (3.43) \end{aligned}$$

In the absence of initial correlations, $c(k) = 0$ and $S(k) = 1 + nh(k) = 1$. Then Eq. 3.43 reduces to the Fokker-Planck equation derived in standard weak coupling theories of many body systems.¹¹⁸ In this sense, then, Eq. 3.42 can be regarded as a “generalized Fokker-Planck” equation.

iii *Low density approximations.* In a very similar manner, one can expand the propagator in the memory kernel in a power series in system

density and retain only lowest order terms to arrive at a low density kinetic equation that is valid for arbitrary frequency or wavelength. To lowest order, the memory kernel becomes

$$\begin{aligned} \varphi(\mathbf{v}, \mathbf{v}', s) = & n [M(\mathbf{v}')]^{-1} \left(\frac{\beta}{m\pi} \right) \frac{\partial}{\partial \mathbf{v}} \frac{\partial}{\partial \mathbf{v}'} : \int d^3\alpha \int d^3r \int d^3q e^{-\beta(\alpha^2 + q^2)} \\ & \times \left\{ g(r) \frac{dV}{dr} \left[e^{-i\mathbf{k}\cdot\mathbf{r}/2} \delta(\mathbf{v} - \boldsymbol{\alpha} - \mathbf{q}) - e^{i\mathbf{k}\cdot\mathbf{r}/2} \delta(\mathbf{v} - \boldsymbol{\alpha} + \mathbf{q}) \right] \right. \\ & \left. \times [s - i\mathbf{k}\cdot\boldsymbol{\alpha} - iL(\mathbf{q}, \mathbf{r})]^{-1} \frac{dV}{dr} e^{i\mathbf{k}\cdot\mathbf{r}/2} \delta(\mathbf{v} - \boldsymbol{\alpha} - \mathbf{q}) \right\} + O(n^2) \end{aligned}$$

This generalization of the linearized Boltzmann equation, which is correct for all k, ω , was first derived using diagrammatic methods by Mazenko.¹¹⁴ It has since been rederived by Boley¹¹⁹ and Akcasu¹²⁰ using somewhat simpler methods.

iv *General comments on perturbation methods.* Of course it is possible to continue this game of expanding the memory kernel in various perturbation parameters. For example, the natural parameter to use in plasma physics would be the inverse of the number of particles in a Debye sphere, $\epsilon \equiv (n\lambda_d^3)^{-1}$. The resulting kinetic equation would then represent a generalization of the linearized Balescu-Lenard equation to arbitrary k and ω .¹²¹⁻¹²³

To facilitate such expansions, one can apply a useful identity due to Akcasu:¹²⁰

$$\varphi(\mathbf{v}, \mathbf{v}', s) = \varphi_0(\mathbf{v}, \mathbf{v}', s) + \int d^3v'' \varphi(\mathbf{v}, \mathbf{v}'', s) \left[s - i\mathbf{k}\cdot\mathbf{v} - \Sigma^{(s)} \int d^3v'' \right]^{-1} \varphi_0(\mathbf{v}'', \mathbf{v}', s) \quad (3.44)$$

where $\varphi_0(\mathbf{v}, \mathbf{v}', s)$ is identical to $\varphi(\mathbf{v}, \mathbf{v}', s)$ except that the modified propagator $[s - i(1-P)L]^{-1}$ is replaced by the true propagator $[s - iL]^{-1}$. Since perturbation expansions of the true propagator usually are far easier to obtain, one can use this to generate a perturbation expansion for $\varphi_0(\mathbf{v}, \mathbf{v}', s)$, then iterate using Eq. 3.44 to build up a perturbation expansion for $\varphi(\mathbf{v}, \mathbf{v}', s)$.

Mazenko¹²⁴ has dramatically extended this approach to achieve a renormalized kinetic theory of time correlation functions. To facilitate this, he has reexpressed the memory kernel in terms of an effective two-particle interaction

$$\varphi(12)nM(\mathbf{v}_2) = - \int d^3\bar{3} \int d^3\bar{4} \int d^4\bar{4} V(1; 3\bar{3}) G(3\bar{3}; 4\bar{4}) V(4\bar{4}; 2)$$

where $l = (\mathbf{x}_1, \mathbf{v}_1), \dots, V(1; 3\bar{3})$ is an effective interaction potential, and $G(3\bar{3}; 4\bar{4})$ is the time correlation function characterizing a two-particle field. Mazenko has demonstrated that V and G are quite amenable to approximation (e.g., by way of cluster or cumulant expansions). In this way he has derived a renormalized generalized Boltzmann equation (in its linearized form, of course), including not only so-called ring terms (corresponding to recollision events) and mode-mode coupling terms, but additional cross terms as well.

v Modeled kinetic equations In the preceding sections we have demonstrated that the generalized Langevin kinetic equation represents an ideal starting point to apply standard perturbation methods in order to generate approximate kinetic equations. Such calculations are quite straightforward and do not lead to the secular divergences^{125, 126} encountered by perturbation schemes based on the Liouville equation or the BBGKY hierarchy. Furthermore, it is easy to generate higher order correction terms to the more familiar low order equations (Vlasov, Fokker-Planck, or Boltzmann equations).

The integrodifferential equations generated by such perturbation analyses are very appealing from a physicist's point of view because they represent obvious generalizations of well-known equations. However they are quite repugnant mathematically because they have very complicated collision operators. To circumvent these difficulties, we can adopt a somewhat different approach by attempting to guess or model the form of the damping kernel $\varphi(\mathbf{v}, \mathbf{v}', t)$ in a spirit very similar to that used in more traditional kinetic theory models.¹²⁷

One such model assumes that the kernel is a rapidly decaying function of time, and in fact can be modeled by a simple exponential time decay

$$\varphi(\mathbf{v}, \mathbf{v}', t) = \varphi(\mathbf{v}, \mathbf{v}', 0)e^{-\alpha(k)t} \quad (3.45)$$

where the $t=0$ form of the kernel can be calculated exactly, while the relaxation parameter $\alpha(k)$ is chosen to satisfy various constraints demanded by the known long- and short-time behavior of $C(\mathbf{k}, \mathbf{v}, \mathbf{v}', t)$. The model Eq. 3.45 is actually very closely related to the multiple time scale approach of Bogoliubov in that we are assuming that the time correlation functions involving the modified propagator $[s - i(1 - P)L]^{-1}$ decay much more rapidly (on a "microscopic" time scale) than do time correlation functions involving the direct propagator $(s - iL)^{-1}$ (on a "kinetic" time scale). Such assumptions are supported by molecular dynamics computer experiments.¹²⁸⁻¹³⁰ The use of such simple relaxation models of damping functions is rather common in nonequilibrium statistical mechanics¹³¹ and has frequently yielded excellent results.

If we introduce such a model into the Laplace transformed kinetic equation 3.40, we find the modeled kinetic equation¹³²

$$\begin{aligned} (s - i\mathbf{k} \cdot \mathbf{v})C + i\mathbf{k} \cdot \mathbf{v}M(\mathbf{v})nc(k) \int d^3v' C(\mathbf{k}, \mathbf{v}', \mathbf{v}'', s) \\ + \frac{\mathbf{v}M(\mathbf{v})}{s + \alpha(k)} \cdot \mathfrak{D} \cdot \int d^3v' v' C(\mathbf{k}, \mathbf{v}', \mathbf{v}'', s) \\ - \frac{D(0)}{s + \alpha(k)} \left\{ \frac{\partial}{\partial \mathbf{v}} \cdot \frac{\partial}{\partial \mathbf{v}} + \frac{\beta}{m} \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{v} \right\} C(\mathbf{k}, \mathbf{v}, \mathbf{v}'', s) = C(\mathbf{k}, \mathbf{v}, \mathbf{v}'', 0) \end{aligned}$$

where

$$\begin{aligned} \mathfrak{D}(k) &\equiv \frac{\mathbf{k}\mathbf{k}nc(k)}{m^2} - \left(\frac{\beta^2}{m^2} \right) \mathbf{D}(k) \\ D_{ij}(k) &\equiv \frac{n}{\beta} \int d^3R \frac{\partial^2 V}{\partial R_j^2} g(R) \cos kR_3 \delta_{ij} \\ D(0) &\equiv \frac{n}{\beta} \int d^3R \frac{\partial^2 V}{\partial R_j^2} g(R) = \frac{\langle \nabla^2 V \rangle}{3\beta} \end{aligned}$$

Fortunately this equation can be solved exactly for the density- and current-time correlation functions. We can choose the relaxation parameter $\alpha(k)$ by demanding that the $s=0$ behavior of the correlation functions agrees with the $k \rightarrow 0$ limit given by conventional hydrodynamics and the $k \rightarrow \infty$ limit given by free gas behavior. Such a model predicts the behavior observed in scattering and computer simulation experiments quite well. It also happens (and this is the most important feature of the generalized Langevin method) that the model is rather insensitive to the precise form chosen for the relaxation parameter $\alpha(k)$.^{132, 133} Evidently by using this approach, we have managed to extract most of the relevant dynamical information before having to make any modeling approximations.

A variety of alternative models are possible. Akcasu and Linnebur¹³⁴ have developed a two-time relaxation model in which single particle and collective phenomena are characterized by different relaxation parameters. This allows them to extend the model into the region of small k and ω where a hydrodynamic description is more suitable—thereby making possible an analysis of light scattering experiments from gases.

One major shortcoming of the above mentioned models is that they are isothermal in that although they conserve mass and momentum, they do

not conserve energy. Forster and Jhon^{135,136} and Bergeron and Gross¹³⁷ have extended these models by adding a new variable into Mori's phase space description corresponding to the total energy density. The resulting model now conserves energy, therefore provides the correct hydrodynamic behavior at small k and ω . It can be adjusted to conserve as well the first two sum rules, and in this sense it represents an extrapolation model between the exact large k, ω and small k, ω regimes.

The flexibility of the generalized Langevin approach in describing non-equilibrium behavior in many body systems is impressive. The method has been applied to develop kinetic equation descriptions of neutron scattering from liquids (both simple liquids¹⁰⁶ such as argon and more complex liquids such as liquid metals¹³⁵), light scattering from gases¹³⁴ and gas mixtures,¹³⁸ Thomson scattering from partially¹³⁹ and fully ionized¹⁴⁰ plasmas, and the dynamics of dilute polymer solutions.¹⁴¹⁻¹⁴³

3.5.4 □ Limitations of the Generalized Langevin Method □ The generalized Langevin method has proved to be remarkably powerful and flexible in facilitating studies of an enormous variety of interesting physical phenomena. One can apply this method to select out of a many body problem a reduced description of only the macroscopic variables of interest, thereby extracting most of the relevant physics involved in the physical process (e.g., static or equilibrium behavior, conservation laws, sum rules) before resorting to approximation. In this sense, the generalized Langevin equation allows one to extract a priori the known information concerning a process, then to bury one's ignorance (i.e., the full complexities of the many body dynamics) in terms that are relatively insensitive to approximation.

It should be noted, however, that our analysis to this point has been confined to essentially *linear* transport processes. That is, we have applied the generalized Langevin equation to the study of small disturbances in systems close to thermodynamic equilibrium or to the calculation of equilibrium-time correlation functions. Yet we know that many non-equilibrium processes are strongly nonlinear.^{144,145} For example, the study of the effects of nonlinear coupling of fluctuations on linear transport processes and the concomitant renormalization of bare transport coefficients has become a very lively topic in statistical mechanics during recent years.¹⁴⁶ Yet another area of considerable interest involves the calculation of time correlation functions characterizing nonstationary systems (e.g., light scattering from a slowly varying nonequilibrium plasma).

A somewhat more difficult task involves the microscopic derivation of nonlinear transport equations. For example, how would one apply gener-

alized Langevin methods to derive the nonlinear Boltzmann equation as a low density limit? Or on a different level, could we derive the nonlinear hydrodynamics equations in a spirit analogous to that used in deriving the exact generalization of the linearized hydrodynamics equations?

It is of considerable interest to extend the generalized Langevin method to the description of highly nonequilibrium behavior. It should first be noted that the form of the generalized Langevin equation is certainly not unique, and in fact, alternative forms of this equation are more appropriate for the analysis of nonlinear processes. These alternative formulations depend on how one defines the fluctuating force term $\mathbf{f}(t)$. For example, Mori¹⁴⁷ has considered the following alternative forms of the generalized Langevin equation (all of which are formal identities with the microscopic equations of motion of a many body system):

i Original generalized Langevin equation:⁹⁴

$$\frac{d\mathbf{a}}{dt} - i\Omega \cdot \mathbf{a}(t) + \int_0^t d\tau \varphi(\tau) \cdot \mathbf{a}(t - \tau) = \mathbf{f}(t) \quad (3.46)$$

ii Frequency-modulated generalized Langevin equation:¹⁴⁷

$$\frac{d\mathbf{a}}{dt} - i\Omega \cdot \mathbf{a}(t) + \Psi(t) \cdot \mathbf{a}(t) = \mathbf{g}(t) \quad (3.47)$$

iii Nonlinear generalized Langevin equation:¹⁴⁸⁻¹⁵⁰

$$\frac{d\mathbf{a}}{dt} - \mathbf{V}(\mathbf{a}(t)) + \int_0^t d\tau \mathbf{C}[\tau, \mathbf{a}(t - \tau)] = \mathbf{R}(t) \quad (3.48)$$

In each of these equations, the parameters [e.g., $\varphi(t)$, $\Psi(t)$, or $\mathbf{C}$] can be expressed in terms of microscopic quantities (e.g., ensemble averages and modified time propagators).

For example, Mori and Fujisaka¹⁴⁸ have derived the nonlinear generalized Langevin equation 3.48 by choosing the dynamic variable set $\mathbf{a}$ to be the microscopic analogue of the probability density for the values α assumed by a dynamical variable:

$$g(\alpha, t) = \delta[\mathbf{a}(t) - \alpha]$$

(thereby following an earlier theory developed by Zwanzig). A straightforward application of the generalized Langevin method then leads to a microscopic “generalized master equation” for $g(\alpha, t)$. Then by taking the first moment of this equation with respect to α , one arrives at the nonlinear

generalized Langevin equation in the form of Eq. 3.48. A variety of other approaches to deriving such nonlinear Langevin equations have been studied, including mode-mode coupling and Fokker-Planck methods.

In spite of these various approaches, the mathematical complexity of nonlinear Langevin equations presents a major difficulty in extensions of the generalized Langevin method to nonlinear processes.¹⁵¹ In the linear theory, the major effort involves the derivation of the microscopic analogue of the linear Langevin equation—that is, choosing a set of dynamical variables $\{a_i\}$, then calculating the static correlations in Ω and approximating the damping or memory terms $\varphi(t)$. Once the explicit form of the generalized Langevin equation has been obtained, however, it is a simple matter to solve this equation (using standard linear techniques such as integral transforms) to obtain either equilibrium-time correlation functions or the linear behavior of ensemble averages.

In sharp contrast, the microscopic derivation of a generalized nonlinear Langevin equation still leaves one with the rather formidable mathematical task of solving this equation—or using the equation to generate nonlinear transport equations for ensemble averages or time correlation functions. To date most of the effort has involved a restricted study of the linearized transport equations (i.e., renormalized transport equations) that arise from such nonlinear Langevin equations.^{152,153} The more general problem of nonlinear transport remains largely unexplored.

3.5.5 □ Some Concluding Remarks □ It has been our intention in this section to embed the subject of transport theory within the more general framework of classical nonequilibrium statistical mechanics and to describe one of the more recent approaches to the derivation of transport (kinetic) equations for general many body systems. This approach used the generalized Langevin method to derive exact (but formal) kinetic equations for both distribution functions and time correlation functions of phase space variables. By introducing approximations into these exact equations by way of perturbation theory or modeling, one can obtain approximate kinetic equations useful for the analysis of transport processes. Not only can one obtain the more familiar transport equations (Vlasov, Boltzmann, Fokker-Planck) and their corrections, but new kinetic equations more suited to the description of dense, many particle systems, can be derived, as well.

Such techniques can be readily extended to quantum mechanical calculations by introducing the Wigner-equivalent operators analogous to $g(\mathbf{x}, \mathbf{v}, t)$. Further investigation of nonequilibrium behavior is needed for the analysis of highly nonequilibrium systems and nonlinear processes. Of

course these schemes could be used to rederive the more familiar transport equations for neutron diffusion or radiative transfer. However most current work is devoted to the derivation and study of transport equations to describe transport processes for which no adequate kinetic theory presently exists (e.g., dense gases, liquids, plasmas).

What then is the role of the transport theorist in the study of such transport processes? Perhaps a very limited role if he is concerned only with the mathematical analysis of transport equations. As one can readily see, most of the problems to which we have addressed ourselves in this section are formulated as infinite medium initial value problems. Most theories of transport processes in dense systems have yet to progress to the point at which actual boundary value problems are the focus.

A more detailed mathematical analysis of the kinetic equations that have been derived may tend to be frustrating until the validity of such equations has been thoroughly established. Quite a bit of physics remains before the mathematician can be allowed to take over.

However the mathematical knowledge and physical intuition of one who is well versed in more classical transport theory would certainly be useful in the study of these complicated physical and mathematical transport problems. Furthermore, transport theorists should certainly keep abreast of developments in kinetic theory and statistical mechanics, since their talents are definitely needed at various stages of the analysis.

□ PROBLEMS □

3.1 Consider the neutron transport equation under the assumptions of zero absorption ($\Sigma_a = 0$) and zero sources ($s = 0$). Demonstrate that the only equilibrium solution to this equation is the Maxwell-Boltzmann distribution.

3.2 See if you can repeat the “uniqueness” proof of Problem 3.1 for the Boltzmann equation for gases (ignore the force term $F = 0$).

3.3 Suppose that an absorber characterized by $\Sigma_a(v) = \Sigma_a^0/v$ is suddenly inserted uniformly throughout an infinite medium containing a well-established Maxwell-Boltzmann distribution of neutrons. Show that the total density of neutrons in the medium steadily decreases in time, but that the neutron energy distribution, hence the effective neutron temperature, does not change. Then discuss qualitatively the change in the energy distribution you might expect for a non- $1/v$ absorber.

3.4 Solve the infinite medium spectrum equation for the neutron flux resulting from an arbitrary source $S(E)$ using the synthetic kernel model (ignore time dependence).

3.5 The synthetic kernel model can also be used to study the time-dependent thermalization of a neutron pulse injected into a moderator at an energy E_0 . To this end, consider the initial value problem characterizing an infinite medium subject to the initial condition $\phi(E, 0) = \phi_0 \delta(E - E_0)$. Solve this problem for $\phi(E, t)$, assuming the synthetic scattering kernel model and $1/v$ absorption.

3.6 A useful model of electron transport through massive, elastic scatterers is provided by a simple Fokker-Planck equation in angle

$$\mu \frac{\partial n}{\partial x} = \alpha \frac{\partial}{\partial \mu} \left[(1 - \mu^2) \frac{\partial n}{\partial \mu} \right]$$

Obtain a solution of this equation on a slab domain $0 \leq x \leq 1$ with inhomogeneous boundary conditions as an expansion in eigenfunctions of the Sturm-Liouville equation. Demonstrate that far from the boundary, $n(x, \mu) \sim A - 3\alpha\Gamma x + \frac{3}{2}\Gamma\mu$, where A and Γ are constants. (See References 29 and 154 for assistance.)

3.7 Demonstrate that the Fermi-Dirac distribution is the equilibrium solution to the transport equation characterizing electron conduction in solids.

3.8 Verify the forms taken by the radiative transfer variables J_ν , u_ν , u , $\mathbf{q}$, and $\mathbf{P}$ when the field is in black body equilibrium characterized by the Planck distribution function $B_\nu(T)$.

3.9 Determine an expression for the radiant momentum density in terms of I_ν .

3.10 Determine the number of photons in a given volume V for an equilibrium radiant energy field.

3.11 Can the photon transport equation be generalized to describe (i) amplification of light in a lasing medium, (ii) reflection of light by a mirror, (iii) photon transport through a narrow slit (i.e., diffraction), (iv) photon transport through water? If so, how might you construct such generalizations?

3.12 Derive an integral equation for steady-state photon transport in the absence of scattering. To integrate the differential form of the transport equation, introduce the optical depth. Specialize this equation to the case in which the specific intensity is much less than the equilibrium field, $I_\nu \ll B_\nu$.

3.13 Demonstrate that the Vlasov equation is reversible. That is, if $n(\mathbf{r}, \mathbf{v}, t)$ is a solution, demonstrate that $n(\mathbf{r}, -\mathbf{v}, -t)$ is also a solution. Then demonstrate in a similar fashion that the Boltzmann and Fokker-Planck equations are irreversible.

3.14 Prove that in a binary collision process, $d^3v d^3v_1 = d^3v' d^3v'_1$ by calculating the Jacobian of the transformation.

3.15 Demonstrate that the generalized Maxwell-Boltzmann distribution containing an external potential Φ is indeed an equilibrium solution of the Boltzmann equation.

3.16 Verify the H -theorem for the linearized Boltzmann equation (3.20).

3.17 Multiply the Boltzmann equation by each of the collisional invariants m , mv , and $mv^2/2$ and integrate over velocity to obtain the transfer equations characterizing the macroscopic counterparts to these quantities (see Section 4.3 for assistance).

3.18 Demonstrate explicitly that the BGK model satisfies the collisional invariant property $\int d^3v \psi J(n, n) = 0$.

3.19 Consider a homogeneous binary gas and define the H -function for one of the components of the gas by

$$H_A = \int d^3v n_A \ln n_A$$

Demonstrate that this function need not necessarily decay monotonically to equilibrium, and explain this result using physical arguments.

3.20 Provide the details in the derivation of the Fokker-Planck equation (3.23). (Refer to Reference 84 for assistance.)

3.21 Explicitly demonstrate the equivalence between the Landau form (3.24) and Rosenbluth form (Eq. 3.25) of the Fokker-Planck equation.

3.22 Verify the H -theorem for the Fokker-Planck equation in the Landau form (assuming a homogeneous plasma).

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□ 4 □

The Derivation of Continuum Descriptions from Transport Equations

In earlier chapters our primary concern has been with the solution of transport equations using standard methods of mathematical analysis. Unfortunately, it has become apparent that any direct attempt to solve even linear transport equations very rapidly encounters depressingly severe mathematical complexities for all but the simplest modeled problems (e.g., infinite media, one-speed, isotropic scattering). Certainly the more complicated nonlinear transport equations are even further removed from successful mathematical analysis and solution.

Therefore it is not surprising that a very important aspect of transport theory involves the development of far simpler approximate descriptions, which are more amenable to mathematical treatment. Perhaps the most useful class of such approximate descriptions contains those that remove the velocity dependence of the transport equation to replace it with a set of approximate equations for field variables in configuration space $\mathbf{r}$. Examples include the neutron diffusion equation and the equations of hydrodynamics for a gas or liquid. These equations generally replace the particle phase space density $n(\mathbf{r}, \mathbf{v}, t)$ by field variables such as mass density $\rho(\mathbf{r}, t)$ or temperature $T(\mathbf{r}, t)$. Therefore it is customary to refer to such approximate equations as providing a “continuum” description (as opposed to a “particle” description) of the transport process.

Under certain conditions the solution $n(\mathbf{r}, \mathbf{v}, t)$ to a transport equation indeed approaches a form that can be directly related to a continuum or hydrodynamic description. That is, under certain conditions the transport process approaches a hydrodynamic limit. Our objective in this chapter is to determine the precise form of such continuum descriptions and examine their domain of validity by deriving them directly from transport equations.

4.1 □ SOME GENERAL REMARKS □ Let us begin by considering our standard form for transport equations

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial n}{\partial \mathbf{v}} = \left(\frac{\partial n}{\partial t} \right)_{\text{coll}} \quad (4.1)$$

The most common procedure for obtaining continuum or hydrodynamic descriptions begins by deriving equations for the macroscopic analogues of conserved variables

$$\Psi_i(\mathbf{r}, t) \equiv \int d^3v \psi_i(\mathbf{v}) n(\mathbf{r}, \mathbf{v}, t)$$

where ψ_i corresponds to a collisional invariant, that is,

$$\psi_i(\mathbf{v}') + \psi_i(\mathbf{v}_1') = \psi_i(\mathbf{v}) + \psi_i(\mathbf{v}_1)$$

for a collision process from $(\mathbf{v}', \mathbf{v}_1')$ to $(\mathbf{v}, \mathbf{v}_1)$. For “point” particles (i.e., those without structure), the natural collisional invariants correspond to mass, momentum, and kinetic energy, $\psi_i = m, m\mathbf{v}, mv^2/2$. To construct moment or conservation equations for the $\Psi_i(\mathbf{r}, t)$, one merely multiplies the transport equation (4.1) by each ψ_i and integrates over $\mathbf{v}$ to find

$$\int d^3v \psi_i \frac{\partial n}{\partial t} + \int d^3v \psi_i \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} + \int d^3v \psi_i \frac{\mathbf{F}}{m} \cdot \frac{\partial n}{\partial \mathbf{v}} = \int d^3v \psi_i \left(\frac{\partial n}{\partial t} \right)_{\text{coll}} \quad (4.2)$$

We can simplify these equations a bit. First note that for any suitable collision term $(\partial n / \partial t)_{\text{coll}}$

$$\int d^3v \psi_i(\mathbf{v}) \left(\frac{\partial n}{\partial t} \right)_{\text{coll}} = 0$$

(recall our demonstration of this feature for the Boltzmann equation in Section 3.2.2). If, moreover, we assume that $\psi_i(\mathbf{v})$ depends only on $\mathbf{v}$, we can extract the $\partial/\partial t$ and $\partial/\partial \mathbf{r}$ operators to write Eq. 4.2 in a form known as *Maxwell's moments or transfer equation*:¹

$$\frac{\partial \Psi_i}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot N \langle \mathbf{v} \psi_i \rangle - \frac{\mathbf{F}}{m} N \cdot \left\langle \frac{\partial \psi_i}{\partial \mathbf{v}} \right\rangle = 0 \quad (4.3)$$

where we define $\langle \rangle$ by

$$\langle \chi \rangle \equiv \left[\int d^3v \chi(\mathbf{v}) n(\mathbf{v}) \right] \left[\int d^3v n(\mathbf{v}) \right]^{-1} = N^{-1} \int d^3v \chi(\mathbf{v}) n(\mathbf{v})$$

As we might have expected, these conservation equations do not form a closed set for $\Psi_i = N \langle \psi_i \rangle$, but rather they involve higher order moments such as $\langle \mathbf{v} \psi_i \rangle$. To complete or close the set, one must introduce suitable approximations. In a sense, these approximations are very similar in spirit to those used to derive transport equations from the equations of particle

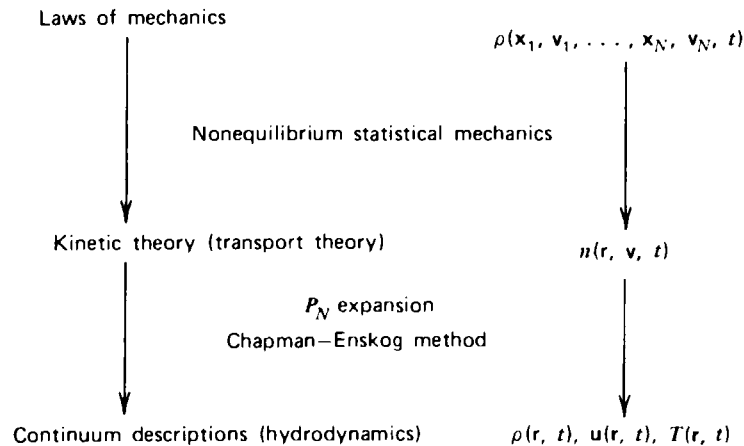


Fig. 4.1 □ Successive “contractions” of the description of a many particle system.

mechanics. One must “contract” the description of the many body system from $n(\mathbf{r}, \mathbf{v}, t)$ to a finite set of velocity moments $\Psi_i(\mathbf{r}, t)$ (see Figure 4.1). We examine how this contracted description can be obtained, both for linear and nonlinear transport processes (i.e., both for self-diffusion and collective motions).

4.2 □ DIFFUSION THEORY □ We begin by studying how a continuum description of self-diffusion processes can be obtained. Since the prototype equation describing such processes is, in fact, just the neutron transport equation

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} + v \Sigma_t n(\mathbf{r}, \mathbf{v}, t) = \int d^3 v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) n(\mathbf{r}, \mathbf{v}', t) + s(\mathbf{r}, \mathbf{v}, t)$$

we use this notation and terminology throughout this section.

4.2.1 □ The One-Speed Diffusion Equation □ To simplify, let us initially restrict our attention to the one-speed transport equation, since it is customary to introduce approximations in the angular dependence separately from those in the energy dependence in neutron or photon transport:

$$\frac{1}{v} \frac{\partial \varphi}{\partial t} + \hat{\Omega} \cdot \nabla \varphi + \Sigma_t \varphi(\mathbf{r}, \hat{\Omega}, t) = \int d\hat{\Omega}' \Sigma_s(\hat{\Omega}' \rightarrow \hat{\Omega}) \varphi(\mathbf{r}, \hat{\Omega}', t) + s(\mathbf{r}, \hat{\Omega}, t) \quad (4.4)$$

Following the procedure outlined in the preceding section, we begin by deriving the appropriate conservation equations from Eq. 4.4 by multiplying it by the various collisional invariants $\psi_i(\hat{\Omega})$, then integrating over $\hat{\Omega}$. However in the self-diffusion process the only conserved quantity is particle mass or number $\psi_i = 1$, and, in fact, even this variable is conserved only in scattering collisions

$$\int d\hat{\Omega} \cdot 1 \cdot \left[\int d\hat{\Omega}' \Sigma_s(\hat{\Omega}' \rightarrow \hat{\Omega}) \varphi(\mathbf{r}, \hat{\Omega}', t) - \Sigma_s \varphi(\mathbf{r}, \hat{\Omega}, t) \right] = 0$$

(absorption processes destroy particles). Hence we find that such self-diffusion processes are characterized by only a single conservation equation. This is obtained by multiplying Eq. 4.4 by $\psi_i = 1$ and integrating to find

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{J} + \Sigma_a \phi(\mathbf{r}, t) = S(\mathbf{r}, t) \quad (4.5)$$

where we recall the definitions:

$$\phi(\mathbf{r}, t) \equiv \int d\hat{\Omega} \varphi(\mathbf{r}, \hat{\Omega}, t), \quad \mathbf{J}(\mathbf{r}, t) \equiv \int d\hat{\Omega} \hat{\Omega} \varphi(\mathbf{r}, \hat{\Omega}, t) \quad (4.6)$$

As expected, we find that the conservation equation (the “particle continuity equation”) contains a higher order moment, $\mathbf{J}(\mathbf{r}, t)$.

Let us continue in this spirit by multiplying Eq. 4.4 by $\hat{\Omega}$ and integrating to find

$$\frac{1}{v} \frac{\partial \mathbf{J}}{\partial t} + \nabla \cdot \int d\hat{\Omega} \hat{\Omega} \hat{\Omega} \varphi(\mathbf{r}, \hat{\Omega}, t) + \Sigma_s \mathbf{J}(\mathbf{r}, t) = \bar{\mu}_0 \Sigma_s \mathbf{J}(\mathbf{r}, t) + \mathbf{S}_1(\mathbf{r}, t) \quad (4.7)$$

Here we have noted that

$$\int d\hat{\Omega} \hat{\Omega} \int d\hat{\Omega}' \Sigma_s(\hat{\Omega}' \rightarrow \hat{\Omega}) \varphi(\mathbf{r}, \hat{\Omega}', t) = \bar{\mu}_0 \Sigma_s \mathbf{J}(\mathbf{r}, t)$$

where $\bar{\mu}_0$ is the average scattering angle cosine defined by

$$\bar{\mu}_0 \equiv \langle \hat{\Omega} \cdot \hat{\Omega}' \rangle = \frac{1}{4\pi \Sigma_s} \int d\hat{\Omega} \int d\hat{\Omega}' \hat{\Omega} \cdot \hat{\Omega}' \Sigma_s(\hat{\Omega}' \rightarrow \hat{\Omega})$$

Thus far we have made no approximations. But then we also have not made any real progress, since the set composed of Eqs. 4.6 and 4.7 represents two equations in three unknowns. To proceed further, we must

introduce an approximation to $\varphi(\mathbf{r}, \hat{\Omega}, t)$ to calculate the moment $\int d\hat{\Omega} \hat{\Omega} \varphi(\mathbf{r}, \hat{\Omega}, t)$.

We introduce this approximation by assuming that the angular flux $\varphi(\mathbf{r}, \hat{\Omega}, t)$ is only weakly dependent on angle. To be more specific, we expand the angular flux in angle as

$$\varphi(\mathbf{r}, \hat{\Omega}, t) \cong \frac{1}{4\pi} \phi(\mathbf{r}, t) + \frac{3}{4\pi} \mathbf{J}(\mathbf{r}, t) \cdot \hat{\Omega} \quad (4.8)$$

and neglect all terms of higher than linear order. Note we have identified the expansion coefficients as ϕ and $\mathbf{J}$, as one can readily verify from the definitions in Eq. 4.6.

We can use this approximate form to evaluate

$$\nabla \cdot \int d\hat{\Omega} \hat{\Omega} \varphi(\mathbf{r}, \hat{\Omega}, t) \cong \frac{\nabla \phi}{3}$$

Hence the set Eqs. 4.5 and 4.7 can now be written as

$$\begin{aligned} \frac{1}{v} \frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{J} + \Sigma_a \phi(\mathbf{r}, t) &= S_0(\mathbf{r}, t) \\ \frac{1}{v} \frac{\partial \mathbf{J}}{\partial t} + \frac{1}{3} \nabla \phi + \Sigma_{tr} \mathbf{J}(\mathbf{r}, t) &= \mathbf{S}_1(\mathbf{r}, t) \end{aligned} \quad (4.9)$$

where we have defined the *transport cross section* $\Sigma_{tr} = \Sigma_t - \bar{\mu}_0 \Sigma_s$. These are known as the P_1 equations, since in one-dimensional geometries, Eq. 4.8 corresponds to expanding in Legendre polynomials in $\mu = \cos \theta$ and retaining only through the P_1 term

$$\varphi(x, \mu, t) = \phi(x, t) \frac{1}{2} P_0(\mu) + J(x, t) \frac{3}{2} P_1(\mu)$$

(We consider higher order P_N approximations in the next section.)

In principle we could now use the P_1 equations to describe the distribution of particles. To simplify these equations, however, it is customary to introduce two further approximations. First we assume that the neutron source term $s(\mathbf{r}, \hat{\Omega}, t)$ is isotropic. This implies, of course, that the source term $\mathbf{S}_1(\mathbf{r}, t)$ vanishes in the equation for the current density. As we mentioned earlier, this approximation is usually of reasonable validity in many applications (e.g., nuclear reactor analysis).

As our second approximation we assume that we can neglect the time derivative $v^{-1} \partial \mathbf{J} / \partial t$ in comparison with the remaining terms in Eq. 4.9.

This would imply, for example, that

$$\frac{1}{|\mathbf{J}|} \frac{\partial}{\partial t} |\mathbf{J}| \ll v\Sigma,$$

that is, that the rate of time variation of the current density is much slower than the collision frequency $v\Sigma_i$. Since $v\Sigma_i$ is typically of order 10^5 sec^{-1} or larger, only an extremely rapid time variation of the current would invalidate this assumption. These approximations allow us to rewrite Eq. 4.9 as

$$\frac{1}{3} \nabla \phi(\mathbf{r}, t) + \Sigma_{tr}(\mathbf{r}) \mathbf{J}(\mathbf{r}, t) = 0$$

We can solve this equation for the current density in terms of the flux

$$\mathbf{J}(\mathbf{r}, t) = - \frac{1}{3\Sigma_{tr}(\mathbf{r})} \nabla \phi(\mathbf{r}, t) \quad (4.10)$$

If we define the diffusion coefficient D by

$$D(\mathbf{r}) = [3\Sigma_{tr}(\mathbf{r})]^{-1} = [3(\Sigma_t - \bar{\mu}_0 \Sigma_s)]^{-1} = \lambda_{tr}^{-1}$$

then we can rewrite Eq. 4.10 as

$$\mathbf{J}(\mathbf{r}, t) = -D(\mathbf{r}) \nabla \phi(\mathbf{r}, t) \quad (4.11)$$

Hence we have found that in certain situations the current density is proportional to the spatial gradient of the flux. This very important relation arises quite frequently in other areas of physics, where it is known as Fick's law.² It is also occasionally referred to as the *diffusion approximation*.

Before we consider the physical implications of this relationship, let us use it to simplify the P_1 equations. If we substitute this into Eq. 4.9 we find

$$\frac{1}{v} \frac{\partial \phi}{\partial t} - \nabla \cdot D(\mathbf{r}) \nabla \phi + \Sigma_a(\mathbf{r}) \phi(\mathbf{r}, t) = S(\mathbf{r}, t) \quad (4.12)$$

This very important result is known as the *one-speed diffusion equation*. It is perhaps the simplest description of particle transport processes.³

We can use the initial and boundary conditions for the transport equation (cf. Section 1.2) to develop comparable conditions for the diffusion equation (4.12). By integrating the transport initial condition over angle, we find we must specify the initial value $\phi(\mathbf{r}, 0)$ throughout the

region of interest. Boundary conditions are a bit harder to come by, since diffusion theory can only approximate the actual transport boundary conditions. Consider, for example, the interface boundary condition that demands that the angular flux $\varphi(\mathbf{r}, \hat{\Omega}, t)$ be continuous across the interface. Since diffusion theory describes only the first two moments of the angular flux, we can demand at most continuity of flux $\phi(\mathbf{r}, t)$ and current density $\mathbf{J}(\mathbf{r}, t)$ across the interface (and can say nothing about continuity of higher order moments).

The free surface boundary condition $\varphi(\mathbf{R}_s, \hat{\Omega}, t) = 0$ for $\hat{\Omega} \cdot \hat{\mathbf{e}}_s < 0$ is even more difficult to approximate. One approach would be to require the inwardly directed partial current density $J_-(\mathbf{r}, t)$ to vanish on the surface. However diffusion theory yields only an approximate description of this quantity and therefore of the corresponding boundary condition

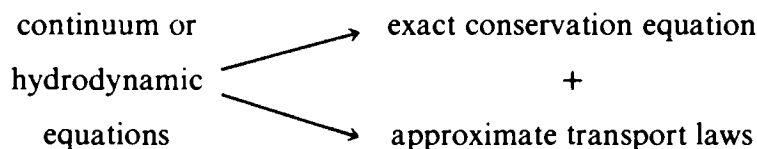
$$J_-(x_s) \cong \frac{\phi(x_s)}{4} + \frac{D}{2} \left. \frac{d\phi}{dx} \right|_{x_s} = 0 \quad (4.13)$$

(written here in one dimension for convenience). A popular alternative to this boundary condition is obtained by recognizing that if we extrapolated the flux described by Eq. 4.13 linearly beyond the boundary, it would vanish at a point $2D = 2\lambda_{tr}/3$ outside this boundary. Therefore the free surface boundary condition $J_-(x_s) = 0$ is commonly replaced by the simpler condition $\phi(\tilde{x}_s) = 0$, where $\tilde{x}_s$ represents the "extrapolated" boundary that has been extended by the extrapolation length $z_0 = 2\lambda_{tr}/3$. We noted in Chapter 2 that the transport theory solution to the Milne problem indicated that a more accurate expression for the extrapolation length is given by $z_0 = 0.7104\lambda_{tr}$.

It should be stressed here that the true flux does not vanish outside the boundary. Furthermore, the diffusion theory flux is a poor representation of the true flux near the boundary. Rather, the extrapolated boundary conditions are intended to yield the proper flux only in the interior of the region of interest several mean free paths away from the surface.

To summarize then, we can see that the derivation of the diffusion equation involves essentially three steps: (i) the derivation of conservation equations by taking moments of the transport equation using the collisional invariants; (ii) closing this set by approximating the form of the angular flux, which appears in the higher order moments (e.g., moments that do not correspond to collisional invariants); (iii) ignoring time derivatives that appear in any higher order moment equations that do not correspond to conservation equations. Such a procedure results in an expression for the current density in terms of gradients of the conserved variable (e.g., $\mathbf{J} = -D \nabla \phi$). Such approximate relations are known as

transport laws, and the proportionality constant D is known as a *transport coefficient*. Such relations play a very important role in any continuum description. Indeed we will find that such continuum descriptions can always be decomposed into *exact* conservation equations augmented by *approximate* transport laws:



From a more general point of view, we can see from Eq. 4.3 that the higher order moments are generated by the streaming term $\mathbf{v} \cdot \nabla$ in the transport equation and appear in the conservation equations as

$$\nabla \cdot \int d^3v \mathbf{v} \psi_i n(\mathbf{r}, \mathbf{v}, t)$$

—that is, as the divergence of a current or flux corresponding to the collisional invariant (i.e., to the macroscopic analogue of the flux $\mathbf{v} \psi_i n$). And since all approximations to the distribution function $n(\mathbf{r}, \mathbf{v}, t)$ involve a series of functions of $\mathbf{v}$ (or $\hat{\Omega}$) in which the coefficients are expressed as derivatives of the moments $\Psi_i = \int d^3v \psi_i n$, the transport laws in general are found to take the form

$$\int d^3v \mathbf{v} \psi_i n \cong - \sum_j \alpha_{ij} \nabla \psi_j$$

where α_{ij} are the corresponding transport coefficients. These ideas will become more apparent as we provide still further examples.

Before proceeding to examine higher order approximations, it is useful to mention an alternative approach that has become quite popular in radiative transfer problems, namely, the variable Eddington factor approximation.^{4,5} Return for a moment to the equations that result from taking the first two angular moments of the transport equation (4.4), rewritten here for one-dimensional geometry with isotropic sources and scattering for convenience:

$$\begin{aligned} \frac{1}{v} \frac{\partial \phi}{\partial t} + \frac{\partial J}{\partial x} + \Sigma_a \phi &= S_0 \\ \frac{1}{v} \frac{\partial J}{\partial t} + \frac{\partial \Pi}{\partial x} + \Sigma_r J &= 0 \end{aligned}$$

Here we have denoted the second moment by $\Pi(x, t)$:

$$\Pi(x, t) \equiv \int_{-1}^{+1} d\mu \mu^2 \varphi(x, \mu, t) \quad (4.14)$$

The key idea is now to postulate that $\Pi(x, t)$ can be reexpressed in terms of $\phi(x, t)$ as

$$\Pi(x, t) = f(x, t) \phi(x, t) \quad (4.15)$$

where $f(x, t)$ is known as the *variable Eddington factor*. Of course we could formally write (from Eq. 4.14)

$$f(x, t) = \left[\int_{-1}^{+1} d\mu \mu^2 \varphi(x, \mu, t) \right] \left[\int_{-1}^{+1} d\mu \varphi(x, \mu, t) \right]^{-1} \equiv \langle \mu^2 \rangle$$

But since $\varphi(x, \mu, t)$ is unknown, we must guess some suitable form for the Eddington factor $f(x, t)$ to implement this postulate. Two limiting cases immediately suggest themselves. If we take $f(x, t) = \frac{1}{3}$, we find just the diffusion approximation. By way of contrast, a choice of $f(x, t) = 1$ yields the moment equations characterizing particle streaming in the forward direction. Hence by an appropriate choice of $\frac{1}{3} \leq f(x, t) \leq 1$, the variable Eddington approximation is capable of modeling both diffusive and streaming behavior. A variety of schemes for estimating $f(x, t)$ have been utilized in radiative transfer problems, particularly in the context of numerical methods suitable for implementation in coupled radiation transport hydrodynamics computer codes.⁵

4.2.2 □ The P_N Equations □

One-Dimensional Form □ A very common scheme for developing higher order corrections to the diffusion equation involves expanding the angular dependence of the flux in spherical harmonics $Y_{lm}(\hat{\Omega})$.⁶⁻⁸ To illustrate this scheme, it is simplest to consider the one-dimensional, one-speed, time-independent transport equation:

$$\mu \frac{\partial \varphi}{\partial x} + \Sigma_t \varphi(x, \mu) = \Sigma_s \int_0^{2\pi} d\phi' \int_{-1}^{+1} d\mu' f(\hat{\Omega}' \cdot \hat{\Omega}) \varphi(x, \mu') + s(x, \mu) \quad (4.16)$$

where $f(\hat{\Omega}' \cdot \hat{\Omega})$ is the scattering probability function. If we denote the cosine of the scattering angle by $\mu_0 \equiv \hat{\Omega}' \cdot \hat{\Omega}$, we can expand the scattering

probability in Legendre polynomials as

$$f(\hat{\Omega}' \cdot \hat{\Omega}) = \sum_{l=0}^L \left(\frac{2l+1}{4\pi} \right) b_l P_l(\mu_0)$$

where

$$b_l = 2\pi \int_{-1}^{+1} d\mu_0 f(\mu_0) P_l(\mu_0)$$

Note here that $b_0 = 1, b_1 = \overline{\mu_0}$. We have also noted that in general only a Legendre representation of finite order L will be required to adequately describe $f(\hat{\Omega}' \cdot \hat{\Omega})$. (Indeed, $f(\hat{\Omega}' \cdot \hat{\Omega})$ is only given for several values of l in a nuclear data set such as ENDF/B.)

Next we use the addition theorem^{9,10} to write $P_l(\mu_0)$ in terms of the spherical harmonics functions $Y_{lm}(\hat{\Omega})$ as

$$P_l(\hat{\Omega}' \cdot \hat{\Omega}) = \sum_{m=-l}^l \left(\frac{4\pi}{2l+1} \right) Y_{lm}^*(\hat{\Omega}') Y_{lm}(\hat{\Omega}) \quad (4.17)$$

Here we should note that the spherical harmonics functions $Y_{lm}(\hat{\Omega})$ can be defined in terms of the associated Legendre polynomials $P_l^m(\mu)$ as

$$Y_{lm}(\hat{\Omega}) = Y_{lm}(\theta, \phi) = \left[\left(\frac{2l+1}{4\pi} \right) \frac{(l-|m|)!}{(l+|m|)!} \right]^{1/2} P_l^m(\cos\theta) e^{im\phi}$$

Of particular importance are the orthogonality and normalization properties of these functions

$$\int d\hat{\Omega} Y_{l'm'}^*(\hat{\Omega}) Y_{lm}(\hat{\Omega}) = \delta_{ll'} \delta_{mm'}$$

If we substitute the expansion (4.17) into the transport equation, we find that the scattering term simplifies to

$$\int_0^{2\pi} d\phi' \int_{-1}^{+1} d\mu' f(\hat{\Omega}' \cdot \hat{\Omega}) \varphi(x, \mu') = \sum_{l=0}^L \frac{1}{2} \int_{-1}^{+1} d\mu' P_l(\mu') P_l(\mu) (2l+1) b_l \varphi(x, \mu')$$

Therefore the transport equation (4.16) can be written as follows:

$$\mu \frac{\partial \varphi}{\partial x} + \Sigma_s \varphi = \frac{\Sigma_s}{2} \sum_{l=0}^L (2l+1) b_l P_l(\mu) \int_{-1}^{+1} d\mu' P_l(\mu') \varphi(x, \mu') + s(x, \mu) \quad (4.18)$$

The essence of the P_N method consists of expanding the angular flux in a complete set of Legendre polynomials

$$\varphi(x, \mu) = \sum_{l=0}^{\infty} \left(\frac{2l+1}{4\pi} \right) \varphi_l(x) P_l(\mu)$$

A similar expansion is used to represent the source term

$$s(x, \mu) = \sum_{l=0}^{\infty} \left(\frac{2l+1}{4\pi} \right) s_l(x) P_l(\mu)$$

where we can use orthogonality

$$\int_{-1}^{+1} d\mu P_l(\mu) P_{l'}(\mu) = \frac{2}{2l+1} \delta_{ll'}$$

to find

$$s_l(x) = 2\pi \int_{-1}^{+1} d\mu s(x, \mu) P_l(\mu)$$

If we substitute these expansions into the transport equation (4.18), multiply by $P_{l'}(\mu)$, integrate over μ , and use orthogonality and the identity⁹

$$(l+1)P_{l+1} + lP_{l-1} = (2l+1)\mu P_l$$

we arrive at an infinite set of coupled ordinary differential equations for the expansion coefficients $\varphi_l(x)$:

$$\left(\frac{l+1}{2l+1} \right) \frac{d\varphi_{l+1}}{dx} + \left(\frac{l}{2l+1} \right) \frac{d\varphi_{l-1}}{dx} + (\Sigma_t - \Sigma_s b_l) \varphi_l(x) = s_l(x), \quad l=0, 1, \dots$$

This infinite set of equations is equivalent in informational content to the transport equation itself; but the set is of formal interest only until an approximation is introduced to truncate the set to a more manageable size. The most common truncation scheme is known as the P_N approximation and consists of demanding that

$$\frac{d\varphi_l}{dx} \equiv 0, \quad l > N$$

This yields a finite set of $N+1$ equations for the $N+1$ unknowns

$\varphi_0, \varphi_1, \dots, \varphi_N$ known as the P_N equations:

$$\left(\frac{l+1}{2l+1}\right) \frac{d\varphi_{l+1}}{dx} + \left(\frac{l}{2l+1}\right) \frac{d\varphi_{l-1}}{dx} + (\Sigma_t - \Sigma_s b_l) \varphi_l(x) = s_l(x),$$

$$l=0, 1, \dots, N \quad (4.19)$$

In some sense, then, as we make the set larger and larger, the representation of the angular flux as an expansion in a truncated set of Legendre polynomials converges more closely to the exact solution of the transport equation

$$\varphi_{\text{approx}}(x, \mu) \equiv \sum_{l=0}^N \left(\frac{2l+1}{4\pi}\right) \varphi_l(x) P_l(\mu) \xrightarrow{N \rightarrow \infty} \varphi_{\text{exact}}(x, \mu) \quad (4.20)$$

It should be noted that this truncation scheme is not unique.⁷ One could just as well have demanded

$$\varphi_l \equiv 0, \quad l > N$$

The latter approximation can be motivated by the recognition that since $P_l(\mu)$ oscillates more and more for large l , then presumably

$$\varphi_{N+1}(x) = 2\pi \int_{-1}^{+1} d\mu \varphi(x, \mu) P_{N+1}(\mu) \rightarrow 0$$

for sufficiently large N . This implies a finite Legendre polynomial representation of the angular flux such as that given by Eq. 4.20.

To make this more explicit, let us consider the form taken by the P_1 equations:

$$\frac{d\varphi_1}{dx} + (\Sigma_t - \Sigma_s) \varphi_0 = s_0$$

$$\frac{1}{3} \frac{d\varphi_0}{dx} + (\Sigma_t - \bar{\mu}_0 \Sigma_s) \varphi_1 = s_1$$

If we let $\varphi_0 = \phi$, $\varphi_1 = J$, and furthermore assume isotropic sources such that $s_1 = 0$, we find that the P_1 equations reduce to just the diffusion equation:

$$-\frac{d}{dx} \left(\frac{1}{3\Sigma_{tr}} \frac{d\phi}{dx} \right) + \Sigma_a \phi = S_0$$

It is useful to examine the structure of the solution to the more general P_N equations. To this end we seek elementary solutions of the form

$$\varphi_l(x) = a_l e^{-\kappa x}$$

Then if we substitute this form into the P_N equations (4.19), we find that the characteristic determinant for κ is given by

$$\begin{vmatrix} (1-c)\Sigma_l & \kappa & 0 & 0 & \dots \\ \kappa & 3\Sigma_l & 2\kappa & 0 & \dots \\ 0 & 2\kappa & 5\Sigma_l & 3\kappa & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{vmatrix} = 0$$

One can demonstrate^{7,8} that for the P_N approximation with N odd, there will be $N+1$ roots $\pm \kappa_j$, corresponding to a solution

$$\varphi_l(x) = \sum_{j=0}^N A_j a_l^j e^{-\kappa_j x}$$

In particular, one finds that the number of roots does not increase in going from odd to even order expansions. Furthermore, even order P_N expansions have been found to lead to boundary condition problems as well. Hence it is customary to implement only odd order expansions (i.e., P_1 , P_3 , P_5 , etc.).

It is of interest to compare the structure of the solution for the total flux, $\phi(x) = \varphi_0(x)$, given by the P_N equations (say, for a plane source at the origin of an infinite medium):

$$\phi(x) = \sum_{j=0}^{N/2} A_j a_0^j e^{-\kappa_j x}, \quad x > 0$$

with the exact transport theory expression for the flux (cf. Section 2.2.4)

$$\phi(x) = a_0 e^{-\kappa_0 x} + \int_{\Sigma_l}^{\infty} d\kappa A(\kappa) e^{-\kappa x}$$

In particular, we can identify the $j=0$ term as the asymptotic or diffusion theory portion of the solution:

$$a_0^0 e^{-\kappa_0 x} \rightarrow a_0 e^{-\kappa_0 x} \sim a_0 e^{-x/L}$$

while the remaining terms $j > 1$ can be identified as the transient terms

$$\sum_{j=1}^{N/2} A_j a_0^j e^{-\kappa_j x} \rightarrow \int_{\Sigma_l}^{\infty} d\kappa A(\kappa) e^{-\kappa x}$$

From a more mathematical perspective, it is apparent that in implementing the P_N approximation, we have represented the continuous spectrum of the transport equation by a discrete set of point eigenvalues (see Figure 4.2).

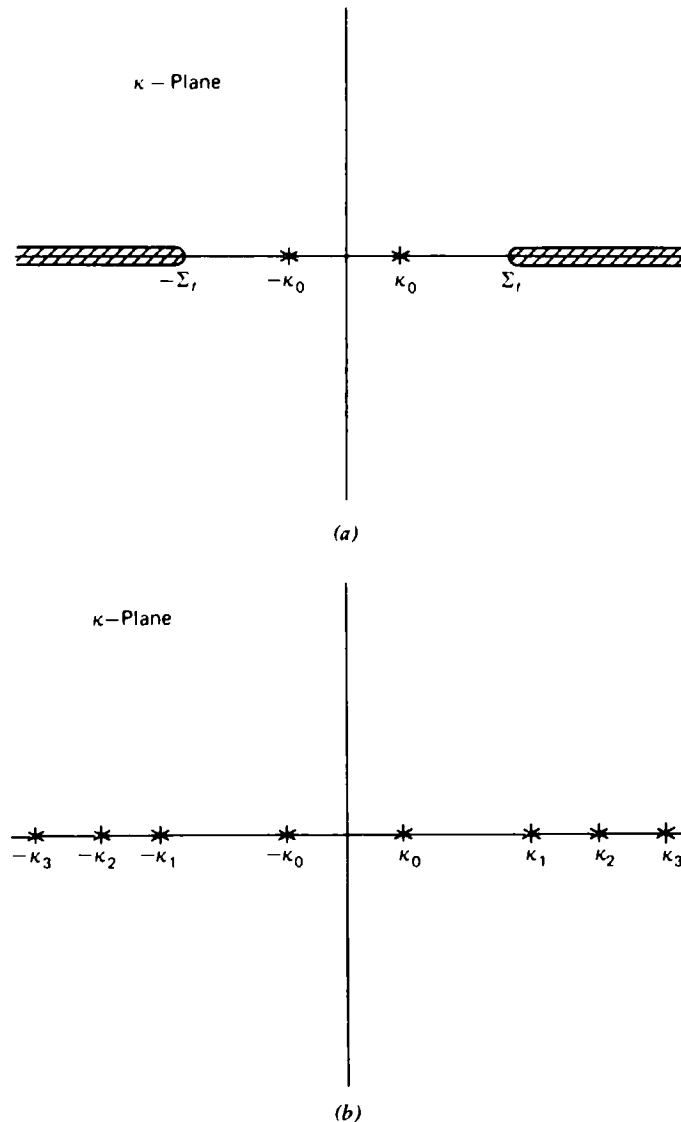


Fig. 4.2 □ Comparison of the eigenvalue spectra of (a) the transport equation and (b) the P_N equations.

This feature is quite characteristic of continuum descriptions of particle transport such as the P_N equations (or the hydrodynamics equations generated by the Chapman-Enskog method).

Boundary Conditions □ We can develop the boundary conditions for the P_N equations directly from the boundary conditions for the transport equation:

i *Boundary conditions at infinity:*

$$\lim_{|x| \rightarrow \infty} \varphi(x, \mu) = 0 \Rightarrow \lim_{|x| \rightarrow \infty} \varphi_l(x) = \lim_{|x| \rightarrow \infty} 2\pi \int_{-1}^{+1} d\mu \varphi(x, \mu) P_l(\mu) = 0$$

ii *Interface boundary conditions:*

$$\varphi_I(x_s, \mu) = \varphi_{II}(x_s, \mu) \Rightarrow 2\pi \int_{-1}^{+1} d\mu \varphi_I(x_s, \mu) P_l(\mu) = 2\pi \int_{-1}^{+1} d\mu \varphi_{II}(x_s, \mu) P_l(\mu)$$

or

$$\varphi_{II}(x_s) = \varphi_{II}(x_s)$$

iii *Vacuum (or free surface) boundary conditions.* To be specific, consider a slab geometry (see Figure 4.3) for which the transport boundary conditions are

$$\varphi(0, \mu) = 0, \quad 0 \leq \mu \leq 1; \quad \varphi(a, \mu) = 0, \quad -1 \leq \mu \leq 0$$

Now recall that since we have represented the angular flux in the P_N approximation as

$$\varphi(x, \mu) = \sum_{l=0}^N \left(\frac{2l+1}{4\pi} \right) \varphi_l(x) P_l(\mu)$$

where

$$\varphi_l(x) = \sum_{j=0}^N A_j a_j^l e^{-\kappa_j x}$$

we must determine $N+1$ boundary conditions to evaluate the $N+1$ parameters A_j —that is, $(N+1)/2$ boundary conditions on each side of the slab. But here we have a problem, since the transport boundary conditions are given over only half of the angular range. This introduces a degree of

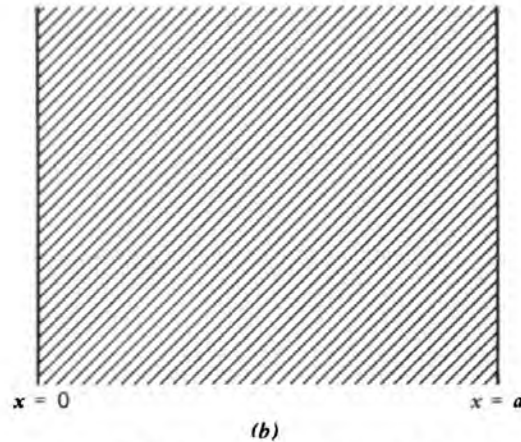
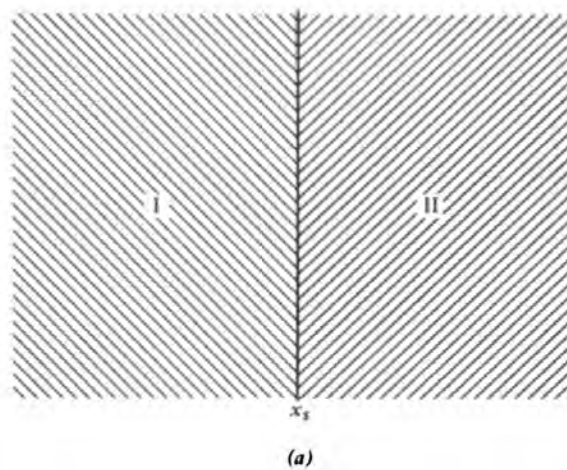


Fig. 4.3 □ (a) Interface and (b) slab boundaries.

arbitrariness into our choice of boundary conditions for the P_N equations. One possibility (known as the Marshak¹¹ boundary conditions) would be to choose

$$\begin{aligned} \int_0^1 d\mu \varphi(0, \mu) P_l(\mu) &= 0 \\ \int_{-1}^0 d\mu \varphi(a, \mu) P_l(\mu) &= 0 \end{aligned} \quad \text{for } l = 1, 3, \dots, N \text{ odd}$$

In particular, for the P_1 approximation, these conditions become

$$\int_0^1 d\mu \varphi(0, \mu) P_1(\mu) = J_+(0) = 0; \quad \int_{-1}^0 d\mu \varphi(a, \mu) P_1(\mu) = J_-(a) = 0$$

which are consistent with the zero reentrant partial current density boundary conditions commonly employed in diffusion theory.

An alternative choice known as the Mark¹² boundary conditions sets

$$\varphi(0, \mu_i) = \varphi(a, -\mu_i) = 0, \quad i = 1, 2, \dots, \frac{N+1}{2}$$

where the μ_i are the positive zeros of $P_{N+1}(\mu)$. One can show that the Mark boundary conditions are equivalent to replacing the vacuum by a purely absorbing medium. They also allow one to directly relate the P_N equations to the discrete ordinate or S_N equations as we demonstrate in Chapter 8.

General Form of the P_N Equations □ We can generalize the P_N equations further to include energy, time, and full three-dimensional spatial dependence by starting with the general form of the transport equation:

$$\frac{1}{v} \frac{\partial \varphi}{\partial t} + \hat{\Omega} \cdot \nabla \varphi + \Sigma_t \varphi = \int_0^\infty dE' \int d\hat{\Omega}' \Sigma_s(E' \rightarrow E, \hat{\Omega}' \cdot \hat{\Omega}) \varphi(\mathbf{r}, E', \hat{\Omega}', t) + s \quad (4.21)$$

and expanding the angular flux in spherical harmonics:

$$\varphi(\mathbf{r}, E, \hat{\Omega}, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^l \left(\frac{2l+1}{4\pi} \right)^{1/2} \varphi_{lm}(\mathbf{r}, E, t) Y_{lm}(\hat{\Omega}) \quad (4.22)$$

In a similar fashion we expand the scattering kernel in Legendre polynomials and use the addition theorem to write

$$\begin{aligned} \Sigma_s(E' \rightarrow E, \hat{\Omega}' \cdot \hat{\Omega}) &= \sum_{l=0}^L \left(\frac{2l+1}{4\pi} \right) \Sigma_l(E' \rightarrow E) P_l(\hat{\Omega}' \cdot \hat{\Omega}) \\ &= \sum_{l=0}^L \sum_{m=-l}^l \Sigma_l(E' \rightarrow E) Y_{lm}^*(\hat{\Omega}') Y_{lm}(\hat{\Omega}) \end{aligned}$$

If we substitute this expansion into the collision term, we find that it simplifies considerably to

$$\begin{aligned} \int_0^\infty dE' \int d\hat{\Omega}' \Sigma_s(E' \rightarrow E, \hat{\Omega}' \cdot \hat{\Omega}) \varphi(\mathbf{r}, E', \hat{\Omega}', t) \\ = \sum_{l=0}^L \sum_{m=-l}^l Y_{lm}(\hat{\Omega}) \int_0^\infty dE' \Sigma_l(E' \rightarrow E) \varphi_{lm}(\mathbf{r}, E', t) \end{aligned}$$

Thus when we substitute the spherical harmonic expansion Eq. 4.22 of the angular flux into the transport equation 4.21, we find

$$\sum_{l,m} \left\{ \frac{1}{v} \frac{\partial \varphi_{lm}}{\partial t} + \hat{\Omega} \cdot \nabla \varphi_{lm} + \Sigma_l \varphi_{lm} - \int_0^\infty dE' \Sigma_l(E' \rightarrow E) \varphi_{lm}(\mathbf{r}, E', t) - s_{lm} \right\} Y_{lm}(\hat{\Omega}) = 0$$

In the usual manner, we can now multiply by $Y_{l'm'}^*(\hat{\Omega})$, integrate over $\hat{\Omega}$, and implement orthogonality and recursion relations to find the general form of the P_N equations. Unfortunately, the streaming term contributes the matrix elements

$$\int d\hat{\Omega} Y_{l'm'}^*(\hat{\Omega}) \hat{\Omega} Y_{lm}(\hat{\Omega})$$

which are quite complicated; therefore the general form of the P_N equations is rather ugly:¹³

$$\begin{aligned} & \frac{1}{v} \frac{\partial \varphi_{lm}}{\partial t} + \left[\frac{(l+2+m)(l+1+m)}{(2l+3)^2} \right]^{1/2} \left[-\frac{1}{2} \frac{\partial \varphi_{l+1,m+1}}{\partial x} - \frac{i}{2} \frac{\partial \varphi_{l+1,m+1}}{\partial y} \right] \\ & + \left[\frac{(l+1-m)(l+2-m)}{(2l+3)^2} \right]^{1/2} \left[\frac{1}{2} \frac{\partial \varphi_{l+1,m-1}}{\partial x} - \frac{i}{2} \frac{\partial \varphi_{l+1,m-1}}{\partial y} \right] \\ & + \left[\frac{(l-m-1)(l-m)}{(2l+1)^2} \right]^{1/2} \left[\frac{1}{2} \frac{\partial \varphi_{l-1,m+1}}{\partial x} + \frac{i}{2} \frac{\partial \varphi_{l-1,m+1}}{\partial y} \right] \\ & + \left[\frac{(l+m)(l+m-1)}{(2l-1)^2} \right]^{1/2} \left[-\frac{1}{2} \frac{\partial \varphi_{l-1,m-1}}{\partial x} + \frac{i}{2} \frac{\partial \varphi_{l-1,m-1}}{\partial y} \right] \\ & + \left[\frac{(l+1+m)(l+1-m)}{(2l+3)^2} \right]^{1/2} \frac{\partial \varphi_{l+1,m}}{\partial z} \\ & + \left[\frac{(l+m)(l-m)}{(2l-1)^2} \right]^{1/2} \frac{\partial \varphi_{l-1,m}}{\partial z} \\ & + \Sigma_l \varphi_{lm} = \int_0^\infty dE' \Sigma_l(E' \rightarrow E) \varphi_{lm}(\mathbf{r}, E', t) + s_{lm} \end{aligned} \quad (4.23)$$

The only simple example of the structure taken by this set of equations occurs for the lowest order, the P_1 equations. Then if we identify

$$\Omega_x = \left(\frac{2\pi}{3}\right)^{1/2} (Y_{1,-1}^* - Y_{11}), \quad \Omega_y = -i \left(\frac{2\pi}{3}\right)^{1/2} (Y_{1,-1}^* + Y_{11})$$

$$\Omega_z = \left(\frac{4\pi}{3}\right)^{1/2} Y_{10}^*$$

and

$$J_x = \left(\frac{1}{\sqrt{2}}\right) (\varphi_{1,-1} - \varphi_{11}), \quad J_y = -\left(\frac{i}{\sqrt{2}}\right) (\varphi_{1,-1} + \varphi_{11}), \quad J_z = \varphi_{10}$$

we find that the P_1 representation of the angular flux is just

$$\varphi(\mathbf{r}, E, \hat{\Omega}, t) = (1/4\pi)\phi(\mathbf{r}, E, t) + (3/4\pi)\hat{\Omega} \cdot \mathbf{J}(\mathbf{r}, E, t)$$

and the P_1 equations take the general form

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{J} + \Sigma_t \phi = \int_0^\infty dE' \Sigma_0(E' \rightarrow E) \phi(\mathbf{r}, E', t) + S_0$$

$$\frac{1}{v} \frac{\partial \mathbf{J}}{\partial t} + \frac{1}{3} \nabla \phi + \Sigma_t \mathbf{J} = \int_0^\infty dE' \Sigma_1(E' \rightarrow E) \mathbf{J}(\mathbf{r}, E', t) + \mathbf{S}_1 \quad (4.24)$$

DP_N Methods □ As a variation on the foregoing theme, it is occasionally useful to perform a half-range P_N expansion.^{14,15} More specifically, near the boundaries of a system, the angular distribution of the angular flux is highly anisotropic (e.g., discontinuous at $\mu=0$). An accurate description of this angular dependence would require a P_N expansion of very high order. To circumvent this, we can use a separate expansion in each range over which the angular distribution is slowly varying. In particular, at an interface one would use an expansion in two series of Legendre polynomials, one for $\mu \in [-1, 0]$ and one for $\mu \in [0, 1]$

$$\varphi(x, \mu) = \sum_{l=0}^{\infty} \left(\frac{2l+1}{4\pi} \right) [\varphi_l^+(x) P_l^+(\mu) + \varphi_l^-(x) P_l^-(\mu)]$$

where we define

$$P_l^+(\mu) \equiv \begin{cases} P_l(2\mu-1), & 0 \leq \mu \leq 1 \\ 0, & -1 \leq \mu < 0 \end{cases} \quad P_l^-(\mu) \equiv \begin{cases} 0, & 0 \leq \mu \leq 1 \\ P_l(2\mu+1), & -1 \leq \mu < 0 \end{cases}$$

while

$$\varphi_l^+(x) = 2\pi \int_0^1 d\mu \varphi(x, \mu) P_l^+(\mu), \quad \varphi_l^-(x) = 2\pi \int_{-1}^0 d\mu \varphi(x, \mu) P_l^-(\mu)$$

If we substitute these expansions into the transport equation and apply orthogonality, we arrive at a set known as the DP_N (the “double” P_N) equations:

$$2l \frac{d\varphi_{l-1}^\pm}{dx} \pm (2l+1) \frac{d\varphi_{l+1}^\pm}{dx} + 2(2l+1) \Sigma_l \varphi_l^\pm(x) = \Sigma_s [\varphi_0^+ + \varphi_0^-] + 2s_0 \delta_{l0}$$

Some Further Comments □ Although P_N or spherical harmonic methods are of great value in obtaining a formal solution to the transport equation, they have found little application to practical problems because the P_N equations are quite ill-suited to numerical solution.¹⁶ These equations are tightly coupled and difficult to solve. Furthermore, as we have noted, there is some ambiguity in formulating boundary conditions. Hence most numerical transport calculations are based on discrete ordinate, finite element, or Monte Carlo methods (discussed in some detail in Chapters 8 and 9).

The P_N method does provide a general approach for contracting the description given by the full transport equation for the angular flux to a reduced or contracted (albeit approximate) description for only a few angular moments of the angular flux such as $\phi(\mathbf{r}, t)$ or $\mathbf{J}(\mathbf{r}, t)$. Viewed in a somewhat different light,¹⁷ we have used this method to project the original transport equation onto a restricted subspace as illustrated in Figure 4.4. That is, if we write the transport equation as

$$\mathcal{L}\varphi = s$$

then we have projected this equation onto an N -dimensional subspace, a procedure we can symbolize as

$$\mathcal{P}_N \mathcal{L}\varphi = \mathcal{P}_N s$$

We then sought the solution φ_{approx} to the projected problem in this restricted subspace as a linear combination of the basis functions ψ_n that span the subspace (e.g., the $Y_{lm}(\hat{\Omega})$ functions):

$$\varphi \rightarrow \varphi_{\text{approx}} = \sum_{n=1}^N \varphi_n \psi_n$$

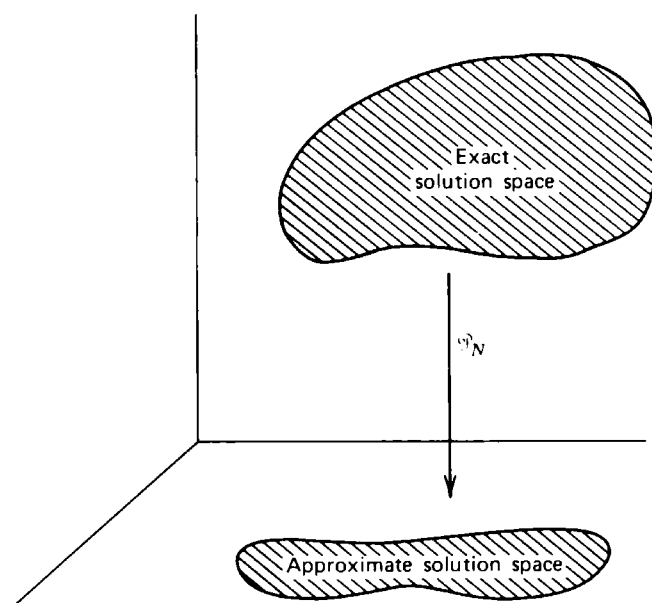


Fig. 4.4 □ Projection of the exact solution space onto an approximate or “contracted” solution space.

Then by substituting this form into the projected equation, we obtained a set of N equations for the expansion coefficients.

To illustrate this more specifically, in deriving the P_1 equations we projected onto the zeroth and first angular moments of $\varphi(\mathbf{r}, \hat{\Omega}, t)$:

$$\mathcal{P}_N \rightarrow \int d\hat{\Omega} \cdot \mathbf{l} \cdot \left\{ \frac{1}{v} \frac{\partial \varphi}{\partial t} + \hat{\Omega} \cdot \nabla \varphi + \Sigma_t \varphi - \frac{\Sigma_s}{4\pi} \int d\hat{\Omega}' \varphi = s \right\}$$

↓

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{J} + \Sigma_a \phi = S_0$$

$$\frac{1}{v} \frac{\partial \mathbf{J}}{\partial t} + \nabla \cdot \int d\hat{\Omega} \hat{\Omega} \hat{\Omega} \varphi + \Sigma_t \mathbf{J} = S_1$$

We then restricted the approximate solution to these equations to lie in the subspace spanned by 1 and $\hat{\Omega}$:

$$\varphi \rightarrow \varphi_{\text{approx}} = \frac{1}{4\pi} \phi + \frac{3}{4\pi} \hat{\Omega} \cdot \mathbf{J}$$

to arrive at the P_1 equations for the “expansion coefficients” $\phi(\mathbf{r}, t)$ and $\mathbf{J}(\mathbf{r}, t)$:

$$\text{projection onto } 1, \hat{\Omega} \left\{ \begin{array}{l} \text{transport} \\ \text{equation} \end{array} \right. (\varphi_{\text{approx}}) \Big\} = P_1 \text{ equations}$$

This identification of the P_N method as just a *projection* of the transport equation onto a reduced dimensional subspace to achieve a contracted description of the particle transport process can be made considerably more precise. Indeed, as we now demonstrate, it is not necessary to introduce an approximation of any sort to achieve such a contracted description. One can use projection operator algebra¹⁸ to obtain an exact (although formal) contracted description.

4.2.3 □ An Alternative Derivation of the Diffusion Equation and Its Generalizations □ To point out some of the important concepts involved in “contracting” a kinetic or transport theory description to a continuum description, we provide a somewhat different (and far more elegant) derivation of the diffusion equation. We use projection operator algebra to obtain formally exact contracted descriptions of particle transport processes. For example, we derive an exact “generalized diffusion equation” for the scalar flux, as well as corresponding exact generalizations of the P_N equations. It should be stressed at the outset that there is nothing magic about these exact generalized diffusion equations. They are merely formal identities with the original transport equation, and as such, they would require all the labor for their solution that would be required by a more direct attack on the transport equation itself. Rather, the value of such projection operator methods is that they recast the original transport equation into a form more suitable for approximation. The generalized diffusion (or P_N) equations not only are a somewhat more direct point of departure for the development of the traditional approximations in transport theory (e.g., P_N methods or asymptotic transport theory), but they also act as a natural bridge to a class of hybrid approximations such as generalized diffusion coefficients,^{16,19} variable Eddington factors,^{20,21} or flux limiters,^{22,23} which attempt to correct the diffusion equation for transport (e.g., streaming) effects.

We begin by applying a particularly simple projection operator to the simplest of all transport equations, that characterizing one-speed transport with isotropic sources and scattering (although, as we demonstrate later, it is a trivial matter to extend these methods to the more general forms of this equation). This will yield an exact generalization of the familiar one-speed

diffusion equation. Then we demonstrate how the traditional approximate theories of particle transport (diffusion theory, P_1 , P_N , asymptotic transport theory) fall directly from this equation. We also illustrate how this equation can be used to develop a variety of modeled diffusion theories that interpolate between particle streaming and diffusive behavior. We then present a variety of more sophisticated projection operator theories that are capable of treating the more general form of the transport equation.

A Simple Example □ To illustrate how projection operator methods can be applied to study transport problems, we first consider the simplest form of the transport equation in which the assumptions of one-speed transport, uniform media, and isotropic scattering and sources have been introduced. Indeed, this problem is sufficiently simple that it can be solved exactly for many situations—which makes it all the more useful for illustrating the projection operator method. The transport equation under these assumptions becomes

$$\frac{1}{v} \frac{\partial \varphi}{\partial t} = -\hat{\Omega} \cdot \nabla \varphi - \Sigma_t \varphi + \frac{\Sigma_s}{4\pi} \int d\hat{\Omega}' \varphi(\mathbf{r}, \hat{\Omega}', t) + \frac{1}{4\pi} S_0(\mathbf{r}, t) \quad (4.25)$$

or in an obvious operator notation

$$\frac{1}{v} \frac{\partial \varphi}{\partial t} = L\varphi + \frac{S_0}{4\pi} \quad (4.26)$$

We regard this (for the moment) as an initial value problem in an infinite medium, therefore leaving boundary conditions unspecified.

Our primary goal is to obtain an equation for the scalar flux

$$\phi(\mathbf{r}, t) = \int d\hat{\Omega} \varphi(\mathbf{r}, \hat{\Omega}, t)$$

—that is, we wish to contract our description of particle transport from $\varphi(\mathbf{r}, \hat{\Omega}, t)$ to $\phi(\mathbf{r}, t)$. We define an operator

$$P \circ \equiv \frac{1}{4\pi} \int d\hat{\Omega} \circ \quad (4.27)$$

which accomplishes this contraction,

$$\phi(\mathbf{r}, t) = 4\pi P\varphi \equiv 4\pi\varphi_{\parallel}$$

Note that P is a *projection operator* in the sense that $P^2 = P$. In particular, P projects out the isotropic component $\varphi_{\parallel}$ of φ .

We now use P to project out the piece of the transport equation that is “relevant” to the calculation of $\phi(\mathbf{r}, t)$. To this end, we first operate on Eq. 4.26 with P and then $(1 - P)$, respectively, to find

$$\frac{1}{v} \frac{\partial \varphi_{\parallel}}{\partial t} = PL\varphi_{\parallel} + PL\varphi_{\perp} + \frac{S_0}{4\pi} \quad (4.28a)$$

$$\frac{1}{v} \frac{\partial \varphi_{\perp}}{\partial t} = (1 - P)L\varphi_{\parallel} + (1 - P)L\varphi_{\perp} \quad (4.28b)$$

where we have identified

$$\varphi_{\parallel} \equiv P\varphi, \quad \varphi_{\perp} \equiv (1 - P)\varphi$$

and noted

$$\varphi = P\varphi + (1 - P)\varphi = \varphi_{\parallel} + \varphi_{\perp}$$

We also have used the fact that $(1 - P)S_0 = 0$. Next we formally solve Eq. 4.28b for $\varphi_{\perp}(t)$ in terms of $\varphi_{\parallel}(t)$:

$$\varphi_{\perp}(t) = e^{iv(1-P)L} \varphi_{\perp}(0) + \int_0^t d\tau e^{\tau v(1-P)L} v(1-P)L\varphi_{\parallel}(t - \tau)$$

and substitute this into Eq. 4.28a to find

$$\begin{aligned} \frac{1}{v} \frac{\partial \varphi_{\parallel}}{\partial t} - PL\varphi_{\parallel}(t) &= \int_0^t d\tau PL e^{\tau v(1-P)L} v(1-P)L\varphi_{\parallel}(t - \tau) \\ &+ \frac{S_0}{4\pi} + PL e^{iv(1-P)L} \varphi_{\perp}(0) \end{aligned} \quad (4.29)$$

We now have arrived at a closed equation for the projected component $\varphi_{\parallel}(t)$ of $\varphi(t)$. (In the literature of statistical mechanics, Eq. 4.29 is sometimes referred to as the “generalized master equation”.¹⁸⁾

To simplify Eq. 4.29, we make the following observations:

- i $PL\varphi_{\parallel} = -\Sigma_a \varphi_{\parallel}(t)$
- ii $(1 - P)L\varphi_{\parallel} = -\hat{\Omega} \cdot \nabla \varphi_{\parallel}$
- iii $PL e^{\tau v(1-P)L} (1 - P)L\varphi_{\parallel} = P \left[\hat{\Omega} \cdot \nabla e^{\tau v(1-P)L} \hat{\Omega} \cdot \nabla \varphi_{\parallel}(t - \tau) \right]$

If we use these results in Eq. 4.29 along with the substitution $\varphi_{\parallel}(t) = (4\pi)^{-1} \phi(t)$, we find

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \Sigma_a \phi = \int_0^t d\tau \nabla \cdot \frac{v}{4\pi} \int d\hat{\Omega} \hat{\Omega} e^{\tau v(1-P)L} \hat{\Omega} \cdot \nabla \phi(\mathbf{r}, t - \tau) + S_0(\mathbf{r}, t) + \mathcal{D}(\mathbf{r}, t) \quad (4.30)$$

Now notice that if we define a generalized diffusion “coefficient” (although it is actually both a tensor and an operator)

$$\mathbf{D}(\mathbf{r}, \tau) \equiv \frac{v}{4\pi} \int d\hat{\Omega} \hat{\Omega} e^{\tau v(1-P)L} \hat{\Omega}$$

we can rewrite Eq. 4.30 in the form of a *generalized diffusion equation* for $\phi(\mathbf{r}, t)$

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \Sigma_a \phi = \int_0^t d\tau \nabla \cdot \mathbf{D}(\mathbf{r}, \tau) \cdot \nabla \phi(\mathbf{r}, t - \tau) + S_0(\mathbf{r}, t) + \mathcal{D}(\mathbf{r}, t) \quad (4.31)$$

Here $\mathcal{D}(\mathbf{r}, t)$ is the initial value term arising from the solution of Eq. 4.28b

$$\mathcal{D}(\mathbf{r}, t) \equiv -\nabla \cdot \frac{v}{4\pi} \int d\hat{\Omega} \hat{\Omega} e^{tv(1-P)L} \left[\varphi(\mathbf{r}, \hat{\Omega}, 0) - \frac{1}{4\pi} \phi(\mathbf{r}, 0) \right]$$

Our exact (but still formal) generalized diffusion equation differs from the usual diffusion equation in two very important respects. First, the diffusion coefficient has now been replaced by an operator $\mathbf{D}(\mathbf{r}, t)$ that is nonlocal in space and time—that is, the diffusion term exhibits “memory.” Second, there is an initial value term that depends on the initial value of the angular density $\varphi(\mathbf{r}, \hat{\Omega}, 0)$, not just the projected component $\varphi_{||}(0) = (4\pi)^{-1} \phi(0)$. [One of the classic problems in kinetic theory is the so-called Hilbert paradox,^{24,25} which involves the role played by the initial data for the transport equation, $\varphi(\mathbf{r}, \hat{\Omega}, 0)$, in the time evolution of the continuum description for $\phi(\mathbf{r}, t)$. We can see quite clearly that this appears through the initial value term $\mathcal{D}(\mathbf{r}, t)$.]

To provide an alternative perspective of this equation, suppose we ignore the source term $S_0(\mathbf{r}, t)$ for the moment and consider the transport equation 4.25 as an initial value problem in an infinite medium. Then we can introduce a Fourier-Laplace transform

$$\tilde{\phi}(k, s) \equiv \int d^3r e^{-i\mathbf{k} \cdot \mathbf{r}} \int_0^\infty dt e^{-st} \phi(\mathbf{r}, t)$$

to transform the generalized diffusion equation 4.31 into

$$\left(\frac{s}{v} + \Sigma_a \right) \tilde{\phi}(k, s) = -k^2 \tilde{D}(k, s) \tilde{\phi}(k, s) + \phi_0(k, 0)$$

or solving

$$\tilde{\phi}(k, s) = \frac{v \phi_0(k)}{s + v \Sigma_a + v k^2 \tilde{D}(k, s)} \quad (4.32)$$

[Here we have followed a convenient custom in projection operator theories by ignoring, at least for the moment, the initial value term $\varphi_{\perp}(0)$ by postulating an isotropic initial distribution $\varphi(\mathbf{r}, \hat{\Omega}, 0) = (4\pi)^{-1} \phi_0(\mathbf{r})$.] We have defined

$$\tilde{D}(k, s) = \left(\frac{v}{4\pi k^2} \right) \int d\hat{\Omega} (\mathbf{k} \cdot \hat{\Omega}) [s - v(1 - P)L]^{-1} (\mathbf{k} \cdot \hat{\Omega})$$

The nonlocal nature of the generalized diffusion coefficient is readily apparent by its dependence on wave number k and frequency $\omega = is$. Its formal nature is also apparent, since any explicit treatment of the propagator $[s - v(1 - P)L]^{-1}$ is tantamount to solving the original transport equation.

But we recall that we can easily solve the original transport equation 4.25 exactly for this very simple situation (cf. Section 2.5) to find

$$\tilde{\phi}(k, s) = \frac{\chi(k, s)}{\Lambda(k, s)} = \frac{\frac{v\phi_0}{2ik} \ln \left(\frac{s + v\Sigma_t + ikv}{s + v\Sigma_t - ikv} \right)}{1 - \frac{\Sigma_s}{2ik} \ln \left(\frac{s + v\Sigma_t + ikv}{s + v\Sigma_t - ikv} \right)}$$

thereby obtaining an explicit form for the generalized diffusion coefficient:

$$\tilde{D}(k, s) = \frac{\phi_0(k) \Lambda(k, s)}{k^2 \chi(k, s)} - \left(\frac{s + v\Sigma_a}{vk^2} \right)$$

Of course, such an explicit form for $\tilde{D}(k, s)$ will not be available for more complicated problems. Rather, we must develop procedures for approximately calculating the nonlocal generalized diffusion coefficient $\tilde{D}(k, s)$.

Approximations to the Generalized Diffusion Equation □ The primary utility of the generalized diffusion equation (aside from being a rather elegant reformulation of the transport equation) rests on its suitability for developing approximate descriptions of particle transport. We illustrate this feature by first demonstrating how the standard approximations can be obtained from Eq. 4.31, then we introduce a new class of modeled theories of particle transport.

i *P₁-Diffusion theory.* We begin by noting that the “modified” time propagator $\exp[\tau v(1 - P)L]$ can be explicitly written as

$$\begin{aligned} & \exp[\tau v(1 - P)L](1 - P)L\varphi_{\parallel} \\ &= \exp\{ -\tau v[(1 - P)\hat{\Omega} \cdot \nabla(1 - P) + \Sigma_t] \} (1 - P)L\varphi_{\parallel} \end{aligned}$$

But if we identify $\|(1-P)\hat{\Omega} \cdot \nabla(1-P)\|$ as essentially a measure of the spatial gradient of the flux, it is apparent that the usual diffusion approximation should arise from the condition

$$\Sigma_t^{-1} \|(1-P)\hat{\Omega} \cdot \nabla(1-P)\| = \left(\frac{mfp}{l} \right) \ll 1$$

where l is a characteristic length scale. In this case

$$\exp\{-\tau v[(1-P)\hat{\Omega} \cdot \nabla(1-P) + \Sigma_t]\} \cong \exp[-\tau v \Sigma_t]$$

If we next note that this approximation to the propagator yields

$$\frac{v}{4\pi} \int d\hat{\Omega} \Omega_i e^{\tau v(1-P)L} \Omega_j \cong e^{-\tau v \Sigma_t} \frac{v}{4\pi} \int d\hat{\Omega} \Omega_i \Omega_j = e^{-\tau v \Sigma_t} \frac{v}{3} \delta_{ij} \quad (4.33)$$

and neglect the initial value term $\phi_{\perp}(0)$, we can write

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \Sigma_a \phi(\mathbf{r}, t) = \int_0^t d\tau \left(\frac{v}{3} \right) e^{-\tau v \Sigma_t} \nabla^2 \phi(\mathbf{r}, t - \tau) + S_0(\mathbf{r}, t)$$

Although this form may at first appear a bit unfamiliar, it is, in fact, equivalent to the time-dependent P_1 equations:

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{J} + \Sigma_a \phi = S_0 \quad (4.34a)$$

$$\frac{1}{v} \frac{\partial \mathbf{J}}{\partial t} + \frac{1}{3} \nabla \phi + \Sigma_t \mathbf{J} = 0 \quad (4.34b)$$

in which the second equation has been solved for $\mathbf{J}$ in terms of ϕ , and this expression has been substituted into the first equation.

To obtain the more familiar diffusion equation, we must assume that $\phi(\mathbf{r}, t)$ varies slowly in time compared to $(v \Sigma_t)^{-1}$ so that we can expand $\phi(\mathbf{r}, t - \tau)$ about t and retain only the leading term to find

$$\int_0^t d\tau e^{-\tau v \Sigma_t} \phi(\mathbf{r}, t - \tau) \cong \int_0^{\infty} d\tau e^{-\tau v \Sigma_t} \phi(\mathbf{r}, t) = (v \Sigma_t)^{-1} \phi(\mathbf{r}, t) \quad (4.35)$$

If this is substituted into Eq. 4.34a, we arrive at the usual diffusion equation

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \Sigma_a \phi(\mathbf{r}, t) = D \nabla^2 \phi + S_0 \quad (4.36)$$

where we have identified $D = (3 \Sigma_t)^{-1}$. The approximation represented by

Eq. 4.35 is sometimes referred to as the “Markov” approximation, since it eliminates the “memory” or nonlocal time behavior in the diffusion coefficient in such a fashion that $\partial\phi/\partial t$ in Eq. 4.36 depends only on the flux $\phi(t)$ evaluated at time t .

One can easily develop the higher order P_N approximations by simply retaining more terms in an expansion of the propagator in the gradient operator $\Sigma_i^{-1}(1-P)\hat{\Omega}\cdot\nabla(1-P)$. Although such propagator expansions are straightforward, they can become somewhat tedious; therefore we develop a more direct method for deriving the P_N equations (and their generalizations), using a more suitable projection operator, later in this section.

ii *Asymptotic transport theory.* A common approximation in transport theory involves retaining only the asymptotically dominant portion of the solution to the transport equation, thereby neglecting all transport “transient” contributions.^{22,26} This particular approximation is, in fact, nothing more than the Chapman-Enskog approximation²⁷ familiar from kinetic theory (which we develop in detail in Section 4.3). To demonstrate this fact,²⁴ we note that inherent in the Chapman-Enskog method is the fundamental assumption that the distribution function is a time-independent functional of its hydrodynamic moments. That is,

$$\varphi(\mathbf{r}, \hat{\Omega}, t) = \varphi(\mathbf{r}, \hat{\Omega}; \phi(t))$$

For our linear transport equation this is equivalent to assuming (in $k-s$ transform space, for convenience)

$$\tilde{\varphi}_{\perp}(k, \hat{\Omega}, s) = F(k, \hat{\Omega}) \tilde{\varphi}_{\parallel}(k, s) \quad (4.37)$$

where $F(k, \hat{\Omega})$ is an unknown (but time- and frequency-independent) function of k and $\hat{\Omega}$. To implement this assumption and to evaluate $F(k, \hat{\Omega})$ and $\tilde{\varphi}_{\parallel}(k, s)$, we begin by substituting this ansatz into the Fourier-Laplace transforms of 4.28 to find

$$\tilde{\varphi}_{\parallel}(s) = \frac{v\varphi_{\parallel}(0)}{s + v\Sigma_a + vP[i\mathbf{k}\cdot\hat{\Omega}F(k, \hat{\Omega})]} \equiv \frac{v\varphi_{\parallel}(0)}{s + \lambda_0(k)} \quad (4.38)$$

and

$$\tilde{\varphi}_{\parallel}(s) = \frac{vF\varphi_{\parallel}(0)}{(s + i\mathbf{k}\cdot\hat{\Omega} + v\Sigma_i)F - vP[i\mathbf{k}\cdot\hat{\Omega}F] + i\mathbf{k}\cdot\hat{\Omega}v} \quad (4.39)$$

Here we have noted that $P[i\mathbf{k}\cdot\hat{\Omega}F]$ depends only on k , and we have

furthermore defined (for a reason that will become apparent in a moment)

$$\lambda_0(k) \equiv v \Sigma_a + v P[i \mathbf{k} \cdot \hat{\Omega} F(\mathbf{k}, \hat{\Omega})]$$

If we now eliminate $\tilde{\varphi}_{||}(s)$ and $\varphi_{||}(0)$ between these two equations, we can solve for

$$(1 + F) = \frac{\Sigma_s}{i \mathbf{k} \cdot \hat{\Omega} + \Sigma_s - P[i \mathbf{k} \cdot \hat{\Omega} F]} \quad (4.40)$$

But since we can show $P(1 + F) = 1$, we can apply the projection operator P to Eq. 4.40 to arrive at an equation for $P[i \mathbf{k} \cdot \hat{\Omega} F(k, \hat{\Omega})]$ or equivalently $\lambda_0(k)$, which takes the familiar form

$$\Lambda(k, -\lambda_0) = 1 - \frac{\Sigma_s}{2ik} \ln \left(\frac{-\lambda_0 + v \Sigma_s + ikv}{-\lambda_0 + v \Sigma_s - ikv} \right) = 0 \quad (4.41)$$

which is the usual dispersion relation for the “discrete” or asymptotic time relaxation parameter $\lambda_0(k)$

$$\lambda_0(k) = v \Sigma_s - kv \operatorname{ctn} \left(\frac{k}{\Sigma_s} \right)$$

Hence, if we now recall the form Eq. 4.38 has taken by $\tilde{\varphi}_{||}(\mathbf{k}, s)$ under the ansatz Eq. 4.37, it is apparent that this ansatz has led immediately to the familiar asymptotic transport form for the scalar flux

$$\phi(k, t) = \phi(k, 0) e^{-\lambda_0(k)t}$$

Thus we find once again that projection operator methods have provided a very convenient starting point for deriving the standard approximations to the transport equation. But these methods also facilitate a somewhat different and more physical approach, since they recast the original transport equation into a form that represents an exact generalization of the well-known diffusion equation, but with a nonlocal diffusion coefficient. Hence one is tempted to guess or model the relevant properties of this term directly, thereby avoiding the complexity of a perturbation expansion in (mfp/l) , for example.

iii *Modeled theories.* It is easiest to guess or model the behavior of the generalized diffusion coefficient in $k-s$ transform space. Recall that the

exact form for $\tilde{D}(k, s)$ is given by

$$\tilde{D}(k, s) = \frac{v}{4\pi k^2} \int d\hat{\Omega} (\mathbf{k} \cdot \hat{\Omega}) [s + v(1 - P)L]^{-1} (\mathbf{k} \cdot \hat{\Omega})$$

The simplest such model would be to ignore the k, s dependence of $\tilde{D}(k, s)$ entirely by replacing

$$\tilde{D}(k, s) \rightarrow \tilde{D}(0, 0) = \frac{\Sigma_s}{3\Sigma_t^2} \equiv D_0$$

But of course this “Markovian” model corresponds to traditional diffusion theory.

A somewhat more interesting model can be developed by retaining a non-Markovian behavior in $\tilde{D}(k, s)$ and postulating a single relaxation time form

$$\tilde{D}(k, s) = \frac{D(k, t=0)}{s + \alpha(k)} = \frac{v/3}{s + \alpha(k)}$$

where we have noted that the $t \rightarrow 0$ (or $s \rightarrow \infty$) limit of $\tilde{D}(k, s)$ can be calculated exactly as $\tilde{D}(k, 0) = v/3$.

Our attention now is directed to choosing some appropriate model for the k -dependent relaxation parameter $\alpha(k)$. We begin by demanding that our model yield the known limiting behavior of $\tilde{\phi}(k, s)$ for small and large values of k, s . In particular, for small k, s , we know that $\tilde{\phi}(k, s)$ is given by P_1 -diffusion theory

$$\tilde{\phi}(k, s) \xrightarrow{s, k \rightarrow 0} v\phi_0 \left[s + v\Sigma_a + \frac{k^2 v^2/3}{s + v\Sigma_t} \right]^{-1}$$

which implies that $\tilde{D}(k, s) \rightarrow \Sigma_s/3\Sigma_t^2$ as $s, k \rightarrow 0$ or $\alpha(k) \rightarrow v\Sigma_t^2/\Sigma_s$ as $k \rightarrow 0$. One such model would be the k -independent form $\alpha(k) = v\Sigma_t^2/\Sigma_s \sim v\Sigma_t$. But of course this “local” model of $\alpha(k)$ leads directly to P_1 theory and therefore is of only passing interest.

We can generate more sophisticated models for $\alpha(k)$ by demanding that our model approximate as well the large k, s behavior of $\tilde{\phi}(k, s)$. This behavior is a bit more complicated to study because it is obviously related to the free streaming limit and therefore depends quite sensitively on the particular source and initial conditions of interest. For example, if our problem were to involve an initial condition corresponding to a forward directed beam at the origin plane of an infinite medium, then evidently we

would have

$$\tilde{\phi}(k, s) \xrightarrow{s, k \rightarrow \infty} v\phi_0[s + v\Sigma_t + ikv]^{-1}$$

which implies $\tilde{D}(k, s) \rightarrow (\Sigma_s + ik)/k^2$ as $k, s \rightarrow \infty$, or $\alpha(k) \rightarrow (vk^2/3)/(\Sigma_s + ik)$ as $k \rightarrow \infty$.

We could now choose $\alpha(k)$ to be a simple form that interpolates between these limits. For example, if we are interested in the forward beam streaming problem, we might choose $\alpha(k) = (v\Sigma_t^2 + vk^2/3)/(\Sigma_s + ik)$.

But this discussion suggests a far more satisfying prescription for modeling $\tilde{D}(k, s)$. Suppose we return to consider the exact transport solution for an initial condition localized at the origin plane:

$$\tilde{\phi}(k, s) = \left[\int_{-1}^{+1} d\mu \frac{\varphi_0(0, \mu)}{s + v\Sigma_t + ikv\mu} \right] \left[1 - \frac{\Sigma_s}{2ik} \ln \left(\frac{s + v\Sigma_t + ikv}{s + v\Sigma_t - ikv} \right) \right]^{-1}$$

This solution exhibits a simple pole at $s = -\lambda_0(k)$ and the usual transport branch cut from $-v\Sigma_t - ikv$ to $-v\Sigma_t + ikv$ as shown in Figure 4.5. Furthermore, as $k \rightarrow k^* = \pi\Sigma_t/2$, we recall that $\lambda_0(k) \rightarrow \lambda^* \equiv v\Sigma_t$, and eventually “disappears” into the branch cut, although the discrete pole can be followed onto the analytic continuation of $\Lambda(k, s)$ if desired for $k > k^*$.

A particularly interesting model would be one that yields not only the correct asymptotic behavior due to the pole at $-\lambda_0(k)$, but also simulates streaming behavior by including contributions from the branch points at $-v\Sigma_t \pm ikv$. That is, we could try to construct $\tilde{D}(k, s)$ so that it yields a dispersion relation of the form

$$\Lambda(k, s) = [(s + v\Sigma_t)^2 + k^2v^2][s + \lambda_0(k)] \quad (4.42)$$

It is apparent that such a model would require $\tilde{D}(k, s)$ to take the form

$$k^2v\tilde{D}(k, s) = \frac{\gamma(k)}{s^2 + \xi(k)s + \alpha(k)}$$

[essentially a two-time relaxation model of $D(k, t)$]. If we insert this form into Eq. 4.32 and compare the resulting dispersion relation with Eq. 4.42, we find it necessary to choose

$$k^2v\tilde{D}(k, s) = \frac{(v^2\Sigma_s^2 + k^2v^2)(\lambda_0(k) - v\Sigma_a)}{(s + v\Sigma_t)^2 + k^2v^2 + (\lambda_0(k) - v\Sigma_a)(s + v\Sigma_s)}$$

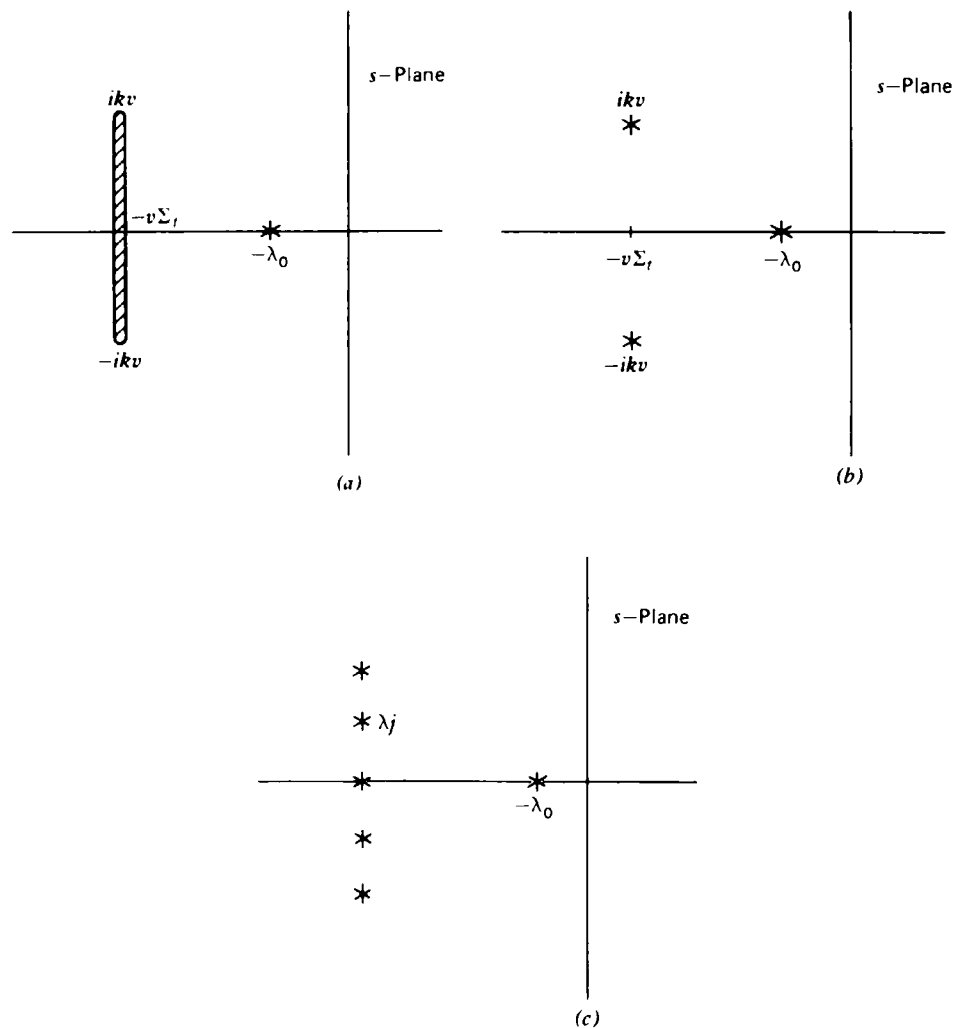


Fig. 4.5 □ s -Plane structure for various transport models. (a) Exact transport solution. (b) Generalized diffusion model. (c) Higher order model.

This form not only yields the complex s -plane structure, which simulates both asymptotic and streaming contributions (see Figure 4.5), but furthermore yields the correct Markovian limit for small k, s .

This s -plane comparison suggests a systematic scheme for improving our model. We would choose a form for $\tilde{D}(k, s)$ that sprinkles additional poles along the cut from $-v\Sigma_l \pm ikv$ for large k to better describe the transport transients.

Such models that “interpolate” between diffusive and streaming behavior are very similar in spirit to the generalized diffusion coefficients,¹⁹ variable Eddington factor,^{20,21} and flux limiter schemes,^{22,23} which have

been used in the past in an attempt to correct or patch up the diffusion equation for transport or streaming effects. For example, in the variable Eddington factor method, one introduces the ad hoc assumption that the second-order moment of the angular flux is simply related to the scalar flux

$$\Pi(x, t) = \int_{-1}^{+1} d\mu \mu^2 \varphi(x, \mu, t) \equiv f(x, t) \phi(x, t) \quad (4.43)$$

The burden now falls on estimating or guessing the form of the “variable Eddington factor” $f(x, t)$. A very similar spirit is adopted in flux limiting schemes that interpolate the current density between diffusive and streaming behavior in an ad hoc fashion

$$J(x, t) \sim \left[\left(-D \frac{\partial \phi}{\partial x} \right)^{-1} + c \left(\frac{\phi}{4} \right)^{-1} \right]^{-1} \quad (4.44)$$

But there is one very important distinction in our generalized diffusion theory: it is nonlocal in space and time. That is, $\tilde{D}(k, s)$ depends on k and s :

$$\tilde{\mathbf{J}}(k, s) = -\tilde{D}(k, s) \nabla \tilde{\phi}(k, s)$$

The corresponding variable Eddington factor is then (exactly)

$$\tilde{f}(k, s) = (s + v \Sigma_t) \tilde{D}(k, s)$$

This, of course, is a major disadvantage from the viewpoint of practical calculations, since nonlocal (i.e., *integral*) equations are awkward to solve numerically compared to local (i.e., *differential*) equations. But, in fact, when we recognize that our theory is formally *exact*, it is apparent that any approximation (such as Eq. 4.43 or 4.44) that attempts to remove this nonlocal feature is mutilating the transport nature of the process. Particle transport (at least on the macroscopic level of the scalar flux) is simply not a local process, unless the traditional approximations that rely on $(mfp/l) \ll 1$ are valid.

Alternative Choices of the Projection Operator □ A variety of alternative choices of projection operators can be introduced in a very similar manner to achieve contracted descriptions of transport processes. A particularly useful class of projection operators takes the form²⁸

$$P \circ \equiv \langle \circ \mathbf{a}^* \rangle \cdot \langle \mathbf{a} \mathbf{a}^* \rangle^{-1} \cdot \mathbf{a} \quad (4.45)$$

where the angular average is defined by

$$\langle \circ \rangle \equiv \frac{1}{4\pi} \int d\hat{\Omega} \circ \longrightarrow \frac{1}{2} \int_{-1}^{+1} d\mu \circ$$

and $\mathbf{a}$ is a column vector of functions of angle (which comprise the basis spanning the approximation subspace), $\mathbf{a} = \text{col}(a_1, \dots, a_N)$. Several examples (confined, for convenience, to one-dimensional plane symmetry) illustrate this class of projection operators more clearly.

i $\mathbf{a} = 1$. Then P reduces to our original choice of a projection

$$P \rightarrow P_1 \circ \equiv \frac{1}{2} \int_{-1}^{+1} d\mu \circ$$

ii $\mathbf{a} = \text{col}(1, \mu)$. We now note that

$$P \rightarrow P_2 \circ \equiv \langle \circ \rangle + 3\mu \langle \circ \mu \rangle$$

projects $\varphi(x, \mu, t)$ onto its first two angular moments

$$P_2 \varphi = \frac{1}{2} \phi(x, t) + \frac{3}{2} \mu J(x, t)$$

If we now imitate our earlier procedure for deriving the generalized diffusion equation with this new projection operator, we arrive at a set of two coupled equations

$$\begin{aligned} \frac{1}{v} \frac{\partial \phi}{\partial t} + \frac{\partial J}{\partial x} + \Sigma_a \phi &= S_0 \\ \frac{1}{v} \frac{\partial J}{\partial t} + \frac{1}{3} \frac{\partial \phi}{\partial x} + \Sigma_r J &= \int_0^t d\tau \frac{\partial}{\partial x} \left\langle \left(\frac{3\mu^2 - 1}{2} \right) e^{\tau v(1-P)L} \left(\frac{3\mu^2 - 1}{2} \right) \right\rangle \frac{\partial}{\partial x} J(x, t - \tau) + \mathcal{Q}_2(x, t) \end{aligned}$$

which we immediately recognize as an exact generalization of the conventional P_1 equations (4.33).

iii $\mathbf{a} = \text{col}(P_0(\mu), P_1(\mu), \dots, P_N(\mu))$. Obviously this particular choice of projection operator decomposes φ into its Legendre polynomial components

$$P\varphi = \sum_{l=1}^N \left(\frac{2l+1}{2} \right) \phi_l(x, t) P_l(\mu)$$

where

$$\phi_l(x, t) \equiv \int_{-1}^{+1} d\mu P_l(\mu) \varphi(x, \mu, t)$$

This will generate an exact generalization of the P_N equations:

$$\begin{aligned} \frac{1}{v} \frac{\partial \phi_0}{\partial t} + \frac{\partial \phi_1}{\partial x} + \Sigma_a \phi_0 &= S_0 \\ \vdots & \\ \frac{1}{v} \frac{\partial \phi_l}{\partial t} + \left(\frac{l+1}{2l+1} \right) \frac{\partial \phi_{l+1}}{\partial x} + \left(\frac{l}{2l+1} \right) \frac{\partial \phi_{l-1}}{\partial t} + (\Sigma_t - \Sigma_s b_l) \phi_l &= S_l \\ \vdots & \\ \frac{1}{v} \frac{\partial \phi_N}{\partial t} + \left(\frac{N}{2N+1} \right) \frac{\partial \phi_{N+1}}{\partial x} + (\Sigma_t - \Sigma_s b_N) \phi_N &= \\ &= \int_0^t d\tau \frac{\partial}{\partial x} \left[\int_{-1}^{+1} d\mu P_{N+1}(\mu) e^{\tau v(1-P)} P_{N+1}(\mu) \right] \frac{\partial}{\partial x} \phi_N(x, t-\tau) + \mathcal{D}_N(x, t) \end{aligned}$$

These equations differ from the conventional P_N equations in that the projection operator method has exactly (although formally) truncated the set at order N by solving for ϕ_{N+1} in terms of ϕ_N .

iv *Energy dependence.* Although our study of projection operator methods has been restricted thus far to one-speed problems, the method can easily be extended to handle energy dependence or anisotropic scattering. Consider, by way of example, the transport equation characterizing time-dependent neutron thermalization

$$\frac{\partial n}{\partial t} = \left[-\mathbf{v} \cdot \nabla \circ - v \Sigma_t \circ + \int d^3 v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) \circ \right] n(\mathbf{r}, \mathbf{v}, t) \equiv \mathcal{L} n \quad (4.46)$$

To simplify, we avoid the explicit treatment of the source term and treat this as an initial value problem. We also assume $1/v$ absorption for convenience, $\Sigma_a(v) = \Sigma_a^0/v$. The simplest choice of a projection operator would be

$$P \circ \equiv M(\mathbf{v}) \int d^3 v' \circ$$

where $M(\mathbf{v})$ is the normalized Maxwellian distribution. This projection

operator selects out the number density

$$n_{\parallel} = Pn = M(\mathbf{v}) \int d^3v n(\mathbf{r}, \mathbf{v}, t) \equiv M(\mathbf{v}) N(\mathbf{r}, t)$$

If we now apply this projection operator to Eq. 4.46 in the usual fashion to find

$$\frac{\partial n_{\parallel}}{\partial t} - P \mathcal{L} n_{\parallel} = \int_0^t d\tau P \mathcal{L} e^{\tau(1-P)\mathcal{L}} (1-P) \mathcal{L} n_{\parallel}(t-\tau) + P \mathcal{L} e^{t(1-P)\mathcal{L}} n_{\perp}(0)$$

then integrate this equation over energy and angle, we arrive at a generalized diffusion equation of the form

$$\frac{\partial N}{\partial t} + \Sigma_a^0 N(\mathbf{r}, t) = \int_0^t d\tau \nabla \cdot \mathbf{D}(\mathbf{r}, \tau) \cdot \nabla N(\mathbf{r}, t-\tau) + \mathcal{S}(\mathbf{r}, t)$$

where

$$\mathbf{D}(\mathbf{r}, t) \equiv \int d^3v \mathbf{v} e^{\tau(1-P)\mathcal{L}} \mathbf{v} M(\mathbf{v})$$

v Linearized Boltzmann equation. The same idea can be used to develop contracted descriptions for any linear transport equation.^{29,30} For example, consider the linearized Boltzmann equation

$$\frac{\partial \varphi}{\partial t} + \mathbf{v} \cdot \nabla \varphi = \int d^3v_1 \int d\hat{\Omega} |\mathbf{v} - \mathbf{v}_1| \sigma n_0(\mathbf{v}_1) [\varphi(\mathbf{v}') + \varphi(\mathbf{v}'_1) - \varphi(\mathbf{v}) - \varphi(\mathbf{v}_1)]$$

Then the appropriate projection to generate a continuum description seeks to contract the description of $\varphi(\mathbf{r}, \mathbf{v}, t)$ to its hydrodynamic moments

$$\begin{bmatrix} \frac{n_1(\mathbf{r}, t)}{n_0} \\ \frac{\mathbf{u}(\mathbf{r}, t)}{T_1(\mathbf{r}, t)} \\ \frac{T_1(\mathbf{r}, t)}{T_0} \end{bmatrix} \equiv \int d^3v \varphi(\mathbf{r}, \mathbf{v}, t) \begin{bmatrix} 1 \\ \mathbf{v} \\ \frac{mv^2}{3kT_0} - 1 \end{bmatrix} \equiv \int d^3v \varphi(\mathbf{v}) \mathbf{a}(\mathbf{v})$$

The corresponding projection operator then becomes

$$P\varphi = \langle \varphi \mathbf{a}^* \rangle \cdot \langle \mathbf{a} \mathbf{a}^* \rangle^{-1} \cdot \mathbf{a} = \frac{n_1}{n_0} + \frac{m}{kT_0} \mathbf{u} \cdot \mathbf{v} + \frac{3}{2} \frac{T_1}{T_0} \left(\frac{mv^2}{3kT_0} - 1 \right)$$

Then if we apply this projection operator to the linearized Boltzmann equation, we arrive at a generalization of the linearized hydrodynamics equations.^{29,30} Although these equations are of considerable interest, we postpone their study until we have generalized this projection or contraction procedure to nonlinear transport equations.

4.3 □ THE EQUATIONS OF HYDRODYNAMICS □ We now turn our attention to the derivation of a continuum description of collective phenomena.³¹⁻³⁵ That is, we consider how one can derive the equations of hydrodynamics for a fluid (whether liquid, gas, or plasma). For simplicity, we take as our starting point the transport equation describing a single species fluid

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial n}{\partial \mathbf{v}} = \left(\frac{\partial n}{\partial t} \right)_{\text{coll}} \quad (4.47)$$

We leave the collision term unspecified for now, requiring only that it be local in both time and space and that it conserve particle mass, momentum, and energy in a collision.

We first develop the conservation equations corresponding to these conserved quantities, then describe the most popular schemes for closing this set of equations and generate the corresponding transport laws.

4.3.1 □ The Conservation Equations □ We begin by taking the moments of the transport equation (4.47) with respect to the collisional invariants

$$\psi_1 = m, \quad \psi_2 = m\mathbf{v}, \quad \psi_3 = \frac{1}{2} m |\mathbf{v} - \mathbf{u}(\mathbf{r}, t)|^2$$

The macroscopic counterparts of these variables correspond to mass density,

$$\rho(\mathbf{r}, t) \equiv \int d^3v m n(\mathbf{r}, \mathbf{v}, t) \equiv \Psi_1(\mathbf{r}, t)$$

momentum density,

$$\rho(\mathbf{r}, t) \mathbf{u}(\mathbf{r}, t) \equiv \int d^3v m \mathbf{v} n(\mathbf{r}, \mathbf{v}, t) \equiv \Psi_2(\mathbf{r}, t)$$

and kinetic energy density

$$\frac{3}{2m} \rho(\mathbf{r}, t) \theta(\mathbf{r}, t) \equiv \int d^3v \frac{m}{2} |\mathbf{v} - \mathbf{u}(\mathbf{r}, t)|^2 n(\mathbf{r}, \mathbf{v}, t) \equiv \Psi_3(\mathbf{r}, t)$$

where $\mathbf{u}(\mathbf{r}, t)$ is the local fluid velocity and $\theta(\mathbf{r}, t) = kT(\mathbf{r}, t)$ is the local (kinetic) temperature.

The general form of the moment (or Maxwell transfer) equations can be written as follows:

$$\begin{aligned} \frac{\partial}{\partial t} \int d^3v \psi_i n - \int d^3v \frac{\partial \psi_i}{\partial t} n + \frac{\partial}{\partial \mathbf{r}} \cdot \int d^3v \mathbf{v} \psi_i n \\ - \int d^3v \mathbf{v} \cdot \frac{\partial \psi_i}{\partial \mathbf{r}} n - \frac{\mathbf{F}}{m} \cdot \int d^3v \frac{\partial \psi_i}{\partial \mathbf{v}} n = 0 \end{aligned} \quad (4.48)$$

where we recall that the moment of the collision term $(\partial n / \partial t)_{\text{coll}}$ with respect to a collisional invariant ψ_i vanishes. We can specialize these to the case of each moment of interest. First consider $\psi_1 = m$. Since this variable does not depend on $\mathbf{r}$, $\mathbf{v}$, or t , we find immediately that the moment equation becomes

$$\frac{\partial}{\partial t} \int d^3v m n + \frac{\partial}{\partial \mathbf{r}} \cdot \int d^3v m \mathbf{v} n = 0$$

or

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot \rho \mathbf{u} = 0$$

which is identified as the usual mass *continuity equation*.

Next we consider $\psi_2 = m\mathbf{v}$, which depends only on the velocity $\mathbf{v}$. Then Eq. 4.48 becomes

$$\frac{\partial}{\partial t} \int d^3v m v_i n + \frac{\partial}{\partial x_j} \int d^3v v_j v_i m n - \frac{F_j}{m} \int d^3v \frac{\partial v_i}{\partial v_j} m n = 0 \quad (4.49)$$

where we have chosen to employ the summation convention to handle the vector calculus. To simplify this equation, we can write

$$\int d^3v v_j v_i m n = m \int d^3v (v_j - u_j)(v_i - u_i) n + \rho u_j u_i$$

and define the pressure tensor P_{ij} by

$$P_{ij} \equiv m \int d^3v (v_i - u_i)(v_j - u_j) n$$

This allows us to write Eq. 4.49 as

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) + \frac{\partial}{\partial x_j} P_{ij} - \rho \frac{F_i}{m} = 0$$

or in vector notation

$$\rho \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \frac{\partial}{\partial \mathbf{r}} \right) \mathbf{u} - \frac{\rho}{m} \mathbf{F} = - \frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{P}$$

—the equation of motion for the fluid.

Finally we consider $\psi_3 = (m/2)|\mathbf{v} - \mathbf{u}(\mathbf{r}, t)|^2$. We must be somewhat more careful, since ψ_3 depends on $\mathbf{r}$ and t as well as $\mathbf{v}$. The moment equation is then

$$\int d^3v \frac{m}{2} (v_j - u_j)(v_j - u_j) \frac{\partial n}{\partial t} + \int d^3v \frac{m}{2} (v_j - u_j)(v_j - u_j) v_i \frac{\partial n}{\partial x_i} = 0 \quad (4.50)$$

If we define the heat flux vector

$$q_i \equiv m \int d^3v \frac{m}{2} (v_i - u_i) |\mathbf{v} - \mathbf{u}|^2 n$$

and use the continuity equation, we can manipulate Eq. 4.50 into the form

$$\rho c_v \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \frac{\partial}{\partial \mathbf{r}} \right) \theta = - \frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{q} - \mathbf{P} : \Lambda$$

where $c_v = \frac{3}{2}$ for this ideal, single species fluid and we define

$$\Lambda_{ij} \equiv \frac{m}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

For convenience, we collect together the conservation equations:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} &= 0 & (\text{mass}) \\ \rho \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{u} - \frac{\rho}{m} \mathbf{F} &= - \nabla \cdot \mathbf{P} & (\text{momentum}) \\ \rho c_v \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \theta &= - \nabla \cdot \mathbf{q} - \mathbf{P} : \Lambda & (\text{energy}) \end{aligned} \quad (4.51)$$

Notice that though exact, these equations are as yet incomplete, since both $\mathbf{P}$ and $\mathbf{q}$ are given only in terms of the full distribution function $n(\mathbf{r}, \mathbf{v}, t)$

$$P_{ij} = m \int d^3v (v_i - u_i)(v_j - u_j) n(\mathbf{r}, \mathbf{v}, t) \quad (4.52)$$

$$q_i = m \int d^3v \frac{m}{2} (v_i - u_i) |\mathbf{v} - \mathbf{u}|^2 n(\mathbf{r}, \mathbf{v}, t) \quad (4.53)$$

Hence we next evaluate these quantities.

4.3.2 □ A Zeroth Order Approximation: The Euler Equations □ We now introduce suitable approximations to the distribution function $n(\mathbf{r}, \mathbf{v}, t)$ that will facilitate the calculation of $\mathbf{P}$ and $\mathbf{q}$. The simplest such approximation would be to replace $n(\mathbf{r}, \mathbf{v}, t)$ by the local Maxwell-Boltzmann distribution

$$n(\mathbf{r}, \mathbf{v}, t) \sim n_0(\mathbf{v}) \equiv N(\mathbf{r}, t) \left(\frac{m}{2\pi\theta(\mathbf{r}, t)} \right)^{3/2} \exp\left(-\frac{m}{2\theta} |\mathbf{v} - \mathbf{u}|^2 \right)$$

Substituting this into Eqs. 4.52 and 4.53, we find

$$P_{ij} \cong m \int d^3v (v_i - u_i)(v_j - u_j) n_0 = N(\mathbf{r}, t) \theta(\mathbf{r}, t) \delta_{ij} \equiv p(\mathbf{r}, t) \delta_{ij}$$

$$q_i \cong m \int d^3v \frac{m}{2} (v_i - u_i) |\mathbf{v} - \mathbf{u}|^2 n_0 = 0$$

where we have identified the local hydrostatic pressure

$$p(\mathbf{r}, t) = N(\mathbf{r}, t) \theta(\mathbf{r}, t)$$

Thus we have closed the set of equations (4.51) to find

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\rho \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{u} - \rho \frac{\mathbf{F}}{m} = -\nabla p$$

$$\rho c_v \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \theta = -(\nabla \cdot \mathbf{u}) \theta$$

which are, of course, just the *Euler equations* for an inviscid fluid.³⁶ But we

know that real fluids exhibit dissipative phenomena such as viscosity and thermal conduction. Therefore replacing $n(\mathbf{r}, \mathbf{v}, t)$ by $n_0(\mathbf{v})$ is not sufficient to yield the known behavior of real fluids. We must seek a better approximation to $n(\mathbf{r}, \mathbf{v}, t)$.

4.3.3 □ The Chapman-Enskog Expansion³⁶ □ We now specify the collision term as the Boltzmann collision operator (although the technique we describe applies to a variety of other collision operators as well):

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial n}{\partial \mathbf{v}} = \int d^3v_1 \int d\hat{\Omega} |\mathbf{v} - \mathbf{v}_1| \sigma(n' n'_1 - n n_1) = J(n, n) \quad (4.54)$$

One of the most popular problems in kinetic theory concerns the derivation of the equations of hydrodynamics (including the transport laws) directly from this equation. Although Hilbert³⁷ was the first to prove the existence of a class of solutions to the Boltzmann equation (so-called normal solutions) that were determined entirely by the initial values of hydrodynamic variables corresponding to collisional invariants (mass, momentum, and kinetic energy), Chapman and Enskog³⁸ were the first to develop a systematic procedure to derive the corresponding hydrodynamic equations (and their higher order corrections) for these variables. Although a variety of alternative schemes have been proposed to generate approximate solutions to the Boltzmann equation (including the 13-moment method of Grad,³⁹ generalized polynomial expansions,⁴⁰ bimodal distribution functions⁴¹⁻⁴³), the Chapman-Enskog method (and equations) remain the most popular scheme for generating hydrodynamic equations from Boltzmann-like kinetic equations.

We have noted that the simple-minded replacement of $n(\mathbf{r}, \mathbf{v}, t)$ by a local Maxwell-Boltzmann distribution $n_0(\mathbf{v})$ is too crude for most applications. Suppose instead that we seek an approximation to n which like n_0 is not explicitly a function of time,^{31,36} but rather depends on time only through its dependence on the hydrodynamic variables $\rho(\mathbf{r}, t)$, $\mathbf{u}(\mathbf{r}, t)$, and $\theta(\mathbf{r}, t)$ as $n(\mathbf{r}, \mathbf{v}, t) = n(\mathbf{r}, \mathbf{v} | \rho, \mathbf{u}, \theta)$. More specifically, we seek a solution by successive approximation

$$n = \zeta^{-1} n^{(0)} + n^{(1)} + \zeta n^{(2)} + \dots \quad (4.55)$$

where ζ is merely an order parameter to keep track of the size of the terms. (We set it equal to 1 eventually.)

We will require that $n^{(0)}$, whatever it turns out to be, yield the correct moments corresponding to collisional invariants

$$\int d^3v \left[\begin{matrix} m \\ m\mathbf{v} \\ \frac{m}{2}|\mathbf{v}-\mathbf{u}|^2 \end{matrix} \right] n^{(0)}(\mathbf{v}) = \left[\begin{matrix} \rho \\ \rho\mathbf{u} \\ \frac{3}{2}N\theta \end{matrix} \right]$$

Then, of course, we must also require

$$\int d^3v \left[\begin{matrix} m \\ m\mathbf{v} \\ \frac{m}{2}|\mathbf{v}-\mathbf{u}|^2 \end{matrix} \right] n^{(l)}(\mathbf{v}) = 0, \quad l > 0$$

If we can evaluate each of the terms in the expansion Eq. 4.55, we can compute

$$P_{ij} = \sum_{l=0}^{\infty} \zeta^l P_{ij}^{(l)}$$

$$q_i = \sum_{l=0}^{\infty} \zeta^l q_i^{(l)}$$

where

$$P_{ij}^{(l)} \equiv m \int d^3v (v_i - u_i)(v_j - u_j) n^{(l)}$$

$$q_i^{(l)} \equiv m \int d^3v \frac{m}{2} (v_i - u_i) |\mathbf{v} - \mathbf{u}|^2 n^{(l)}$$

Therefore all we need to do is develop a consistent scheme to calculate the $n^{(l)}$. To accomplish this, we decompose the Boltzmann equation (4.54) into successive equations for the $n^{(l)}$.

First note that if we assume that the distribution function $n(\mathbf{r}, \mathbf{v}, t)$ we are trying to construct depends on time only implicitly through $\rho(\mathbf{r}, t)$, $\mathbf{u}(\mathbf{r}, t)$, and $\theta(\mathbf{r}, t)$, then

$$\frac{\partial n}{\partial t} = \frac{\partial n}{\partial \rho} \frac{\partial \rho}{\partial t} + \frac{\partial n}{\partial u_i} \frac{\partial u_i}{\partial t} + \frac{\partial n}{\partial \theta} \frac{\partial \theta}{\partial t}$$

We can expand each term in this derivative as

$$\frac{\partial n}{\partial \rho} = \frac{1}{\zeta} \left(\frac{\partial n^{(0)}}{\partial \rho} + \zeta \frac{\partial n^{(1)}}{\partial \rho} + \cdots \right), \dots$$

and then identify orders as

$$\frac{\partial}{\partial t} = \frac{\partial_0}{\partial t} + \zeta \frac{\partial_1}{\partial t} + \zeta^2 \frac{\partial_2}{\partial t} + \dots$$

where the $\partial_n/\partial t$ are defined by

$$\frac{\partial_0}{\partial t} \rho \equiv - \frac{\partial}{\partial x_i} (\rho u_i); \quad \frac{\partial_n}{\partial t} \rho \equiv 0, \quad n > 0$$

$$\frac{\partial_0}{\partial t} u_i \equiv - u_j \frac{\partial u_i}{\partial x_j} + \frac{F_i}{m} - \frac{1}{\rho} \frac{\partial P_{ij}^{(0)}}{\partial x_j}; \quad \frac{\partial_n}{\partial t} u_i \equiv \frac{1}{\rho} \frac{\partial P_{ij}^{(n)}}{\partial x_j}, \quad n > 0$$

$$\frac{\partial_0}{\partial t} \theta \equiv - u_j \frac{\partial \theta}{\partial x_j} - \frac{2}{3} \frac{1}{\rho} \frac{\partial q_i^{(0)}}{\partial x_i} - \frac{2}{3} \frac{1}{\rho} \Lambda_{ij} P_{ij}^{(0)};$$

$$\frac{\partial_n}{\partial t} \theta = - \frac{2}{3} \frac{1}{\rho} \left(\frac{\partial q_i^{(n)}}{\partial x_i} + \Lambda_{ij} P_{ij}^{(n)} \right), \quad n > 0$$

That is, we identify the lowest order with the Euler equations (as we see later), while higher orders correspond to the dissipative transport terms.

Therefore we can expand

$$\frac{\partial n}{\partial t} = \frac{1}{\zeta} \left(\frac{\partial_0}{\partial t} + \zeta \frac{\partial_1}{\partial t} + \zeta^2 \frac{\partial_2}{\partial t} + \dots \right) (n^{(0)} + \zeta n^{(1)} + \zeta^2 n^{(2)} + \dots)$$

In a similar fashion,

$$\begin{aligned} \left(\mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial}{\partial \mathbf{v}} \right) n &= \frac{1}{\zeta} \left[\left(\mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial}{\partial \mathbf{v}} \right) n^{(0)} \right. \\ &\quad + \zeta \left(\mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial}{\partial \mathbf{v}} \right) n^{(1)} \\ &\quad \left. + \zeta^2 \left(\mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial}{\partial \mathbf{v}} \right) n^{(2)} + \dots \right] \end{aligned}$$

Finally, we expand the collision term as

$$J(n, n) = \frac{1}{\zeta^2} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \zeta^{n+m} J(n^{(n)}, n^{(m)}) \equiv \frac{1}{\zeta^2} \sum_{n=0}^{\infty} \zeta^n J^{(n)}$$

where

$$J^{(n)}(n^{(0)}, n^{(1)}, \dots, n^{(n)}) \equiv \sum_{r+s=n} J(n^{(r)}, n^{(s)})$$

If we now put all these pieces together, we can write Eq. 4.54 as

$$\begin{aligned} \frac{1}{\zeta} \left[\left(\frac{\partial_0}{\partial t} + \zeta \frac{\partial_1}{\partial t} + \zeta^2 \frac{\partial_2}{\partial t} \right) + \left(\mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial}{\partial \mathbf{v}} \right) \right] [n^{(0)} + \zeta n^{(1)} + \zeta^2 n^{(2)} + \dots] \\ = \frac{1}{\zeta^2} [J^{(0)}(n^{(0)}, n^{(0)}) + \zeta J^{(1)}(n^{(0)}, n^{(1)}) + \zeta^2 J^{(2)}(n^{(0)}, n^{(1)}, n^{(2)}) + \dots] \end{aligned}$$

Now we follow the usual procedure for dealing with such ordered expansions by demanding that the coefficients of each power of ζ vanish separately:

$$\begin{aligned} (0) \quad J^{(0)}(n^{(0)}, n^{(0)}) &= 0 \\ (1) \quad \frac{\partial_0}{\partial t} n^{(0)} + \left(\mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial}{\partial \mathbf{v}} \right) n^{(0)} &= J^{(1)}(n^{(0)}, n^{(1)}) \\ (2) \quad \frac{\partial_0}{\partial t} n^{(1)} + \frac{\partial_1}{\partial t} n^{(0)} + \left(\mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial}{\partial \mathbf{v}} \right) n^{(1)} &= J^{(2)}(n^{(0)}, n^{(1)}, n^{(2)}) \end{aligned}$$

One can verify that such a scheme will indeed produce a solution of the form of Eq. 4.55.

Let us examine the more practical question of how these equations can be solved. The zeroth order equation is just

$$J(n^{(0)}, n^{(0)}) = 0$$

which yields the expected zeroth order solution

$$n^{(0)} = n_0 = \left(\frac{\rho}{m} \right) \left(\frac{m}{2\pi\theta} \right)^{3/2} \exp \left(- \frac{m|\mathbf{v} - \mathbf{u}|^2}{2\theta} \right)$$

To solve for the next order, we first note

$$\begin{aligned} \left[\frac{\partial_0}{\partial t} + \left(\mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial}{\partial \mathbf{v}} \right) \right] n_0 &= \left[U_i \left(\frac{m}{2\theta} U^2 - \frac{5}{2} \right) \frac{1}{\theta} \frac{\partial \theta}{\partial x_i} \right. \\ &\quad \left. + \frac{1}{\theta} \left(U_i U_j - \frac{1}{3} \delta_{ij} U^2 \right) \Lambda_{ij} \right] n_0 \end{aligned}$$

where $\mathbf{U} \equiv \mathbf{v} - \mathbf{u}$. Furthermore, we note

$$\begin{aligned} J^{(1)}(n^{(0)}, n^{(1)}) &= \int d^3 v_1 \int d\hat{\Omega} |\mathbf{v} - \mathbf{v}_1| \sigma n_0 [n^{(1)}(\mathbf{v}') + n^{(1)}(\mathbf{v}_1') - n^{(1)}(\mathbf{v}) - n^{(1)}(\mathbf{v}_1)] \\ &\equiv L[n^{(1)}] \end{aligned}$$

which is just the linearized Boltzmann collision operator L .

Therefore we must solve

$$L[n^{(1)}] = \left[\frac{1}{\theta} \left(\frac{m}{2\theta} U^2 - \frac{5}{2} \right) U_i \frac{\partial \theta}{\partial x_i} + \frac{1}{\theta} \left(U_i U_j - \frac{1}{3} \delta_{ij} U^2 \right) \Lambda_{ij} \right] n_0$$

Let us suppose we can invert L , and continue to study the implications of the first order solutions. Then we find³¹

$$\begin{aligned} P_{ij}^{(1)} &= -\frac{m}{\theta} \Lambda_{kl} \int d^3U U_i U_j L^{-1} \left[\left(U_k U_l - \frac{1}{3} \delta_{kl} U^2 \right) n_0(U) \right] \\ &= -\frac{2\mu}{m} \left(\Lambda_{ij} - \frac{m}{3} \delta_{ij} \nabla \cdot \mathbf{u} \right) \end{aligned} \quad (4.56)$$

and

$$q_i^{(1)} = -\frac{m^2}{2} \int d^3U U_i U^2 L^{-1} \left[U_j \left(\frac{m}{2\theta} U^2 - \frac{5}{2} \right) n_0(U) \right] \frac{\partial \theta}{\partial x_j} = -k \frac{\partial \theta}{\partial x_j} \quad (4.57)$$

Here we have introduced some simplifications that arise from the parity of the integrands and formally defined the thermal conductivity k and the shear viscosity μ .

Of course the general inversion of the linearized Boltzmann collision operator L is quite difficult and usually involves a numerical evaluation. A particularly simple example³² corresponds to the BGK model in which $L^{-1} \rightarrow \nu^{-1}$. Then Eqs. 4.56 and 4.57 can be evaluated to find

$$k = \frac{5}{2} \frac{\rho \theta}{m \nu}, \quad \mu = \frac{\rho \theta}{m \nu}$$

The hydrodynamics equations to first order are therefore

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 \\ \rho \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{u} - \frac{\rho \mathbf{F}}{m} &= -\nabla p + \frac{1}{3} \nabla \mu \nabla \cdot \mathbf{u} + \mu \nabla^2 \mathbf{u} \\ \rho c_v \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \theta &= -\rho (\nabla \cdot \mathbf{u}) \theta + \nabla \cdot k \nabla \theta \end{aligned}$$

The equation of motion is now referred to as the *Navier-Stokes equation*, and the expression for the thermal heat flux is known as *Fourier's law*. For

this reason the first order of the Chapman-Enskog method is sometimes known as *Navier-Stokes* or *Navier-Stokes-Fourier hydrodynamics*.

Higher orders $n^{(l)}$ can be worked out in a very similar fashion (although the technical details become quite complicated). For example, the second order is known as the *Burnett equations*.³⁶ As we indicate later, however, these higher order corrections to conventional (i.e., Navier-Stokes) hydrodynamics are rarely worth the extra calculational effort required for their implementation.

4.3.4 □ Alternative Expansion Schemes □ In the Chapman-Enskog method, the Navier-Stokes equations (and their generalizations) appear as first (or higher) order corrections to the Euler equations. It is natural to develop the approximate form of the distribution function in terms of its first five moments (number or mass density, fluid velocity, and temperature) and their gradients. That is, one demands that the distribution function $n(\mathbf{r}, \mathbf{v}, t)$ be a time-independent functional of the hydrodynamic variables ρ , $\mathbf{u}$, and θ .

Certainly, to the extent that the solutions of the Boltzmann equation approach local equilibrium, such a constraint seems appropriate. But for highly nonequilibrium behavior, $n(\mathbf{r}, \mathbf{v}, t)$ may not approach a time-independent functional of ρ , $\mathbf{u}$, and θ —and, indeed, the system may not be adequately described by conventional hydrodynamics (or its generalizations as constructed by the Chapman-Enskog method).

An alternative scheme for developing approximations to the phase space density seeks to expand $n(\mathbf{r}, \mathbf{v}, t)$ about some known “zeroth order” function $n^{(0)}(\mathbf{r}, \mathbf{v}, t)$ as

$$n(\mathbf{r}, \mathbf{v}, t) = n^{(0)}(\mathbf{r}, \mathbf{v}, t) \sum_p a_p(\mathbf{r}, t) M_p(\mathbf{v}; \mathbf{r}, t)$$

where the M_p are some appropriately chosen complete set of functions in velocity space (which may depend on $\mathbf{r}$ and t).⁴⁴ The unknown expansion coefficients $a_p(\mathbf{r}, t)$ then play the role of state variables in this reduced description of the system. For example, one might choose $n^{(0)} = n_0$, the LTE distribution, and the $M_p(\mathbf{v})$ would be some appropriate set of polynomials in velocity, such as the Hermite polynomials (this is the particular approximation first studied by Grad).⁴⁵

We can obtain a set of equations for the $a_p(\mathbf{r}, t)$ as follows: first multiply the Boltzmann equation (4.47) by M_p and integrate over $\mathbf{v}$ to obtain a set of moment equations

$$\begin{aligned} \frac{\partial}{\partial t} \int d^3v M_p n - \int d^3v \frac{\partial M_p}{\partial t} n + \frac{\partial}{\partial \mathbf{r}} \cdot \int d^3v \mathbf{v} M_p n \\ - \int d^3v \mathbf{v} \cdot \frac{\partial M_p}{\partial \mathbf{r}} n - \frac{\mathbf{F}}{m} \cdot \int d^3v \frac{\partial M_p}{\partial \mathbf{v}} n = C[M_p] \end{aligned} \quad (4.58)$$

where we have transformed the collision term into

$$\int d^3v M_p(\mathbf{v}) J(n, n) = \int d^3v \int d^3v_1 \int d\hat{\Omega} |\mathbf{v} - \mathbf{v}_1| \sigma n n_1 [M_p(\mathbf{v}') - M_p(\mathbf{v})] \\ \equiv C[M_p]$$

Since the set $\{M_p\}$ is complete, all the derivatives $\partial M_p / \partial t$, $\partial M_p / \partial \mathbf{v}$, and $\partial M_p / \partial \mathbf{r}$ can be expressed in terms of other M_p (generally an infinite series). It is useful to choose the M_p to be orthogonal with weight function $n^{(0)}$

$$\int d^3v n^{(0)} M_p M_q = \delta_{pq}$$

Then the first term in Eq. 4.58 simplifies to

$$\frac{\partial}{\partial t} \int d^3v M_p n = \frac{\partial}{\partial t} \sum_q a_q \int d^3v n^{(0)} M_p M_q = \frac{\partial a_p}{\partial t}$$

In practice then, one would truncate this expansion at some (usually low) order.

By way of example, consider *Grad's 13-moment* approximation⁴⁵ in which $n(\mathbf{r}, \mathbf{v}, t)$ is approximated by the expansion

$$n(\mathbf{r}, \mathbf{v}, t) = n_0(\mathbf{r}, \mathbf{v}, t) \left\{ 1 + \frac{P_{ij}}{2pRT} v_i v_j - \frac{q_i}{pRT} v_i \left(1 - \frac{v^2}{5RT} \right) \right\}$$

(the name arises since only part of the third order state variables are retained, corresponding to 13 such variables: ρ , u_i , T , P_{ij} , and q_i).

This particular approach then yields the usual conservation equations for ρ , u_i , and T :

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0$$

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j + P_{ij}) = 0$$

$$\frac{\partial}{\partial t} \left[\rho \left(e + \frac{1}{2} u^2 \right) \right] + \frac{\partial}{\partial x_j} \left[\rho u_j \left(e + \frac{1}{2} u^2 \right) + u_k P_{kj} + q_j \right] = 0$$

Here, $p \equiv (\frac{1}{3}) P_{ii}$ and the reduced stress tensor or stress deviation is $p_{ij} \equiv P_{ij} - p \delta_{ij}$, which has the property that $p_{ii} = 0$. The temperature is given by $T = p / R \rho = 2e / 3R$, where R is the gas constant. The equations for p_{ij} and

q_i are rather complex:

$$\begin{aligned} \frac{\partial p_{ij}}{\partial t} + \frac{\partial}{\partial x_r} (u_r p_{ij}) + \frac{2}{5} \left(\frac{\partial q_i}{\partial x_j} + \frac{\partial q_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial q_r}{\partial x_r} \right) + p_{ir} \frac{\partial u_j}{\partial x_r} + p_{jr} \frac{\partial u_i}{\partial x_r} \\ - \frac{2}{3} \delta_{ij} p_{rs} \frac{\partial u_r}{\partial x_s} + p \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_r}{\partial x_r} \right) + \beta p_{ij} \rho = 0 \\ \frac{\partial q_i}{\partial t} + \frac{\partial}{\partial x_r} (u_r q_i) + \frac{7}{5} q_r \frac{\partial u_i}{\partial x_r} + \frac{2}{5} q_r \frac{\partial u_r}{\partial x_i} + \frac{2}{5} q_i \frac{\partial u_r}{\partial x_r} + RT \frac{\partial p_{ir}}{\partial x_r} \\ + \frac{7}{2} p_{ir} \frac{\partial}{\partial x_r} RT - \frac{p_{ir}}{\rho} \frac{\partial p_{rs}}{\partial x_s} + \frac{5}{2} p \frac{\partial}{\partial x_i} RT + \frac{2}{3} \beta \rho q_i = 0 \end{aligned}$$

It should be noted, however, that only the single collision parameter β enters. This is given by

$$\beta(RT) = \frac{2}{5} (2\pi)^{1/2} \int_0^\infty dx x^6 e^{-x^2/2} \left[\int d\theta \sin^2 \theta \cos^2 \theta \sigma(x \sqrt{2RT}, \theta) \right]$$

Hence in the Grad 13-moment method, the conventional hydrodynamics equations are augmented by separate equations for the pressure tensor p_{ij} and heat flux q_i which replace the traditional laws of Stokes and Fourier.

4.3.5 □ Perturbation Theory Derivations of Continuum Descriptions □

Both the Chapman-Enskog and Hilbert methods can be interpreted as perturbation expansions in the Knudsen number³⁵

$$\text{Kn} = \frac{\text{mfp}}{\text{characteristic length}} \equiv \epsilon$$

This parameter enters the Boltzmann equation as

$$\epsilon \left(\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} \right) = J(n, n)$$

Since we note that $\epsilon \rightarrow \infty$ corresponds to streaming or free molecular flow, while $\epsilon \rightarrow 0$ corresponds to continuum flow, it is apparent that we wish to develop approximations that are valid for small ϵ . But since ϵ multiplies the derivatives in the Boltzmann equation, it is also apparent that we have a singular perturbation problem.

Hilbert³⁷ proposed to seek the distribution function as a power series in ϵ

$$n = \sum_{n=0}^{\infty} \epsilon^n n^{(n)}$$

This expansion yields to each order in ε a sequence of equations of the form

$$\frac{\partial}{\partial t} n^{(n-1)} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} n^{(n-1)} = J_n(n)$$

where

$$J_0 \equiv 0, \quad J_n \equiv 2J(n^{(0)}, n^{(n)}) + \sum_{k=1}^{n-1} J(n^{(k)}, n^{(n-k)})$$

One can construct solutions to these equations and extract a continuum theory in terms of the usual mass density, local velocity, and temperature variables. But in Hilbert's expansion, these quantities obey the inviscid fluid (Euler) equations. Furthermore the expansion is asymptotic in the sense that the solution will be valid only for certain limited regions of space and time. Indeed, one finds that the solutions obtained by the Hilbert expansion are invalid in just the regions that couple to the initial and boundary conditions for the Boltzmann equation (the so-called Hilbert paradox).

Hence one turns instead to the Chapman-Enskog method in which not the solution but rather the Boltzmann equation itself is expanded in powers of ε . This procedure, coupled with the functional ansatz that the distribution function depends on time only through its dependence on the hydrodynamic variables $\rho(\mathbf{r}, t)$, $\mathbf{u}(\mathbf{r}, t)$, and $T(\mathbf{r}, t)$, leads to the usual Navier-Stokes-Fourier equations, the Burnett equations, and so on, to each order in ε . Once again, however, one encounters difficulties in "connecting" these solutions to initial and boundary data. Furthermore, the significance of the higher order equations (Burnett, super-Burnett, etc.) is still unknown, and the latter equations are rarely applied in practice.

Such perturbation expansions in $\varepsilon = \text{Kn}$ are basically different from the expansions used to linearize the Boltzmann equation.³⁵ In the latter case, one essentially expands in a parameter characterizing the deviation of the initial or boundary distribution from a global Maxwell-Boltzmann distribution. There have been numerous studies of the convergence properties of the Hilbert and Chapman-Enskog expansions for linearized kinetic equations.^{46,47} However the application of such perturbation expansions to complicated nonlinear equations such as the Boltzmann equation is a difficult mathematical problem that continues to receive active study.

4.3.6 □ Generalized Hydrodynamics Equations □ We noted earlier in this chapter that the derivation of the diffusion equation from a linear transport equation could be interpreted as a projection of the phase space

density $n(\mathbf{r}, \mathbf{v}, t)$ onto a reduced description in terms of continuum variables such as the particle density $N(\mathbf{r}, t)$. The concept of a projection from a phase space to a configuration space or hydrodynamic description was formalized and used to derive an exact generalized diffusion equation. We also noted in passing that the same technique can be used to develop generalized hydrodynamics equations from the linearized Boltzmann equation.

More specifically, one can project the solution of the linearized Boltzmann equation onto an absolute equilibrium distribution, weighted by the usual collisional invariants corresponding to mass, momentum, and kinetic energy.^{29,30} This yields a set of exact (but formal) linearized hydrodynamics equations in which the transport coefficients (viscosity, thermal conductivity) become space- and time-dependent kernels in integral terms. Moreover there are initial value terms in these generalized hydrodynamics equations that cannot be specified in terms of the initial values of hydrodynamic variables alone (i.e., that do not correspond to Hilbert's normal solutions³⁷). If the transport kernels are expanded in terms of the spatial gradients of hydrodynamic variables, one recovers the conventional transport laws and their generalizations (i.e., Navier-Stokes, Burnett, etc.). Such an approach is useful not only because it provides an alternative derivation of the well-known Chapman-Enskog results, but it also suggests alternative types of approximate transport laws that are more capable of describing large frequency,⁴⁸ short wavelength phenomena. Moreover a study of the initial value terms reveals the manner in which a gas approaches a hydrodynamic state, thereby providing a direct resolution of the Hilbert paradox.^{37,34} That is, this approach explains in what sense the initial values of ρ , $\mathbf{u}$, and T alone are sufficient to determine $n(\mathbf{r}, \mathbf{v}, t)$ for later times.

This section demonstrates that very similar techniques can be used to develop exact, generalized hydrodynamics equations from the full *nonlinear* Boltzmann equation (or similar nonlinear Boltzmannlike equations). However such a development requires a generalization of the usual concept of a projection operator to allow the projection onto time-dependent (e.g., local thermodynamic equilibrium) states. Such "projections" then become time dependent as well as nonlinear functionals of the phase space density $n(\mathbf{r}, \mathbf{v}, t)$ itself. Such operators, though certainly rather awkward in many respects, are not completely unfamiliar because Robertson,⁴⁹ Piccirelli,⁵⁰ and others⁵¹ have utilized them in nonequilibrium statistical mechanics (albeit in a formal sense) to derive generalized transport laws.

This section introduces the concept of a projection onto LTE states, then applies it to the Boltzmann equation to generate an exact set of generalized hydrodynamics equations. To provide a very concrete application of these equations, we demonstrate that the more conventional nonlinear hydrody-

dynamic descriptions (i.e., Navier-Stokes and Burnett) are easily generated by this procedure.

We begin by assuming that the gas can be adequately described by the Boltzmann equation (4.47) (or a similar Boltzmannlike equation). Actually, the following analysis uses only very general properties of the collision term $J(n, n)$ that would apply to any collision operator (e.g., the Fokker-Planck operator) that models collisions as point, instantaneous processes. Of course $J(n, n)$ in general will be a nonlinear operator. The external force $\mathbf{F}(\mathbf{r}, t)$ could also depend on $n(\mathbf{r}, \mathbf{v}, t)$, as, for example, in the Vlasov equation.

Our goal is to derive a set of generalized hydrodynamics equations for the traditional hydrodynamic variables corresponding to mass density, local flow velocity, and temperature. We have noted that these quantities can be related to averages of the various collisional invariants $\psi_i(\mathbf{v})$ over the phase space density, which we can denote symbolically by

$$\Psi_i(\mathbf{r}, t) = \int d^3v \psi_i(\mathbf{v}) n(\mathbf{r}, \mathbf{v}, t)$$

For classical point particles, we choose the collisional invariants $\psi_1 = m$, $\psi_2 = m\mathbf{v}$, and $\psi_3 = \frac{1}{2} m|\mathbf{v} - \mathbf{u}|^2$. These yield the corresponding macroscopic variables $\Psi_1(\mathbf{r}, t) = \rho(\mathbf{r}, t)$, $\Psi_2(\mathbf{r}, t) = \rho(\mathbf{r}, t)\mathbf{u}(\mathbf{r}, t)$, and $\Psi_3(\mathbf{r}, t) = (3/2m)\rho(\mathbf{r}, t)\theta(\mathbf{r}, t)$.

One of the first key results of kinetic theory was the demonstration that for long times compared to the mean time between collisions, the phase space density $n(\mathbf{r}, \mathbf{v}, t)$ approaches a time-independent functional of the hydrodynamic variables, $n(\mathbf{r}, \mathbf{v}|\Psi_i(t))$ that corresponds to a local thermodynamic equilibrium

$$n_0(\mathbf{r}, \mathbf{v}|\rho, \mathbf{u}, \theta) = \frac{\rho(\mathbf{r}, t)}{m} \left[\frac{m}{2\pi\theta(\mathbf{r}, t)} \right]^{3/2} \exp \left[-\frac{m|\mathbf{v} - \mathbf{u}(\mathbf{r}, t)|^2}{2\theta(\mathbf{r}, t)} \right]$$

Notice that the variables that appear in n_0 correspond to the true hydrodynamic variables. Hence $n_0(\mathbf{r}, \mathbf{v}, t)$ is *defined* such that

$$\Psi_i(\mathbf{r}, t) \equiv \int d^3v \psi_i(\mathbf{v}) n(\mathbf{r}, \mathbf{v}, t) = \int d^3v \psi_i(\mathbf{v}) n_0(\mathbf{r}, \mathbf{v}, t)$$

Thus $n_0(\mathbf{r}, \mathbf{v}, t)$ contains essentially all the information one needs to calculate the hydrodynamic variables n , $\mathbf{u}$, and θ . Our goal is to derive an exact equation for $n_0(\mathbf{r}, \mathbf{v}, t)$ from the Boltzmann equation (4.47) for $n(\mathbf{r}, \mathbf{v}, t)$.

To begin, let us write the Boltzmann equation Eq. 4.47 in the symbolic notation

$$\frac{\partial n}{\partial t} = -Sn + J(n, n) \quad (4.59)$$

where $S = \mathbf{v} \cdot (\partial / \partial \mathbf{r}) + (\mathbf{F}/m) \cdot (\partial / \partial \mathbf{v})$ is the streaming operator and J is the collision operator. Next we introduce an operator $P(t)$, which is defined by its action on an arbitrary function $g(\mathbf{r}, \mathbf{v}, t)$ as

$$P(t)g(\mathbf{r}, \mathbf{v}, t) = \sum_j \frac{\partial n_0}{\partial \Psi_j} \int d^3v \psi_j(\mathbf{v}) g(\mathbf{r}, \mathbf{v}, t)$$

Notice that $P(t)$ has the property that

$$P(t) \frac{\partial n}{\partial t} = \sum_j \frac{\partial n_0}{\partial \Psi_j} \int d^3v \psi_j(\mathbf{v}) \frac{\partial n}{\partial t} = \frac{\partial n_0}{\partial t}$$

Thus in a sense $P(t)$ projects the time derivative of the phase space density $\partial n / \partial t$ onto the time derivative of the LTE density $\partial n_0 / \partial t$.

To proceed further, suppose we define the deviation of $n(\mathbf{r}, \mathbf{v}, t)$ from equilibrium such that

$$n(\mathbf{r}, \mathbf{v}, t) = n_0(\mathbf{r}, \mathbf{v}, t) + n_1(\mathbf{r}, \mathbf{v}, t) \quad (4.60)$$

We will now operate with $P(t)$ on the Boltzmann equation (4.59) and use Eq. 4.60 to find

$$P \frac{\partial n}{\partial t} = \frac{\partial n_0}{\partial t} = -PSn_0 - PSn_1 + PJ[n, n] \quad (4.61)$$

But notice that

$$PJ(n, n) = \sum_j \frac{\partial n_0}{\partial \Psi_j} \int d^3v \psi_j(\mathbf{v}) J[n, n] = 0$$

since the $\psi_i(\mathbf{v})$ are collisional invariants. Hence Eq. 4.61 simplifies to

$$\frac{\partial n_0}{\partial t} + PSn_0 = -PSn_1 \quad (4.62)$$

To derive the generalized hydrodynamics equations, we now follow the usual approach and take the moments of the “projected” transport equation with respect to each of the collisional invariants $\psi_i(\mathbf{v})$. Avoiding cumbersome details, we merely note the resulting form of these moment

equations here:

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 \\ \rho \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{u} + \nabla p - \frac{\rho}{m} \mathbf{F} &= -m \frac{\partial}{\partial \mathbf{r}} \cdot \int d^3 v (\mathbf{v} - \mathbf{u})(\mathbf{v} - \mathbf{u}) n_1(\mathbf{r}, \mathbf{v}, t) \\ \rho \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \theta + \frac{\rho}{c_V} (\nabla \cdot \mathbf{u}) \theta &= -\frac{m}{2c_V} \frac{\partial}{\partial \mathbf{r}} \cdot \int d^3 v \frac{m}{3} |\mathbf{v} - \mathbf{u}|^2 (\mathbf{v} - \mathbf{u}) n_1(\mathbf{r}, \mathbf{v}, t) \\ &\quad - \frac{2}{3} m \int d^3 v (\mathbf{v} - \mathbf{u})(\mathbf{v} - \mathbf{u}) n_1(\mathbf{r}, \mathbf{v}, t) \cdot \frac{m}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)\end{aligned}$$

Thus we have arrived at a set of hydrodynamiclike equations—except that the transport terms are still expressed in terms of an unknown function $n_1(\mathbf{r}, \mathbf{v}, t)$.

If we subtract our projected equation (4.62) from the Boltzmann equation (4.59), we arrive at an equation for $n_1(\mathbf{r}, \mathbf{v}, t)$

$$\frac{\partial n_1}{\partial t} + [1 - P(t)] S n_1 - L(n_0, n_1) - J(n_1, n_1) = -[1 - P(t)] S n_0 \quad (4.63)$$

where we have identified $L(n_0, n_1) = J(n_0, n_1) + J(n_1, n_0)$ as the usual linearized Boltzmann operator. We must now solve Eq. 4.63 for n_1 in terms of n_0 . Since $J(n_1, n_1)$ is a nonlinear operator, it is not possible to explicitly represent the inversion as a linear operator. Instead we formally write (for the present)

$$n_1(\mathbf{r}, \mathbf{v}, t) = \mathcal{U}(t, 0) n_1(\mathbf{r}, \mathbf{v}, 0) - \int_0^t d\tau \mathcal{U}(t, \tau) [1 - P(\tau)] S n_0(\tau) \quad (4.64)$$

Hence to complete our derivation of generalized hydrodynamic equations, we must evaluate the “transport law”-like terms. This requires a rather tedious calculation of $(1 - P) S n_0$. We once again avoid details and note only the final form of the resulting *generalized hydrodynamics equations*:

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 \\ \rho \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{u} + \nabla p - \frac{\rho}{m} \mathbf{F} &= -\nabla \cdot \mathbf{P}' + \mathcal{D}_u(\mathbf{r}, t) \\ \rho c_V \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \theta + \rho (\nabla \cdot \mathbf{u}) \theta &= -\nabla \cdot \mathbf{q} - \Lambda : \mathbf{P}' + \mathcal{D}_\theta(\mathbf{r}, t)\end{aligned} \quad (4.65)$$

where we have identified the *generalized transport laws*

$$\begin{aligned}
 P'_{ij}(\mathbf{r}, t) &\equiv \int_0^t d\tau \left[\theta^{-1} \int d^3v I_{ij}(\mathbf{r}, \mathbf{v}, t) \mathfrak{Q}_l(t, \tau) I_{kl}(\mathbf{r}, \mathbf{v}, \tau) n_0(\tau) \right] \Lambda_{kl}(\mathbf{r}, \tau) \\
 &\quad + \int_0^t d\tau \left[\theta^{-2} \int d^3v I_{ij}(\mathbf{r}, \mathbf{v}, t) \mathfrak{Q}_l(t, \tau) J_k(\mathbf{r}, \mathbf{v}, \tau) n_0(\tau) \right] \frac{\partial \theta}{\partial r_k}(\mathbf{r}, \tau) \\
 q_i(\mathbf{r}, t) &\equiv \int_0^t d\tau \left[\theta^{-1} \int d^3v J_i(\mathbf{r}, \mathbf{v}, t) \mathfrak{Q}_l(t, \tau) I_{jk}(\mathbf{r}, \mathbf{v}, \tau) n_0(\tau) \right] \Lambda_{jk}(\mathbf{r}, \tau) \\
 &\quad + \int_0^t d\tau \left[\theta^{-2} \int d^3v J_i(\mathbf{r}, \mathbf{v}, t) \mathfrak{Q}_l(t, \tau) J_j(\mathbf{r}, \mathbf{v}, \tau) n_0(\tau) \right] \frac{\partial \theta}{\partial r_j}(\mathbf{r}, \tau)
 \end{aligned} \tag{4.66}$$

Here we have introduced the following convenient definitions:

$$\begin{aligned}
 \Lambda_{ij} &\equiv \frac{m}{2} \left(\frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i} \right), \quad p \equiv \frac{\rho \theta}{m}, \quad U \equiv \mathbf{v} - \mathbf{u}(\mathbf{r}, t) \\
 J_i(\mathbf{r}, \mathbf{v}, t) &\equiv \left(\frac{m}{2} U^2 - \frac{5}{2} \theta \right) U_i, \quad I_{ij}(\mathbf{r}, \mathbf{v}, t) \equiv m \left(U_i U_j - \frac{1}{3} \delta_{ij} U^2 \right)
 \end{aligned}$$

The functions $\mathfrak{Q}_u(\mathbf{r}, t)$ and $\mathfrak{Q}_\theta(\mathbf{r}, t)$ in Eq. 4.65 are the initial value terms corresponding to $\mathfrak{Q}_l(t, 0) n_1(\mathbf{r}, \mathbf{v}, 0)$.

It should be stressed again that the generalized hydrodynamics equations are an exact consequence of the original transport equation (4.47). However they are also of only formal interest until we introduce suitable approximations. To illustrate the usefulness of this formalism, let us demonstrate how these equations can be used to develop the conventional Chapman-Enskog approximations. Since we have already extracted n_0 in our formalism (i.e., the Euler equations), we can move directly to the calculation of the Navier-Stokes and higher order terms by writing Eq. 4.63 as

$$\begin{aligned}
 \frac{\partial n_1}{\partial t} + [1 - P(t)] S n_1 - L(n_0, n_1) - J(n_1, n_1) &= -[1 - P(t)] S n_0 \\
 &= -\theta^{-1} \mathbf{I} : \mathbf{\Lambda} - \theta^{-2} \mathbf{J} \cdot \nabla \theta
 \end{aligned} \tag{4.67}$$

To obtain the Navier-Stokes equations, we retain only lowest order terms

in Eq. 4.67 to write

$$-L(n_0, n_1) = -[1 - P(t)] S n_0$$

or

$$n_1(t) = -L^{-1}[1 - P(t)] S n_0$$

In terms of our propagator representation Eq. 4.64, we can identify that to this order

$$\mathcal{Q}_L(t, \tau) = \delta(t - \tau) L^{-1}$$

Thus our transport laws of Eq. 4.66 become

$$\begin{aligned} P'_{ij} &= \theta^{-1} \left[\int d^3v I_{ij} L^{-1} I_{kl} n_0 \right] \Lambda_{kl} + \theta^{-2} \left[\int d^3v I_{ij} L^{-1} J_k n_0 \right] \frac{\partial \theta}{\partial r_k} \\ q_i &= \theta^{-1} \left[\int d^3v J_i L^{-1} I_{jk} n_0 \right] \Lambda_{jk} + \theta^{-2} \left[\int d^3v J_i L^{-1} J_j n_0 \right] \frac{\partial \theta}{\partial r_j} \end{aligned}$$

Since L is isotropic, we note

$$\int d^3v I_{ij} L^{-1} J_k n_0 = 0 = \int d^3v J_i L^{-1} I_{jk} n_0$$

Furthermore, we can identify the usual transport coefficients

$$k = \left(\frac{1}{3\theta^2} \right) \int d^3v \mathbf{J} \cdot L^{-1} \mathbf{J} n_0$$

and

$$\mu = \left(\frac{1}{10\theta} \right) \int d^3v \mathbf{I} : L^{-1} \mathbf{I} n_0$$

to arrive at the standard Navier-Stokes-Fourier transport laws

$$\mathbf{q} = -k \nabla \theta$$

$$\mathbf{P}' = - \left(\frac{2\mu}{m} \right) \left(\Lambda - \frac{m}{3} \mathbf{I} \nabla \cdot \mathbf{u} \right)$$

To calculate the next order corrections (the Burnett equations), we must actually take into account the non-Markovian behavior. First write

$$\frac{\partial n_1}{\partial t} - L(n_0, n_1) = -[1 - P(t)] S n_0(\tau) - [1 - P(t)] S n_1(\tau) + J(n_1, n_1)$$

We can now solve for

$$\begin{aligned} n_1(t) = & - \int_0^t d\tau \vartheta(t, \tau) [1 - P(t - \tau)] S n_0(t - \tau) \\ & - \int_0^t d\tau \vartheta(t, \tau) [1 - P(t - \tau)] S n_1(t - \tau) \\ & + \int_0^t d\tau \vartheta(t, \tau) J[n_1(t - \tau), n_1(t - \tau)] + \mathcal{V}(t) \end{aligned} \quad (4.68)$$

where $\vartheta(t, \tau)$ is the propagator for the linearized Boltzmann equation

$$\frac{\partial \vartheta}{\partial t} - L[n_0, \vartheta] = \delta(t - \tau)$$

[Note here that since $n_0 = n_0(t)$, $L \rightarrow L(t)$, and we cannot write this as the usual $\exp(+tL)$ without time ordering.] To obtain the Burnett terms, we iterate Eq. 4.68, then expand the non-Markovian integrals in Taylor series expansions about t :

$$\begin{aligned} n_1(t) = & - \int_0^t d\tau \vartheta(t, \tau) \left[[1 - P(t)] S n_0(t) + \tau \frac{\partial}{\partial t} [1 - P(t)] S n_0(t) + \cdots \right] \\ & + \int_0^t d\tau \vartheta(t, \tau) [1 - P(t - \tau)] S \int_0^t d\tau' \vartheta(\tau, \tau') [1 - P(\tau' - \tau)] S n_0(\tau' - \tau) \\ & + \int_0^t d\tau \vartheta(t, \tau) J \left[\int_0^t d\tau \vartheta(t, \tau) [1 - P(t)] S n_0(t), \right. \\ & \quad \left. \times \int_0^t d\tau \vartheta(t, \tau) [1 - P(t)] S n_0(t) \right] + \cdots + \mathcal{V}(t) \end{aligned}$$

If we now take the Markovian limit by letting the upper limit in the integrals approach infinity and define

$$\int_0^\infty d\tau \vartheta(t, \tau) \equiv \mathcal{L}^{-1}, \quad \int_0^\infty d\tau \tau \vartheta(t, \tau) \equiv \mathcal{L}^{-2}$$

we can write

$$\begin{aligned} n_1(t) = & \mathcal{L}^{-1} [1 - P(t)] S n_0(t) + \mathcal{L}^{-1} \frac{\partial}{\partial t} [1 - P(t)] S n_0(t) \\ & + \mathcal{L}^{-1} [1 - P(t)] S \mathcal{L}^{-1} [1 - P(t)] S n_0(t) \\ & + \mathcal{L}^{-1} J[\mathcal{L}^{-1} [1 - P(t)] S n_0(t), \mathcal{L}^{-1} [1 - P(t)] S n_0(t)] + \cdots + \mathcal{V}(t) \end{aligned}$$

We then use once again

$$[1 - P(t)] S n_0(t) = \theta^{-1} I : \Lambda + \theta^{-2} J \cdot \nabla \theta$$

to arrive at the Burnett terms, which take the form

$$\mathbf{q} = -k \nabla \theta + \gamma \frac{\partial}{\partial t} \nabla \theta + \chi \nabla \cdot \Lambda + \dots$$

$$\mathbf{P} = -2\mu \Lambda + \xi \frac{\partial}{\partial t} \Lambda + \psi \nabla \nabla \theta + \dots$$

where the transport coefficients are given by

$$k = (3\theta^2)^{-1} (J \cdot \mathcal{L}^{-1} J), \quad \mu = (10\theta)^{-1} (I : \mathcal{L}^{-1} I)$$

$$\gamma = (3\theta^2)^{-1} (J \cdot \mathcal{L}^{-2} J), \quad \chi = (5\theta)^{-1} (J \mathcal{L}^{-1} (1 - P) \mathcal{D} (1 - P) \mathcal{L}^{-1} : I)$$

$$\xi = (5\theta)^{-1} (I : \mathcal{L}^{-2} I), \quad \psi = (5\theta^2)^{-1} (I : \mathcal{L}^{-1} (1 - P) \mathcal{D} (1 - P) \mathcal{L}^{-1} J)$$

with

$$(f, g) \equiv \int d^3v n_0(\mathbf{v}) f^*(\mathbf{v}) g(\mathbf{v})$$

Finally, we note that the foregoing method for contracting the transport equation to a continuum description has a far wider range of applicability. For example, it can be used to project the solution of any time-dependent equation (e.g., the Liouville equation) on a restricted or contracted form of solution that can be written as a time-independent functional of moments of the original solution. For example, it could be used to express the ensemble density $\rho(\Gamma, t)$ as a time-independent functional of the phase space density $n(\mathbf{r}, \mathbf{v}, t)$, thus yielding a generalization of Bogoliubov's ansatz.⁵²

4.4 □ SOME CONCLUDING REMARKS □ Continuum descriptions of transport processes play an extremely important role in science and engineering. Indeed, they are usually sufficient for the description of most physical phenomena. For example, the conventional hydrodynamics equations (e.g., the Navier-Stokes equations) rarely break down in the description of fluid flow processes. Neutron diffusion theory has become the mainstay of nuclear reactor engineering.

However continuum descriptions sometimes fail quite badly. For example, the diffusion of neutrons in a nuclear reactor core is certainly not described by the traditional form of the diffusion equation. Rather, the coefficients in this equation (i.e., the diffusion coefficient and macroscopic cross sections) and its corresponding boundary conditions must be adjusted (in effect, “fudged”) to take account of transport effects. Without such transport corrections, diffusion theory would simply be inadequate for the analysis of neutron diffusion in nuclear systems.³

A second example of the limited utility of continuum descriptions of particle transport arises in the physics of high temperature plasmas. In such systems, collision effects are so weak that they are usually unable to force the distribution function characterizing the plasma particles (ions and electrons) into even a local thermodynamic equilibrium. Hence the traditional hydrodynamics equations are clearly inadequate for describing such a system (although once again they are frequently applied by adding “transport corrections” such as dissipative coefficients to characterize Landau damping).⁵³

As a final example, one frequently encounters situations in rarefied gas dynamics in which the mean free path is sufficiently large, or gradients or rates are sufficiently large, that a hydrodynamic description is inadequate, and a more detailed analysis based on kinetic theory must be performed.²³

Therefore there are a variety of situations in science and engineering in which we must face the horrifying task of attacking the transport equation directly, without invoking a continuum description. The methods used to analyze such transport problems, the nature and extent of approximations or modeling, depend sensitively on the particular application. However a few general features of transport problems and the methods used to analyze them prove to be useful in a large variety of situations. We develop and discuss these features as we analyze initial and boundary value problems in transport theory in Chapter 5.

□ PROBLEMS □

4.1 Verify the angular integrals

$$\int d\hat{\Omega} \Omega_i \Omega_j = \left(\frac{4\pi}{3}\right) \delta_{ij}, \quad \int d\hat{\Omega} \hat{\Omega} \int d\hat{\Omega}' \Sigma_s(\hat{\Omega}' \cdot \hat{\Omega}) \varphi(\hat{\Omega}') = \bar{\mu}_0 \Sigma_s \mathbf{J}$$

used in the derivation of the one-speed diffusion equation.

4.2 Imagine a diffusing medium in the half-space $x > 0$ with a source of infinite magnitude at infinity such that the boundary condition on the flux

is that $\phi(x) \sim S_0 \exp(x/L)$ as $x \rightarrow \infty$. (This is of course just the Milne problem.) Obtain the flux in this half-space using one-speed diffusion theory using first the boundary condition of zero reentrant current, then using the extrapolated boundary condition. Determine the conditions under which these two boundary conditions might be expected to yield similar results.

4.3 Compute the root-mean-square distance $(\langle x^2 \rangle)^{1/2}$ a particle will travel from a plane source to absorption using one-speed diffusion theory. Compare this result with the rms distance to absorption in a strongly absorbing medium (in which scattering can be neglected).

4.4 Consider the time-dependent P_1 equations in plane geometry. Eliminate one of these equations to obtain an equation for the flux $\phi(x, t)$ and compare this equation with the one-speed diffusion equation. In particular, discuss differences in the solutions to these equations.

4.5 Determine the relaxation constants κ_j for one-speed, isotropic scattering, plane symmetry, and no time dependence for both the P_1 and the P_3 approximations. Indicate the general form of the P_1 and P_3 total flux in an infinite medium with an isotropic plane source at the origin and compare this with the one-speed transport results.

4.6 Derive the P_N equations for the transport equation in spherical coordinates (assume spherical symmetry for convenience).

4.7 Solve the Milne problem (Problem 4.2) for a nonabsorbing medium with isotropic scattering in the P_1 and the P_3 approximation. Compare both results in various regions of interest.

4.8 Derive the general form of the P_N equations in three-dimensional Cartesian geometry.

4.9 Prove the three identities involving the projection operator $P \circ \equiv (4\pi)^{-1} \int d\hat{\Omega} \circ$ given on page 240.

4.10 Apply the projection operator method to the linearized Boltzmann equation to derive the generalization of the linearized hydrodynamics equations.^{29, 30}

4.11 Demonstrate the physical implications of the choice of the Eddington factor as $f = 1$ and $f = \frac{1}{3}$.

4.12 Provide the details necessary to manipulate the moments of the Boltzmann equation with respect to the collisional invariants $m, m\mathbf{v}, \frac{1}{2}m|\mathbf{v} - \mathbf{u}|^2$, into the form of the conventional hydrodynamics equations.

4.13 Demonstrate the explicit form given for $C[M_p]$.

4.14 Determine the Chapman-Enskog solution to the BGK model to first and second order.

- 4.15** Determine the transport coefficients k and μ within the BGK model and compare the ratio μ/k with the value obtained from the full Boltzmann collision term.
- 4.16** Sketch how you would obtain the next order correction to the Navier-Stokes equations using the Chapman-Enskog expansion.
- 4.17** When an ideal monatomic gas undergoes an adiabatic process, thermodynamics implies that the temperature and density are related by $\rho \sim T^{3/2}$. Demonstrate that the hydrodynamics equations to first order in the Chapman-Enskog expansion also satisfy this relation.
- 4.18** Derive the Grad 13-moment equations.
- 4.19** Specialize the Grad 13-moment equations to the case of zero flow ($\mathbf{u}=0$) and develop the corresponding corrections to Fourier's law.
- 4.20** Prove that the time-dependent projection onto the LTE state has the property that $P(t)(\partial n / \partial t) = \partial n_0 / \partial t$.
- 4.21** Provide the details in the derivation of the "projected" moment equations (4.65).

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Basic Problems in Transport Theory

We have confined our attention thus far to solutions of the transport equation under very idealized assumptions. For example, we considered the transport of particles when scattering processes could be ignored entirely or when the energy dependence of the particle phase space density was of secondary concern. When space and time variations are sufficiently weak, we found that we could remove the angular dependence of the transport process by developing various continuum or hydrodynamic descriptions.

We now investigate transport processes in which both the particle speed and flight direction must be considered, that is, neither one-speed nor hydrodynamic approximations are valid. Needless to say, a general analytical solution of most of these problems is usually out of the question. Indeed, even brute force numerical methods frequently prove inadequate. Fortunately in many cases we can use the known properties of the transport equation to infer a good deal about its solutions, even though we may be unable to determine a solution in complete detail.

First we examine a class of problems in which the details of the initial or boundary conditions can be ignored. Such problems involve “asymptotic relaxation” phenomena in which a disturbance is introduced into the particle distribution, and one studies the spatial or temporal relaxation of this disturbance to equilibrium or quasi-equilibrium behavior. These problems are of particular mathematical interest because they are intimately related to the eigenvalue spectrum of the corresponding transport operator. They provide information that facilitates the study of more general and complicated problems.

We then consider typical initial and boundary value problems that arise in a number of areas of particle transport and discuss analytical tools available for the study of such problems. One particular subject of interest is the study of the transport of particles that are initially characterized by kinetic energies very much in excess of the thermal energies of the host medium—“superthermal” particle transport. We deal with both the spatial transport and subsequent slowing down of such particles.

5.1 □ ASYMPTOTIC RELAXATION PROBLEMS (EIGENVALUE PROBLEMS) □

5.1.1 □ Neutron Transport □ We begin by recalling that the transport equation describing the diffusion of neutrons through a medium can be written as follows:

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \nabla n + v \Sigma_t(\mathbf{v}) n(\mathbf{r}, \mathbf{v}, t) = \int d^3v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) n(\mathbf{r}, \mathbf{v}', t) + s(\mathbf{r}, \mathbf{v}, t) \quad (5.1)$$

where any fission sources are included in $s(\mathbf{r}, \mathbf{v}, t)$. We have already noted that the dependence of the cross sections on neutron speed can become quite complicated. Hence the solution of the general velocity-dependent transport equation (5.1) is no easy matter—particularly for realistic cross section behavior. However there is one class of problems to which this equation can be applied and studied in essentially its most general form: the transport theory of *asymptotic relaxation phenomena* in neutron thermalization.

Such problems typically involve the injection of a burst of neutrons (usually fast neutrons) into a sample of material. One studies the relaxation or decay of the asymptotic neutron distribution established in the sample. This process can occur in either space or time, and it corresponds physically to familiar experimental procedures used in neutron physics (e.g., the measurement of the neutron diffusion length in a material, or experiments performed with pulsed neutron sources).

Asymptotic relaxation phenomena are of major theoretical interest because they play an important role in the general subject of kinetic theory. In the case of neutron transport they correspond to the relaxation of a foreign gas (the neutron gas) to thermal equilibrium in a background medium. Their asymptotic nature allows one to avoid a detailed confrontation with boundary conditions and to focus instead on the energy dependence of the transport process. The study of such asymptotic decay or relaxation processes is ideally suited to the mathematical technique of eigenfunction expansions and stimulates a thorough study of the spectral theory of the transport operator. To provide a physical foundation for the types of problem we are going to consider, it is useful to briefly describe several of the physical situations that give rise to these relaxation processes.

i *Pulsed neutron experiments.*¹⁻³ This work involves the injection of a burst of fast neutrons into a sample of material, followed by measurements of the time decay of the neutron population in the sample as neutrons leak out or are absorbed. After a certain length of time, one expects to find an exponential decay of the form $N(t) \sim N_0 e^{-\lambda t}$ (see Figure 5.1a). In the usual experimental procedure this “time relaxation parameter” λ is measured as

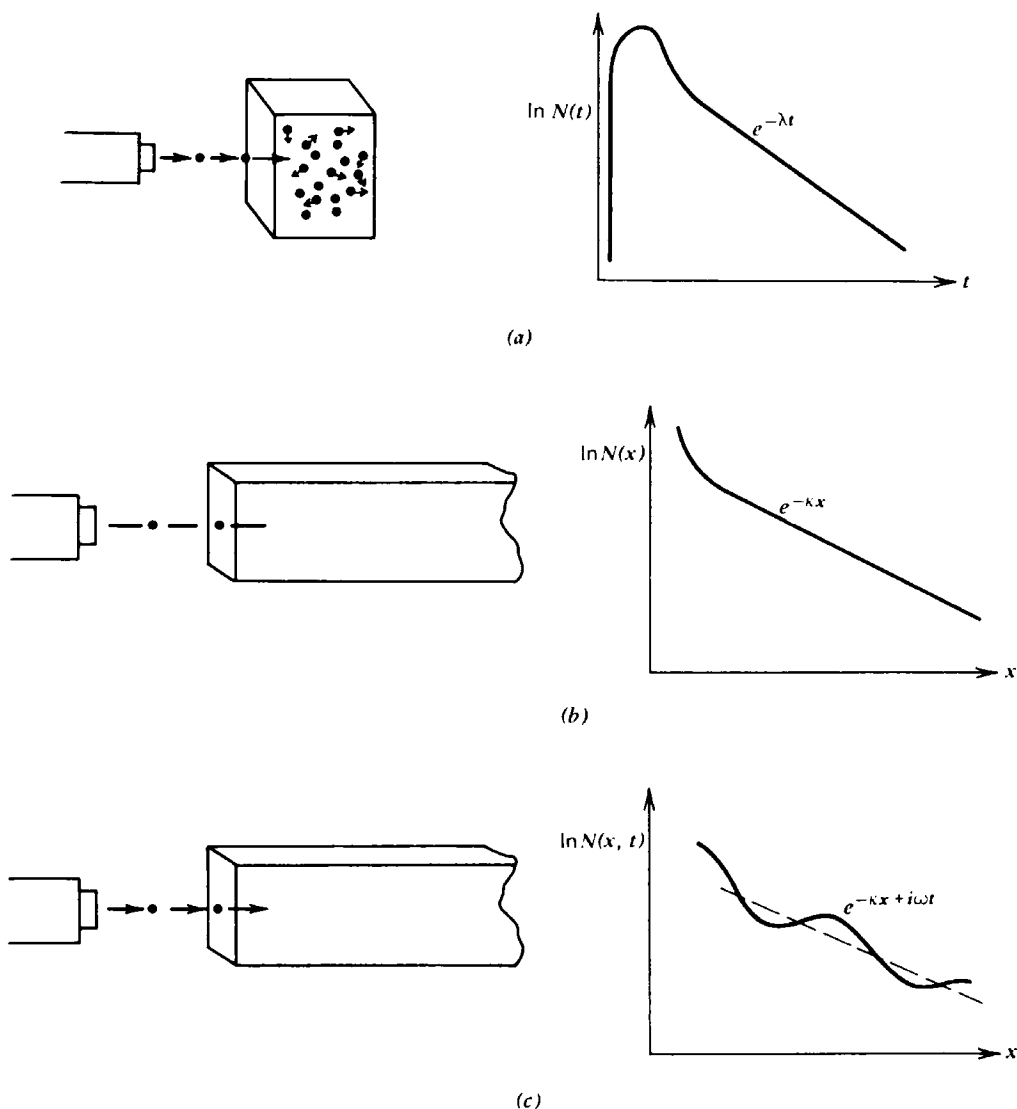


Fig. 5.1 □ Asymptotic relaxation experiments in neutron transport. (a) Pulsed neutron. (b) Diffusion length. (c) Neutron wave.

a function of sample size in an effort to infer information concerning the manner in which neutrons interact with the material in the sample (e.g., cross section information).

ii *Diffusion length experiments.*^{4,5} In these experiments one places a time-independent neutron source up against one end of a column of the material of interest, then measures the spatial attenuation of the neutron density established within the material by the source. Again, at large distances from the source one expects to find an exponential decay $N(x) \sim N_0 e^{-\kappa x}$. (Figure 5.1*b*.) This “spatial relaxation parameter” κ is then measured, usually as a function of absorption (which can be varied by adding small quantities of a strong neutron absorber to the column).

iii *Neutron wave experiments.*⁶⁻⁸ In these variations on the diffusion length experiment, a time-modulated component is added to the source, say of the form $\exp(i\omega t)$. This modulated component excites a time-dependent disturbance in the neutron distribution within the column that will also be modulated as $\exp(i\omega t)$. But since it takes a finite time for neutrons emitted by the source to wander down the column, there will be a phase lag relative to the source. Therefore it becomes possible to measure not only the spatial attenuation of this oscillating component, but its phase lag relative to the source as well. Again we expect to find exponential relaxation at large x , $N(x, t) \sim N_0 \exp(-\kappa x + i\omega t)$, but now the relaxation parameter κ will be complex. Hence the asymptotic form of this disturbance is in the form of a damped plane wave running away from the source (Figure 5.1*c*). Now one measures the “complex spatial relaxation parameter” κ characterizing this “neutron wave” as a function of source frequency. (Note that for $\omega=0$, this becomes just the usual diffusion length experiment.)

These three experiments have a number of features in common. They are all asymptotic in the sense that all measure the decay or relaxation of the neutron density either at long times or at large distances from the source. All three experiments implicitly assume that this asymptotic behavior will be exponential, then attempt to measure the relaxation parameter characteristic of this exponential decay as a function of some independent experimental variable (system size, absorption, or source frequency). Then by comparing the experimentally measured relaxation parameter with theoretical calculations, presumably it is possible to measure various integral transport parameters of the sample (absorption rates, diffusion coefficients, moments of the scattering kernel, etc.).

A very major question whenever such experiments are performed concerns the existence of such asymptotic exponential behavior. That is, if we

wait long enough or make measurements sufficiently far from the source, will we indeed see an exponential decay in the neutron density? Furthermore, we must determine just what macroscopic integral transport parameters (e.g., diffusion coefficients) are involved in the calculation of the appropriate relaxation parameters.

In our analysis of such asymptotic relaxation experiments using the neutron transport equation, we demonstrate that its mathematical formulation takes the form of an eigenvalue problem. However it would be inappropriate to continue further without mentioning yet one more class of eigenvalue problem that plays an extremely important role in neutron physics although it does not involve an asymptotic relaxation process, namely, the criticality problem.

iv *The criticality problem.*⁹ Probably the most important eigenvalue problem encountered in neutron transport theory arises in the study of nuclear fission chain reactions. Mathematically, the neutrons produced in fission reactions appear as an effective source term in the neutron transport equation that takes the form (cf. Section 1.4)

$$Fn \equiv \chi(\mathbf{v}) \int d^3v' \nu(v') v' \Sigma_f(v') n(\mathbf{r}, \mathbf{v}', t)$$

Of key concern is the determination of the combination of system composition and geometry that will yield a steady state or “critical” chain reaction (i.e., a nontrivial solution to the time-independent transport equation). It is customary to formulate this calculation as an eigenvalue problem by introducing a free parameter k into the transport equation with a fission source, written as

$$Ln = \frac{1}{k} Fn$$

where L is the usual time-independent transport operator. Here, k is referred to as the multiplication or criticality eigenvalue. Then if we adjust system composition and geometry so that the eigenvalue $k = k_0$ corresponding to an everywhere positive solution $n_0(\mathbf{r}, \mathbf{v})$ is equal to one ($k_0 = 1$), we achieve a critical chain reacting system. (It is customary in reactor physics⁹ to refer to this eigenvalue as the “effective multiplication factor” and denote it by $k_0 = k_{\text{eff}}$.)

We now study in some detail the mathematical analysis of each of these problems by utilizing the appropriate form of the neutron transport equation. We begin by examining the steady-state or equilibrium solutions to the transport equation characterizing an infinite, uniform medium.

Stationary Neutron Thermalization in an Infinite Medium^{4, 10-12} □ An important problem in nuclear reactor studies involves the determination of the energy dependence of the neutron density (or flux) that is established in an infinite homogeneous medium by a time-independent, spatially uniform source. It is customary to assume that the source neutron energies are far in excess of the thermal energy of the nuclei comprising the host material ($E \gg kT$), and on occasion the source is taken to be just the fission neutron spectrum $\chi(E)$. If we integrate the appropriate form of the transport equation (5.1) over angle $\hat{\Omega} = \mathbf{v}/|\mathbf{v}|$ and define $N(v) = \int d\hat{\Omega} v^2 n(\mathbf{r}, v, \hat{\Omega})$, we arrive at the infinite medium neutron spectrum equation:

$$[v\Sigma_a(v) + v\Sigma_s(v)]N(v) = \int_0^\infty dv' v' \Sigma_s(v' \rightarrow v) N(v') + S(v) \quad (5.2)$$

Of course this equation represents the classic problem of neutron thermalization in which one studies the energy spectrum of neutrons as they slow down into thermal equilibrium with a host material. It is the problem of most interest to thermal reactor calculations, and to the generation of multigroup cross sections in particular. However since it is not a transport problem in the strict sense, but rather a problem in the neutron speed alone, our study of Eq. 5.2 will be rather cursory.

Of course an integral equation such as Eq. 5.2 can be very difficult to solve in general if the full complexities of the cross section dependence on neutron speed are included. One must usually resort to some kind of an approximate model of $\Sigma_s(v' \rightarrow v)$. However there are two limiting cases we can study without resorting to such approximations.

i *Zero absorption and sources:* $\Sigma_a(v) = 0$ and $S(v) = 0$. If we recall the detailed balance condition that must be satisfied by the scattering cross section (cf. Section 3.1), it is apparent that the only solution to

$$v\Sigma_s(v)N(v) = \int_0^\infty dv' v' \Sigma_s(v' \rightarrow v) N(v')$$

is just the Maxwell-Boltzmann distribution at the temperature T of the host medium

$$N(v) = n_0 M(v) = n_0 \frac{4}{\sqrt{\pi}} \left(\frac{m}{2kT} \right)^{3/2} v^2 \exp\left(-\frac{mv^2}{2kT} \right)$$

Hence detailed balance ensures that the only solution to the “equilibrium”

problem is $M(v)$. Of course, sources, absorption, leakage, or time dependence can cause deviations from equilibrium and can give rise to more general solutions $N(v)$.

ii *Large* $v \gg (kT/m)^{1/2}$. For large v , we enter the neutron slowing down regime and (as we demonstrate in Section 5.3) the neutron speed dependence assumes the asymptotic form $N(v) \sim 1/v^2$. Therefore in general we expect the solution to vaguely resemble a Maxwellian with a $1/v^2$ tail.

To obtain more information about the steady-state neutron spectrum, one must resort to either numerical techniques or very approximate models of the scattering kernel (e.g., the proton gas or heavy gas models¹³). We defer a discussion of these approximate methods to Chapter 7 and continue to examine time- and space-dependent relaxation problems.

Time Relaxation Phenomena in Neutron Thermalization □ The prototype relaxation problem in neutron physics involves the time behavior of a burst of fast neutrons injected into a sample of material. These neutrons suffer collisions with the nuclei in the sample and slow down in energy until they are absorbed or leak out. The corresponding neutron density evolves in time and eventually approaches a Maxwell-Boltzmann distribution in energy (characterized by the temperature of the sample), all the while decaying away in magnitude because of absorption and leakage. We can identify the mathematical description of this process as just the initial value problem (or Cauchy problem) for the neutron transport equation

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \nabla n + v \Sigma_t(v) n(\mathbf{r}, \mathbf{v}, t) = \int d^3v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) n(\mathbf{r}, \mathbf{v}', t) \quad (5.3)$$

subject to a given initial condition (i.c.) corresponding to the pulsed source

$$\text{i.c.: } n(\mathbf{r}, \mathbf{v}, 0) = n_0(\mathbf{r}, \mathbf{v})$$

and suitable boundary conditions (b.c.) such as those characterizing a free surface

$$\text{b.c.: } n(\mathbf{R}_s, \mathbf{v}, t) = 0, \hat{\mathbf{e}}_s \cdot \mathbf{v} < 0$$

This is an extremely difficult problem to solve in general. A direct confrontation with the time-dependent transport equation in all its glory (or horror) is perhaps too much at this early stage. Instead, let us ease more slowly into the concepts and mathematical techniques necessary for

analyzing such problems by working our way up a ladder of somewhat simpler problems:

- i Time relaxation in an infinite medium.
- ii Time relaxation assuming asymptotic transport theory.
- iii Time relaxation in bounded geometries.

Naturally we begin with the simplest problem, time relaxation in an infinite medium.

Time relaxation in an infinite medium □ The mathematical statement of the problem of time relaxation of a spatially independent initial distribution of neutrons in an infinite medium involves the solution of

$$\frac{\partial N}{\partial t} + v\Sigma_t(v)N(v,t) = \int_0^\infty dv' v' \Sigma_s(v' \rightarrow v) N(v',t) \quad (5.4)$$

subject to a given initial condition: $N(v,0) = N_0(v)$. One can analyze this problem in a manner very similar to the one-speed transport model by applying integral transforms (in this case, a Laplace transform in time) or separation of variables and eigenfunction expansions. To illustrate these approaches, we first consider a simple example in which the scattering kernel is modeled by a separable kernel of the form¹⁴

$$\Sigma_s(v' \rightarrow v) = \beta \Sigma_s(v') v M(v) \Sigma_s(v), \quad \beta^{-1} \equiv \int_0^\infty dv v M(v) \Sigma_s(v)$$

so that Eq. 5.4 becomes

$$\frac{\partial N}{\partial t} + v\Sigma_t(v)N(v,t) = \beta \Sigma_s(v) v M(v) \int_0^\infty dv' v' \Sigma_s(v') N(v',t) \quad (5.5)$$

Let us first try the integral transform approach by defining the Laplace transform

$$\tilde{N}(v,s) = \int_0^\infty dt e^{-st} N(v,t)$$

Then our transformed equation (5.5) becomes

$$[s + v\Sigma_t(v)] \tilde{N}(v,s) = \beta \Sigma_s(v) v M(v) \int_0^\infty dv' v' \Sigma_s(v') \tilde{N}(v',s) + N_0(v) \quad (5.6)$$

We can solve this simple integral equation in the usual way by first dividing through by $s + v\Sigma_t(v)$, then multiplying through by $v\Sigma_s(v)$, and integrating over v to find (after some rearrangement):

$$\tilde{R}(s) \equiv \int_0^\infty dv v \Sigma_s(v) \tilde{N}(v, s) = \frac{\int_0^\infty dv \frac{v \Sigma_s(v) N_0(v)}{s + v \Sigma_t(v)}}{1 - \beta \int_0^\infty dv \frac{v^2 [\Sigma_s(v)]^2 M(v)}{s + v \Sigma_t(v)}} \equiv \frac{\chi(s)}{\Lambda(s)} \quad (5.7)$$

Hence the transformed solution can be obtained from Eq. 5.6 as

$$\tilde{N}(v, s) = \frac{\beta \Sigma_s(v) v \dot{M}(v)}{s + v \Sigma_t(v)} \frac{\chi(s)}{\Lambda(s)} + \frac{N_0(v)}{s + v \Sigma_t(v)} \quad (5.8)$$

All we have to do now is to invert this Laplace transform. Actually, since we recognize that $\tilde{R}(s)$ as given by Eq. 5.7 is just the response of a detector with cross section $\Sigma_s(v)$, it is convenient at this point to study the inversion of this “detector response” function

$$R(t) = \int_{\sigma - i\infty}^{\sigma + i\infty} ds e^{st} \tilde{R}(s)$$

[the inversion of the full solution (5.8) is only slightly more complicated].

We must determine the analytic structure of $\tilde{R}(s)$ in the complex s -plane to determine how to deform the Bromwich inversion contour. We begin by noting that both $\chi(s)$ and $\Lambda(s)$ contain a Cauchy integral of the form

$$\int_0^\infty dv \frac{f(v)}{s + v \Sigma_t(v)}$$

Thus we can identify a branch cut for $s = -v\Sigma_t(v)$, $v \in [0, \infty)$. Since neutron cross sections behave as $1/v$ for small v (cf. Section 3.1) and approach a constant value at large v , we find that the Cauchy integral gives rise to a branch cut along the negative real axis from $-\lambda^*$ to $-\infty$, where

$$\lambda^* \equiv \min_{v \in [0, \infty)} [v \Sigma_t(v)]$$

Notice here that λ^* defines the lower bound to this cut. We will find that this is a general feature of time-dependent transport problems.

Next we must determine whether $\tilde{R}(s)$ has any isolated singularities such as poles [i.e., zeros of $\Lambda(s)$]. We can distinguish between two cases:

1/v Absorption $\Sigma_a(v) = \Sigma_a^0/v$ (which is not necessarily a bad approximation). Then it is evident that $s = -\Sigma_a^0$ is the only zero of $\Lambda(s)$. We later show that for $1/v$ absorption, $s = -\Sigma_a^0$ is always the least damped pole, although for more general $\Sigma_s(v' \rightarrow v)$ there may be additional poles.

Non-1/v absorbers Again there is one zero of $\Lambda(s)$ on the negative real axis between $-\lambda^*$ and 0. However there is no longer a closed-form expression for this zero.

Therefore we find that $\tilde{R}(s)$ has a simple pole at $s = -\lambda_0$ and a branch cut from $-\lambda^*$ to $-\infty$ (see Figure 5.2). We can deform the inversion contour in the usual way to find

$$R(t) = a_0 e^{-\lambda_0 t} + \int_{\lambda^*}^{\infty} d\lambda A(\lambda) e^{-\lambda t}$$

where we can calculate

$$a_0 = \chi(-\lambda_0) \left[\frac{\partial \Lambda}{\partial s} \Big|_{-\lambda_0} \right]^{-1}; \quad A(\lambda) = \frac{1}{2\pi i} \left[\frac{\chi^+(\lambda)}{\Lambda^+(\lambda)} - \frac{\chi^-(\lambda)}{\Lambda^-(\lambda)} \right]$$

In particular, we should note that for long times

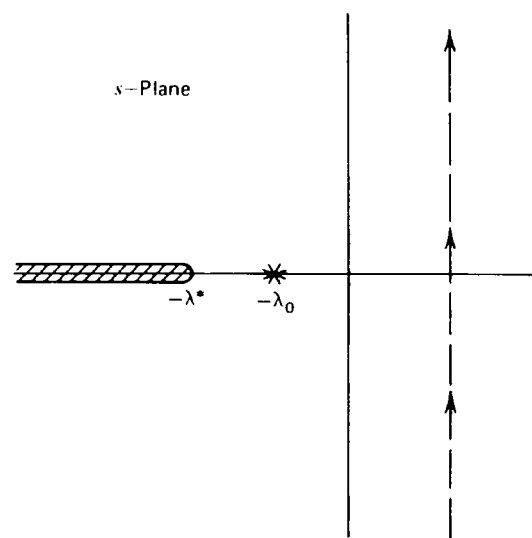
$$R(t) \sim a_0 e^{-\lambda_0 t} + O(e^{-\lambda^* t}) \sim a_0 e^{-\lambda_0 t}$$

which is the desired exponential behavior.

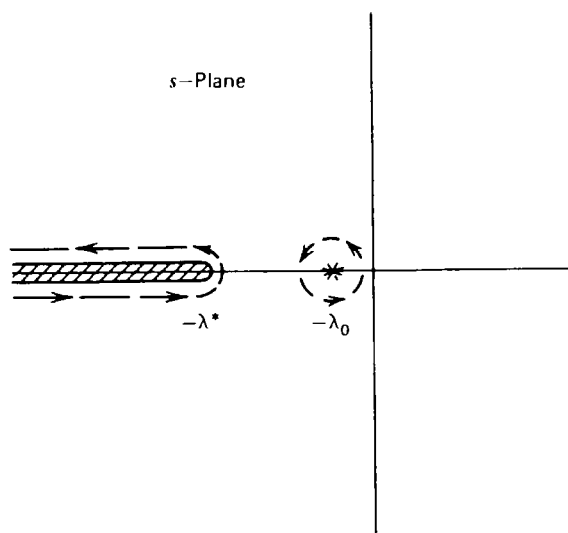
The inversion of the solution for the density $\tilde{N}(v, s)$ as given by Eq. 5.8 is only slightly more complicated due to the presence of an additional simple pole at $s = -v\Sigma_t(v)$; therefore we give only the final result:

$$N(v, t) = a_0 \frac{\beta \Sigma_s(v) v M(v)}{[v \Sigma_t(v) - \lambda_0]} e^{-\lambda_0 t} + \int_{\lambda^*}^{\infty} d\lambda a(\lambda, v) \beta \Sigma_s(v) v M(v) e^{-\lambda t} \\ + N_0(v) e^{-v \Sigma_t(v) t}$$

We note parenthetically that the integral or “transient” term can be attributed to neutrons slowing down from the source energy, whereas the



(a)



(b)

Fig. 5.2 □ s -Plane structure (a) and deformation (b) of Laplace inversion contour.

last term is obviously the contribution from virgin source neutrons.

As a variation on this theme, we can repeat this calculation using the separation of variables approach by seeking a separable solution of the form

$$N(v, t) \sim \psi_\lambda(v) e^{\lambda t}$$

If we substitute this into Eq. 5.5, we find a condition on $\psi_\lambda(v)$ and λ

$$[\lambda + v\Sigma_t(v)]\psi_\lambda(v) = \beta\Sigma_s(v)vM(v) \int_0^\infty dv' v' \Sigma_s(v')\psi_\lambda(v') \quad (5.9)$$

which we recognize as an eigenvalue problem for the eigenvalue λ and the corresponding eigenfunction $\psi_\lambda(v)$. It is convenient to normalize the $\psi_\lambda(v)$ such that

$$\int_0^\infty dv v \Sigma_s(v) \psi_\lambda(v) = 1 \quad (5.10)$$

Then, in analogy to the application of singular eigenfunction methods to the one-speed transport equation in Chapter 2, we expect Eq. 5.9 to have a continuous spectrum of eigenvalues for those values of λ such that $\lambda + v\Sigma_t(v)$ can vanish: $\lambda = -v\Sigma_t(v)$, $v \in [0, \infty)$. Hence for $\lambda \notin (-\infty, -\lambda^*]$, we can divide through to find

$$\psi_\lambda(v) = \frac{\beta\Sigma_s(v)vM(v)}{\lambda + v\Sigma_t(v)}$$

and apply the normalization condition Eq. 5.10 to find that the discrete eigenvalues are given by the condition

$$\Lambda(\lambda) = 1 - \beta \int_0^\infty dv \frac{[v\Sigma_s(v)]^2 M(v)}{\lambda + v\Sigma_t(v)} = 0$$

But we know that this equation has one solution, $\lambda = -\lambda_0$; that is, Eq. 5.9 has one discrete eigenvalue, $-\lambda_0$.

The values $\lambda \in (-\infty, -\lambda^*]$ form the continuous eigenvalue spectrum and have corresponding continuous eigenfunctions

$$\psi_\lambda(v) = P \frac{\beta\Sigma_s(v)vM(v)}{\lambda + v\Sigma_t(v)} + g(\lambda)\delta[\lambda + v\Sigma_t(v)]$$

where the normalization yields

$$g(\lambda) = 1 - \beta P \int_0^\infty dv \frac{[v\Sigma_s(v)]^2 M(v)}{\lambda + v\Sigma_t(v)}$$

We can prove the usual orthogonality and completeness properties (see Koppel's work¹⁵ for details). An expansion of the general solution to the initial value problem in terms of these eigenfunctions and a subsequent

evaluation of the expansion coefficients by applying the initial condition and orthogonality will yield a final solution identical to that obtained by Laplace transform methods. These eigenfunctions in the speed variable are used only to expand functions of v defined for the full range of $v \in [0, \infty)$. That is, we never need to consider the difficulties that arise in half-range expansions in this problem.

Before leaving this simple example, it is useful to note several features that reappear in more general problems: (i) the branch cut of the integral transform approach is identical to the continuous eigenvalue spectrum that occurs in the separation of variables approach, (ii) this continuous spectrum ranges from $-\lambda^*$ to $-\infty$, and (iii) the discrete eigenvalues are real.

Let us now return to the more general problem represented by Eq. 5.4. In operator notation this can be written as

$$\frac{\partial N}{\partial t} = AN \quad (5.11)$$

where we have defined the collision operator

$$A \circ \equiv -v\Sigma_t(v) + \int_0^\infty dv' v' \Sigma_s(v' \rightarrow v) \circ$$

Suppose we apply a Laplace transform to Eq. 5.11—at least in a formal sense—to write

$$s\tilde{N}(v, s) - N_0(v) = A\tilde{N}(v, s)$$

We can then formally solve for the transformed density $\tilde{N}(v, s)$ as

$$\tilde{N}(v, s) = [s - A]^{-1} N_0(v)$$

where $[s - A]^{-1}$ represents the inverse of the operator $[s - A]$. Hence we are faced with inverting

$$N(v, t) = \frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} ds e^{st} [s - A]^{-1} N_0(v)$$

To facilitate this inversion, we must study the analytic behavior of $[s - A]^{-1} N_0(v)$ as a function of the complex variable s .

But how do we study the analytic behavior of an operator expression such as this? Suppose that λ_0 was an eigenvalue of A . Then in some sense (soon to be clarified)

$$[s - A]^{-1} N_0(v) \sim (s - \lambda_0)^{-1} N_0(v)$$

Hence the singularities of $[s - A]^{-1}N_0(v)$ are just the eigenvalues of the operator A . That is, in the more general problem in which the scattering kernel is not in the simple form of a degenerate kernel, we must study the eigenvalue problem

$$A\psi_\lambda = \lambda\psi_\lambda$$

before we can invert the transform.

Of course a more direct approach would be to use separation of variables by trying a solution

$$N(v, t) \sim \psi_\lambda(v) e^{\lambda t}$$

to find the eigenvalue problem directly as

$$A\psi_\lambda = \left[-v\Sigma_t(v) + \int_0^\infty dv' v' \Sigma_s(v' \rightarrow v) \right] \psi_\lambda(v) = \lambda\psi_\lambda(v) \quad (5.12)$$

Unfortunately, we cannot merely follow the singular eigenfunction approach to analyze this more general problem as we could for the synthetic kernel model Eq. 5.5. We must develop a more general mathematical approach.

Let us remind ourselves of the general procedure we have employed in our earlier applications of the separation of variables method:

- i We obtained an eigenvalue problem by substituting the separable form of the solution into the homogeneous equation.
- ii We studied this eigenvalue problem to determine its eigenvalues and eigenfunctions.
- iii We sought the general solution to our initial value problem as a linear combination of these eigenfunctions

$$N(v, t) = \sum_\lambda a_\lambda \psi_\lambda(v) e^{\lambda t}$$

and applied initial conditions (along with orthogonality) to evaluate the expansion coefficients a_λ .

Therefore it is apparent that the eigenvalue problem plays the key role in the mathematical solution of the problem (whether we approach it by integral transforms or by separation of variables). But in asymptotic relaxation processes, the eigenvalue problem also plays a key role in the physical interpretation. The eigenvalue problem tells us what kind of decay modes (eigenfunctions) exist. If there exists an eigenvalue with least real

part λ_0 , its corresponding mode will dominate for long time: $N(v, t) \sim a_0 \psi_0(v) e^{-\lambda_0 t}$. Hence any experiment measuring the asymptotic behavior of the neutron distribution will measure this least damped eigenvalue.

Therefore just by studying the eigenvalue problem, we can frequently determine all we need to know about asymptotic relaxation experiments. It is not necessary to construct the full solution to the initial value problem. That is, the asymptotic behavior of the neutron distribution is determined by the least damped eigenvalue of the appropriate form of the transport operator A . This is a common feature of all such asymptotic relaxation problems (such as those arising in pulsed neutron, diffusion length, and neutron wave experiments), and it explains their rather intimate connection with the spectral theory of the transport operator.

Therefore we now turn our attention to a study of the eigenvalue problem Eq. 5.12. Unfortunately, A is a rather complicated operator—much more complicated, in fact, than the standard operators one encounters in mathematical physics. It is (i) *not* self-adjoint, (ii) *not* completely continuous or compact, and (iii) *unbounded*. This means that our eigenvalue problem is of an extremely general type. Therefore we require rather general mathematical concepts from functional analysis to deal with Eq. 5.12.¹⁶⁻²³

Appendix E introduces very briefly several of the concepts from functional analysis that are necessary to study eigenvalue problems associated with transport theory. Fortunately most of the items we require are merely definitions, since mathematicians have already done most of the work for us by proving the relevant theorems. Our principal remaining task, then, is to determine just which of these theorems can be applied to study our eigenvalue problem.

We can separate this analysis into three steps (which correspond essentially to the steps outlined previously):

- i Classification of the spectrum $\sigma(A)$ of the operator A (i.e., determine the “eigenvalues” of A).
- ii Spectral representation of functions (i.e., determine the corresponding eigenfunctions and demonstrate orthogonality and completeness properties).
- iii Use of this spectral representation to solve the original initial value problem.

In most cases, the analyses presented in the literature complete only the first step, the classification of the spectrum, since this is frequently all that is needed to analyze asymptotic relaxation experiments. Furthermore, in only a few simple cases is it possible to carry through the second and third

steps to complete the solution of the original problem—at least on any but a formal basis.

To demonstrate how to apply the spectral theory of operators to transport problems, we analyze in some detail the initial value problem represented by Eq. 5.4. Later, when we discuss more complicated problems (involving space and angle dependence), we skip the details of classifying the spectrum because they are rather clumsy but straightforward extensions of the steps involved in studying Eq. 5.4.

Before we proceed it is convenient to “symmetrize” the problem by making a change of dependent variable

$$\Psi_\lambda(v) = [M(v)]^{-1/2} \psi_\lambda(v)$$

so that we can rewrite the eigenvalue problem Eq. 5.12 as

$$-v\Sigma_t(v)\Psi_\lambda(v) + \int_0^\infty dv' K(v',v)\Psi_\lambda(v') \equiv (A_1 + A_2)\Psi_\lambda = \lambda\Psi_\lambda \quad (5.13)$$

where $K(v',v) \equiv [M(v')/M(v)]^{1/2} v'\Sigma_s(v' \rightarrow v)$. By using detailed balance, $v'M(v')\Sigma_s(v' \rightarrow v) = vM(v)\Sigma_s(v \rightarrow v')$, we can verify that $K(v',v)$ is a symmetric kernel. This is useful because it will imply that the integral operator A_2 is self-adjoint. We can now proceed to study the eigenvalue problem, Eq. 5.13.

Step 1. Classification of the Spectrum $\sigma(A)$. We have already mentioned that A_2 is self-adjoint in the sense that $(A_2 f, g) = (f, A_2 g)$. Furthermore we note that an integral operator such as A_2 is completely continuous if its kernel $K(v',v)$ or any Neumann iterate of this kernel is square integrable, for example,

$$\int_0^\infty dv \int_0^\infty dv' |K_n(v',v)|^2 < \infty$$

(Such square-integrable, symmetric kernels are called *Hilbert-Schmidt* kernels,²⁴ and they have been extensively studied by mathematicians.)

Hence to determine whether A_2 is a completely continuous integral operator, we must study the square integrability of its kernel $K(v',v)$ for various materials—that is, various types of cross section $\Sigma_s(v' \rightarrow v)$. This is a rather involved procedure, and we state only the results of this investigation for various materials.

i *Monatomic gases.* Detailed calculations by Dorfman²⁵ have demonstrated that although $K(v',v)$ is not itself square integrable, its third iterate

is square integrable. This is sufficient to imply that A_2 is completely continuous for gases.

ii *Solids in the incoherent approximation.* Kuščer and Corngold²⁶ have shown that $K(v', v)$ is well behaved for low and intermediate (v', v) . Since $K(v', v)$ must reduce to the monatomic gas kernel at high (v', v) , they conclude that A_2 is also completely continuous for incoherent scattering from solids.

iii *Liquids.* For liquids, Kuščer and Corngold have shown that $K(v', v)$ also possesses a divergence for low (v', v) . However they conjecture that an iterate of $K(v', v)$ is square integrable, hence permitting them to conclude that A_2 is completely continuous for this case as well.

iv *Coherent, elastic scattering from solids.* We have seen that the cross sections for polycrystalline materials contain δ -functions in both energy and angle. Hence we must conclude that A_2 is not completely continuous in this case.

Therefore for all materials in which coherent scattering is insignificant, we can conclude that A_2 is a self-adjoint, completely continuous integral operator. Furthermore, since the contributions to A_1 and A_2 due to elastic scattering cancel in the infinite medium problem, we can disregard case iv without loss of generality (although for problems in which the spatial dependence must be included, case iv will pose a special problem).

Next we examine $A_1 = -v\Sigma_r(v)$. It is evidently self-adjoint (since it is real). But since $\Sigma_r(v) \sim \text{constant}$ for large v , A_1 is an unbounded operator and certainly not completely continuous. It is a closed operator, however (since a multiplicative operator cannot destroy the convergence of a sequence). Hence we conclude that A_1 is a self-adjoint, closed operator.

We now have enough information about A_1 and A_2 to classify the spectrum of A . We approach this classification in the usual fashion by stating the results as a theorem (see Appendix E for the relevant definitions and details).

Theorem. The operator $A = A_1 + A_2$ decomposes the spectral λ -plane as follows:

$\sigma_c(A) = C$, where $C \equiv \{\lambda : \lambda = -v\Sigma_r(v), v \in [0, \infty)\}$.

$\sigma_p(A)$: A real set contained in the interval $(-\infty, -\lambda^*]$.

$\sigma_r(A)$: An empty set.

$\rho(A)$: All other points in the λ -plane not contained in $\sigma(A)$ (see Figure 5.3).

Proof. We first show that $C \subset \sigma_c(A_1)$ by using the Weyl criterion (see Appendix E). Choose values of $\lambda \in C$ and v_λ such that $\lambda = -v_\lambda \Sigma_r(v_\lambda)$. Now

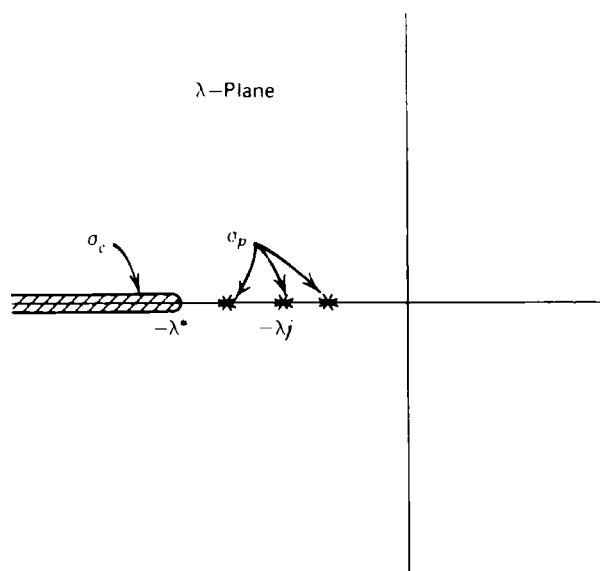


Fig. 5.3 □ Spectrum of the infinite medium transport operator.

construct a set of functions φ_δ that approximate $\delta(v - v_\lambda)$

$$\varphi_\delta(v) = \begin{cases} [M(v)/\delta]^{1/2}, & v_\lambda \leq v \leq v_\lambda + \delta \\ 0, & \text{otherwise} \end{cases}$$

Clearly

$$\|\varphi_\delta\| = \left[\int_{v_\lambda}^{v_\lambda + \delta} dv \frac{M(v)}{\delta} \right]^{1/2} = c \geq 0$$

whereas $\varphi_\delta \rightarrow 0$ [since $(f, \varphi_\delta) \rightarrow 0$ for any $f \in \mathcal{L}_2$]. Furthermore, $\|(A_1 - \lambda)\varphi_\delta\| \rightarrow 0$. Hence by the Weyl criterion, $\lambda \in \sigma_c(A_1) \Rightarrow C \subset \sigma_c(A_1)$.

Next we have to prove that *all* the continuous spectrum is contained in C . To do this, we consider some λ_0 not in C , that is, some $\lambda_0 \neq -v\Sigma_t(v)$ for any $v \in [0, \infty)$. Then

$$(A_1 - \lambda_0)^{-1} = [-v\Sigma_t(v) - \lambda_0]^{-1}$$

is certainly a bounded operator. Hence by the definition of the continuous spectrum, these λ_0 cannot be in $\sigma_c(A_1)$, and $\lambda_0 \notin \sigma_c(A_1) \Rightarrow C \subset \sigma_c(A_1) \Rightarrow C = \sigma_c(A_1)$. Now since A_1 is a closed operator, and A_2 is a completely continuous self-adjoint operator, we can apply the Weyl-von Neumann theorem to show that

$$\sigma_c(A) = \sigma_c(A_1 + A_2) = \sigma_c(A_1) = C$$

Since $A = A_1 + A_2$ is the sum of two self-adjoint operators, hence is itself self-adjoint, it can have no residual spectrum $\sigma_r(A)$.

Finally we consider the point spectrum $\sigma_p(A)$. Using detailed balance, we can demonstrate (just as in the synthetic kernel model) that for $1/v$ absorption, $\Sigma_a(v) = \Sigma_a^0/v$, the smallest eigenvalue is $\lambda_0 = -\Sigma_a^0$. But how do we study the remainder of the point spectrum? This is rather difficult in general, but the idea is to use the fact that $\lambda \notin C$ to rewrite the eigenvalue problem (5.13) as

$$\Phi_\lambda(v) = \int_0^\infty dv' k_\lambda(v', v) \Phi_\lambda(v') \quad (5.14)$$

where

$$k_\lambda(v', v) = \frac{K(v', v)}{[v\Sigma_t(v) + \lambda]^{1/2} [v'\Sigma_t(v') + \lambda]^{1/2}}$$

We now introduce an “artificial” eigenvalue c into this equation

$$c\Phi_\lambda(v) = \int_0^\infty dv' k_\lambda(v', v) \Phi_\lambda(v') \quad (5.15)$$

Since $k_\lambda(v', v)$ is a symmetric, square-integrable kernel (of the Hilbert-Schmidt type), we can frequently determine the eigenvalues c of Eq. 5.15. Then we must plot these eigenvalues $c(\lambda)$ as a function of the parameter λ and pick off the points where $c(\lambda) = 1$ to determine the point eigenvalues of Eq. 5.13 (see Figure 5.4). For incoherent solids, this procedure indicates a finite set of point eigenvalues in $\sigma_p(A)$. For gases we find an infinite set of eigenvalues, with $-\lambda^*$ appearing as a limit point of this set. The situation for liquids is a combination of both these cases and not very well understood.²⁶

Step 2. Construction of the Spectral Representation. There is relatively little information available concerning the spectral representation corresponding to the spectrum $\sigma(A)$. In analogy with our separable kernel model, we might expect that the forms of the eigenfunctions are as follows:

$$\psi_j(v) = \frac{\varphi_j(v)}{v\Sigma_t(v) + \lambda_j}, \quad \lambda_j \in \sigma_p(A)$$

where $\varphi_j(v)$ is defined to be the solution to the integral equation

$$\varphi_j(v) = \int_0^\infty dv' \frac{v'\Sigma_s(v' \rightarrow v)}{v'\Sigma_t(v') + \lambda} \varphi_j(v')$$

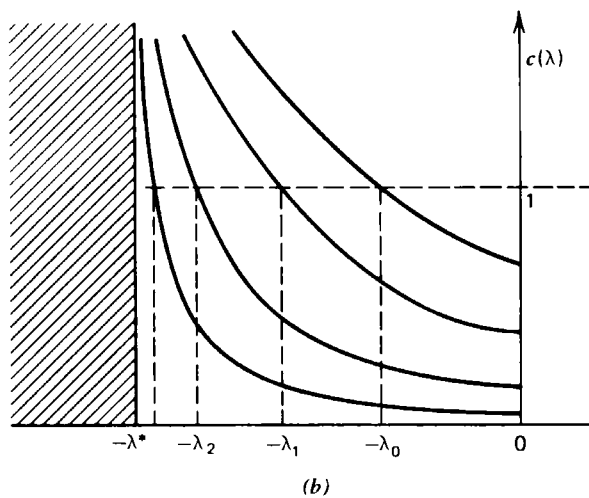
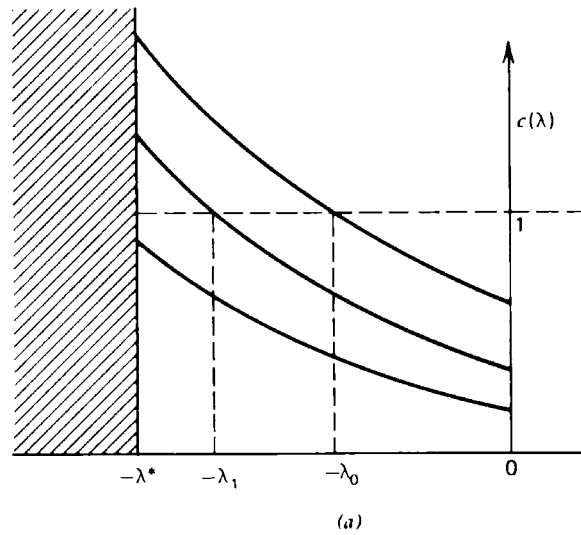


Fig. 5.4 □ Location of the point eigenvalue spectrum for solids (a) and gases (b).

The singular eigenfunctions take a similar form

$$\psi_{\lambda}(v) = P \frac{\varphi_{\lambda}(v)}{v \Sigma_r(v) + \lambda} + g(\lambda) \delta[v \Sigma_r(v) + \lambda], \quad \lambda \in \sigma_c(A)$$

Since we do not have a more explicit form for the eigenfunctions, it is difficult to determine their orthogonality or completeness properties. At this point we can only presume that the form of the solution to the initial

value problem Eq. 5.4 will be

$$N(v, t) = \sum_{\lambda_j \in \sigma_p} a_j \psi_j(v) e^{-\lambda_j t} + \int_{\lambda^*}^{\infty} d\lambda A(\lambda) \psi_\lambda(v) e^{-\lambda t}$$

in analogy to the form we calculated for the synthetic kernel model.

Asymptotic Transport Theory ($e^{i\mathbf{B}\cdot\mathbf{r}}$ approximation) □ We now turn our attention to the more general problem of the decay of a neutron pulse in a finite-sized sample of nonmultiplying material. We implement an approximation known as *asymptotic transport theory*^{27,28} by forcing the solution to have a harmonic spatial dependence. More specifically, we assume that the neutron phase space density can be written as

$$n(\mathbf{r}, \mathbf{v}, t) \sim n_B(\mathbf{v}, t) e^{i\mathbf{B}\cdot\mathbf{r}}$$

where $|\mathbf{B}|$ is a fixed, real number and is frequently identified with the “geometric buckling” or characteristic wave number of the geometry, $B \sim (\pi/\text{characteristic dimension})$. One can provide a more “rigorous” justification for this ansatz by assuming that we are interested in studying only the time decay of the fundamental spatial mode, or that we have just taken a Fourier transform in space and are going to invert this transform eventually (although of course one never completes the last step in practice). Presumably asymptotic transport theory will give an idea about what is going on for long times in systems of dimensions much greater than a mean free path.

Substituting this ansatz into the transport equation, we find that our initial value problem simplifies to

$$\frac{\partial n_B}{\partial t} + i\mathbf{B}\cdot\mathbf{v} n_B + v \Sigma_t(v) n_B(\mathbf{v}, t) = \int d^3v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) n_B(\mathbf{v}', t)$$

$$\text{i.c.: } n_B(\mathbf{v}, 0) = n_0(\mathbf{v})$$

(Of course we no longer have any boundary conditions to worry about.) Once again we can apply our spectral theory approach by using separation of variables

$$n_B(\mathbf{v}, t) = \psi_\lambda(\mathbf{v}) e^{\lambda t}$$

to arrive at an eigenvalue problem of the form

$$(A_1 + A_2) \psi_\lambda \equiv \left[-v \Sigma_t(v) - iB\mu v + \int d^3v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) \circ \right] \psi_\lambda(\mathbf{v}) = \lambda \psi_\lambda$$

(5.16)

where $\mu = \mathbf{v} \cdot \mathbf{B} / |\mathbf{v}| |\mathbf{B}|$. Notice that this is almost the same as the time relaxation problem in an infinite medium, except we now have an additional $iB\mu v$ term in the multiplicative operator A_1 as well as an angle dependence. We can apply essentially the same scheme to classify the eigenvalue spectrum of A . We avoid details and state only results.

Since A_1 is closed and A_2 is self-adjoint and completely continuous (at least for noncrystalline media), we find that by the Weyl–von Neumann theorem

$$\sigma_c(A) = \sigma_c(A_1 + A_2) = \sigma_c(A_1)$$

But if we assume that there are no point eigenvalues embedded in C , we find that the continuous spectrum fills a bullet-shaped region in the left half-plane (see Figure 5.5):

$$\sigma_c(A_1) = C, C \equiv \{ \lambda : \lambda = -v \Sigma_r(v) - iB\mu v, v \in [0, \infty), \mu \in [-1, +1] \}$$

Since A_1 is a non-self-adjoint operator (because of the $iB\mu v$ term), we have a complex continuous spectrum C —in fact, we have a two-dimensional set or area spectrum in the λ -plane. We can again show that the residual spectrum $\sigma_r(A)$ is empty by demonstrating that if $\lambda^* \in \sigma_p(A^\dagger)$ then $\lambda \in \sigma_p(A)$.

To identify the location of the point spectrum $\sigma_p(A)$, we consider the special case of isotropic scattering. Then we can restrict $\lambda \notin C$, divide

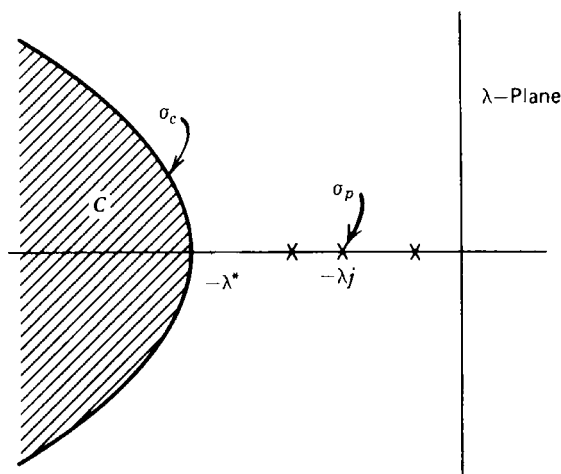


Fig. 5.5 □ Spectrum of the transport operator under the assumption of asymptotic transport theory.

through in Eq. 5.16 by $\lambda + iB\mu v + v\Sigma_t(v)$, and integrate over μ to find

$$\Phi_\lambda(v) = \frac{1}{2iBv} \ln \left[\frac{\lambda + iBv + v\Sigma_t(v)}{\lambda - iBv + v\Sigma_t(v)} \right] \int_0^\infty dv' \Sigma_s(v' \rightarrow v) \Phi_\lambda(v') \quad (5.17)$$

where $\Phi_\lambda(v) = \int_{-1}^1 d\mu \psi_\lambda(v)$. This equation can be used to demonstrate that the point eigenvalues are real. It can also be used to demonstrate the following very interesting property (first noted by Corngold).²⁷

Theorem. ("Maximum B Theorem"). For B sufficiently large, there are no point eigenvalues to the right of $-\lambda^*$.

Proof. Suppose we write Eq. 5.17 as follows:

$$\Phi_\lambda(v) = g(\lambda, B, v) A_2 \Phi_\lambda(v), \quad \lambda \notin C$$

The application of the Schwartz inequality to this equation yields

$$\|\Phi_\lambda\| = \|gA_2\Phi_\lambda\| \leq \|gA_2\| \|\Phi_\lambda\|$$

Hence for Eq. 5.17 to have nontrivial solutions Φ_λ , we demand

$$\|gA_2\| \geq 1 \quad \text{for some } \lambda \notin C$$

But as B becomes very large,

$$g(\lambda, B, v) = \frac{1}{2iBv} \ln \left[\frac{\lambda + iBv + v\Sigma_t(v)}{\lambda - iBv + v\Sigma_t(v)} \right] \sim 0 \left(\frac{1}{B} \right) \quad \text{as } B \rightarrow \infty$$

Therefore we can show that

$$\lim_{B \rightarrow \infty} \|gA_2\| = 0$$

In particular, for some $B^* < \infty$, $B > B^*$ will imply that $\|gA_2\| < 1$, hence that Eq. 5.17 has no nontrivial solutions for any $\lambda \notin C$ —that is, there are no point eigenvalues for $B > B^*$.

Notice that this theorem has a very interesting physical implication. We expect the general solution to the initial value problem to take the form

$$n(\mathbf{r}, \mathbf{v}, t) = \sum_{\lambda \in \sigma_p} a_\lambda \psi_\lambda(\mathbf{v}) e^{i\mathbf{B} \cdot \mathbf{r} + \lambda t} + \int_C d^2\lambda A(\lambda) \psi_\lambda(\mathbf{v}) e^{i\mathbf{B} \cdot \mathbf{r} + \lambda t}$$

For $B < B^*$, the least damped point eigenvalue $-\lambda_0$ will dominate the long

time behavior as

$$n(\mathbf{r}, \mathbf{v}, t) \sim a_0 \psi_0(\mathbf{v}) e^{i\mathbf{B} \cdot \mathbf{r} - \lambda_0 t} \quad \text{as } t \rightarrow \infty$$

But notice that for the case $B > B^*$, we have no point eigenvalues; therefore our solution takes the form

$$n(\mathbf{r}, \mathbf{v}, t) = \int_C d^2\lambda A(\lambda) \psi_\lambda(\mathbf{v}) e^{i\mathbf{B} \cdot \mathbf{r} + \lambda t}$$

which is not an exponential in time (at least manifestly). Hence this theorem suggests that for sufficiently large B , that is, sufficiently small systems, one can no longer observe an asymptotically dominant exponential decay in time. (In this regard, recall our analysis of the analogous one-speed problem in Section 2.5).

The nature of this problem changes somewhat for polycrystalline materials such as graphite or beryllium, since the scattering operator due to coherent elastic scattering (Bragg scattering) is not completely continuous and gives rise to an additional continuous spectrum.²⁸ Furthermore, the irregular, essentially discontinuous behavior of the total cross section for these materials fragments the continuous spectrum $\sigma_c(A)$. However the principal conclusions of our earlier analysis (in particular, the maximum B theorem) remain valid.

The Initial Value Problem in Bounded Geometries²⁹⁻³² □ Let us now return (finally) to consider the most general form of the initial value problem

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \nabla n + v \Sigma_t(v) n(\mathbf{r}, \mathbf{v}, t) = \int d^3v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) n(\mathbf{r}, \mathbf{v}', t)$$

$$\text{i.c.: } n(\mathbf{r}, \mathbf{v}, 0) = n_0(\mathbf{r}, \mathbf{v})$$

$$\text{b.c.: } n(\mathbf{R}_s, \mathbf{v}, t) = 0, \quad \hat{\mathbf{e}}_s \cdot \mathbf{v} < 0$$

We again use separation of variables

$$n(\mathbf{r}, \mathbf{v}, t) = \psi_\lambda(\mathbf{r}, \mathbf{v}) e^{\lambda t}$$

to arrive at the appropriate eigenvalue problem

$$\lambda \psi_\lambda(\mathbf{r}, \mathbf{v}) = \left[\underbrace{-\mathbf{v} \cdot \nabla - v \Sigma_t(v)}_{A_1} - \underbrace{\int d^3v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) \circ}_{A_2} \right] \psi_\lambda(\mathbf{r}, \mathbf{v}) = A \psi_\lambda$$

Notice that since we have a spatial derivative in the operator, we must also

include the boundary conditions in the specification of the eigenvalue problem: $\psi_\lambda(\mathbf{R}_s, \mathbf{v}) = 0, \hat{\mathbf{e}}_s \cdot \mathbf{v} < 0$. As before, we must first classify the spectrum $\sigma(A)$. The situation is now much more difficult because of the $\mathbf{v} \cdot \nabla$ term. Again the idea is to pick a sequence of test functions (which now must also satisfy the boundary conditions). However in this case, we can only construct a sequence $\{\varphi_\delta\}$ such that

$$\begin{aligned} \|\varphi_\delta\| &\geq c > 0 \\ \|(A_1 - \lambda)\varphi_\delta\| &\rightarrow 0, \quad \operatorname{Re}\{\lambda\} < -\lambda^* \end{aligned}$$

(we can no longer show weak convergence $\varphi_\delta \rightarrow 0$). Hence all we can say is that the region to the left of $-\lambda^*$ is in the spectrum of A , we cannot specify just whether it is in $\sigma_c(A)$ or $\sigma_p(A)$ (see Figure 5.6).

Unfortunately we can no longer apply the Weyl-von Neumann theorem, since A_1 is not a closed operator (because of the derivative term). There is an alternative approach to proving that all the continuous spectrum must be to the left of $-\lambda^*$ however. First we restrict $\operatorname{Re}\{\lambda\} > -\lambda^*$. Then we can integrate the integrodifferential form of the transport equation over space to find the integral equation (the “generalized Peierls equation”):

$$\begin{aligned} \Psi_\lambda(\mathbf{r}, \mathbf{v}) &= \int_0^{\tau_1} d\tau \exp\{-[v\Sigma_t(v) + \lambda]\tau\} \int d^3v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) \Psi_\lambda(\mathbf{r} - \mathbf{v}\tau, \mathbf{v}') \\ &\equiv F_\lambda \Psi_\lambda \end{aligned}$$

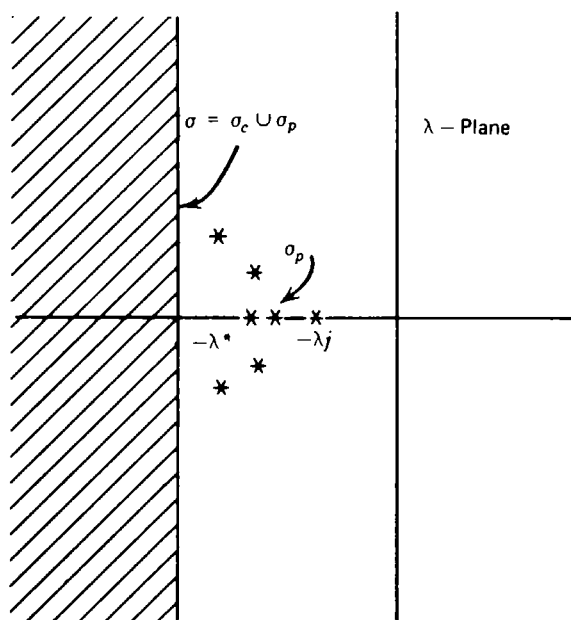


Fig. 5.6 □ Spectrum of the transport operator in bounded geometry.

where $\mathbf{r} - \mathbf{v}\tau_1$ is on the surface of the sample. We now apply a very useful theorem from functional analysis.

Theorem. (Tamarkin and Shmul'yan).³³ If F_λ is defined in a given region $D(\lambda)$ of the λ -plane as a compact operator analytically dependent on λ , any given number c (in our case, $c=1$) is (i) an eigenvalue of F_λ for all $\lambda \in D(\lambda)$ or (ii) belongs to the resolvent set—except for isolated values for which c is an eigenvalue.

To apply this theorem, one notes that by construction F_λ is analytic in λ . Hence all we have to prove is that F_λ is compact. This is rather messy, but it can be done. Then applying the Tamarkin–Shmul'yan theorem (noting that case ii applies), we find that only point eigenvalues can lie to the right of $-\lambda^*$. Here we have again used the fact that there is no residual spectrum.

It is also possible to prove that for small R , where R is some characteristic dimension of the sample (an average chord length),

$$\lim_{R \rightarrow 0} \|F_\lambda\| = 0$$

which implies that for sufficiently small systems, there are no discrete eigenvalues to the right of $-\lambda^*$.

And as in the two simpler problems we considered earlier, there is still very little known about the spectral representation of the solution to the initial value problem using this spectral classification.

***Spatial Relaxation Phenomena in Neutron Thermalization*^{34,35}** □ Let us now turn our attention to the analogous problem involving the spatial decay or relaxation of the neutron distribution away from a localized source. That is, we will study the asymptotic spatial decay of the phase space density at large distances from the source (just as in the time relaxation problem, we studied the asymptotic time decay for long times after the source burst).

To be more precise, consider the time-independent transport equation

$$\mathbf{v} \cdot \nabla n + v \Sigma_t(v) n(\mathbf{r}, \mathbf{v}) = \int d^3v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) n(\mathbf{r}, \mathbf{v}') + s(\mathbf{r}, \mathbf{v}) \quad (5.18)$$

Since we are only interested in the asymptotic form of the solution to this equation, we leave the boundary conditions unspecified.

We can again approach this problem using either integral transforms or separation of variables. Since we have found that both approaches eventually lead to the same eigenvalue problem, we consider only the more direct

separation of variables approach by choosing a separable ansatz

$$n(\mathbf{r}, \mathbf{v}) = \varphi_{\kappa}(\mathbf{v}) e^{-\kappa \cdot \mathbf{r}}$$

where our coordinate system will be chosen such that the wave vector is along the z -axis. Then if we substitute this form into the transport equation (5.18), we arrive at an eigenvalue problem

$$[v\Sigma_t(v) - \kappa\mu v] \varphi_{\kappa}(\mathbf{v}) = \int d^3v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) \varphi_{\kappa}(\mathbf{v}') \quad (5.19)$$

for the eigenvalue κ and the corresponding eigenfunction $\varphi_{\kappa}(\mathbf{v})$. Again we can follow the general approach by (i) classifying the spectrum of Eq. 5.19, (ii) constructing the corresponding spectral representation, and (iii) using this spectral representation to solve the given boundary value problem, say in the form

$$n(\mathbf{r}, \mathbf{v}) = \sum_{\kappa \in \sigma} a_{\kappa} \varphi_{\kappa}(\mathbf{v}) e^{-\kappa \cdot \mathbf{r}}$$

Once again we note that if there exists a least damped eigenvalue κ_0 , then far from sources and boundaries we find the asymptotic form

$$n(\mathbf{r}, \mathbf{v}) \sim a_0 \varphi_0(\mathbf{v}) e^{-\kappa_0 \cdot \mathbf{r}}$$

Hence just as we interpreted the pulsed neutron experiment as the measurement of the least damped *time* eigenvalue of the transport operator, we can interpret the analogous spatial experiment, the neutron diffusion length experiment, as just the measurement of the least damped *spatial* eigenvalue.

We can adapt much of the earlier analysis of the time eigenvalue problem. Again we skip the proofs and merely note results. For the case of incoherent scattering (noncrystalline media) the integral operator in Eq. 5.19 is completely continuous; hence our continuous spectrum $\sigma_c(A)$ is given by the set of all κ for which $[v\Sigma_t(v) - \kappa\mu v]$ vanishes; that is,

$$\kappa = \frac{\Sigma_t(v)}{\mu}, \quad v \in [0, \infty), \quad \mu \in [-1, +1]$$

Hence the continuous spectrum falls on the real axis from $-\infty$ to $-\Sigma_M$ and from $+\Sigma_M$ to $+\infty$, where we define $\Sigma_M \equiv \min \Sigma_t(v)$. It should be noted here that Σ_M is the analogue to λ^* in the time-dependent problem. However, whereas λ^* occurred as $v \rightarrow 0$, Σ_M usually occurs as $v \rightarrow \infty$ (see Figure 5.7).

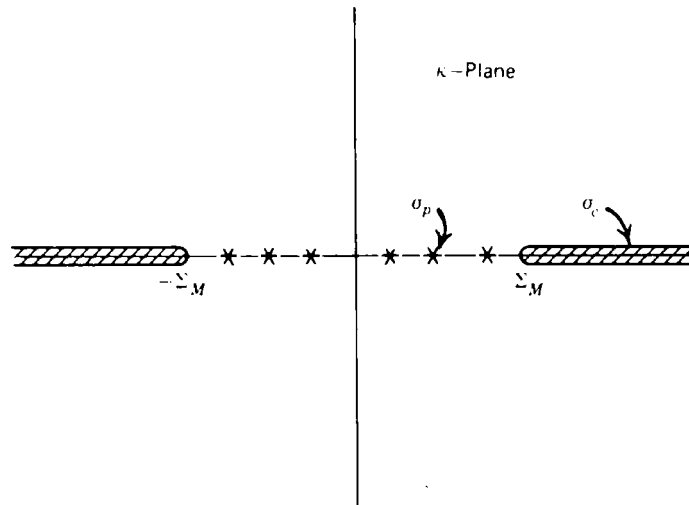


Fig. 5.7 □ Spatial eigenvalue spectrum of the transport operator.

Since the operators in Eq. 5.19 are self-adjoint, the spectrum must be real. We can prove that the point spectrum must lie in the range $[-\Sigma_M, \Sigma_M]$. If we further assume that scattering is isotropic, we can rewrite Eq. 5.19 for the point spectrum as

$$\Phi_\kappa(v) = \frac{1}{2\kappa v} \ln \left[\frac{\Sigma_t(v) + \kappa}{\Sigma_t(v) - \kappa} \right] \int_0^\infty dv' v' \Sigma_s(v' \rightarrow v) \Phi_\kappa(v') \equiv G_\kappa \Phi_\kappa$$

where $\Phi_\kappa(v) = \int_{-1}^1 d\mu \varphi_\kappa(v)$. Once again one can force the point spectrum to disappear, this time by adding absorption to the medium. That is, if we assume that we have $1/v$ absorption, $\Sigma_a = \Sigma_a^0/v$, it can be shown that $\|G_\kappa\| \rightarrow 0$ as $\Sigma_a^0 \rightarrow \infty$. Thus we can prove another theorem.

Theorem. (“Maximum Absorption Theorem”).²⁷ For sufficiently large absorption, there are no spatial eigenvalues.

If we suppose the spectral representation to take the form

$$n(\mathbf{r}, v) = \sum_{\kappa \in \sigma_p} a_\kappa \varphi_\kappa(v) e^{-\kappa \cdot \mathbf{r}} + \int_{\sigma_c} d\kappa A(\kappa) \varphi_\kappa(v) e^{-\kappa \cdot \mathbf{r}}$$

then for $\Sigma_a^0 < \Sigma_a^*$ we find the desired exponential behavior

$$n(\mathbf{r}, v) \sim a_0 \varphi_0(v) e^{-\kappa_0 \cdot \mathbf{r}}, \quad |\mathbf{r}| \rightarrow \infty$$

while for $\Sigma_a^0 > \Sigma_a^{0*}$

$$n(\mathbf{r}, \mathbf{v}) \sim \int_{\sigma_c} d\kappa A(\kappa) \varphi_\kappa(\mathbf{v}) e^{-\kappa \cdot \mathbf{r}}, \quad |\mathbf{r}| \rightarrow \infty$$

Since we define the neutron diffusion length $L = \kappa_0^{-1}$, we can conclude that for $\Sigma_a^0 > \Sigma_a^{0*}$ there is no diffusion length (at least in the traditional sense).

A very closely related problem is the neutron wave experiment,³⁶ which involves the asymptotic response of the neutron distribution to a time-modulated source (more precisely, a time-modulated component of the source, since a negative source function would not be defined). This can be described by the transport equation

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \nabla n + v \Sigma_t n = \int d^3 v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) n(\mathbf{r}, \mathbf{v}', t) + s_\omega(\mathbf{r}, \mathbf{v}) e^{i\omega t}$$

where ω is real and fixed. Of course for $\omega = 0$, we have the static source typical of the diffusion length experiment, and in this sense, the diffusion length problem is only a special case of the more general neutron wave problem in which $\omega > 0$.

We assume that all time transients have decayed away so that the time behavior of the neutron distribution is identical to that of the source. Hence our ansatz is taken as

$$n(\mathbf{r}, \mathbf{v}, t) = \varphi_\kappa(\mathbf{v}) \exp -(\kappa \cdot \mathbf{r} + i\omega t)$$

and on substitution into the transport equation, this leads to the eigenvalue problem for κ

$$[i\omega - \kappa \mu v + v \Sigma_t(v)] \varphi_\kappa(\mathbf{v}) = \int d^3 v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) \varphi_\kappa(\mathbf{v}')$$

Notice that the $i\omega$ has now made the problem non-self-adjoint. Hence we expect to find complex eigenvalues. The continuous spectrum for this problem is an area in the complex κ -plane (see Figure 5.8). Furthermore, the point spectrum is also complex (with symmetry between the first and third quadrants corresponding to wave propagation either to the left or to the right). As $\omega \rightarrow 0$, the area continuous spectra collapse to the cuts along the real axis characteristic of the diffusion length experiment.

Once again we encounter situations in which the point spectrum may vanish.³⁶

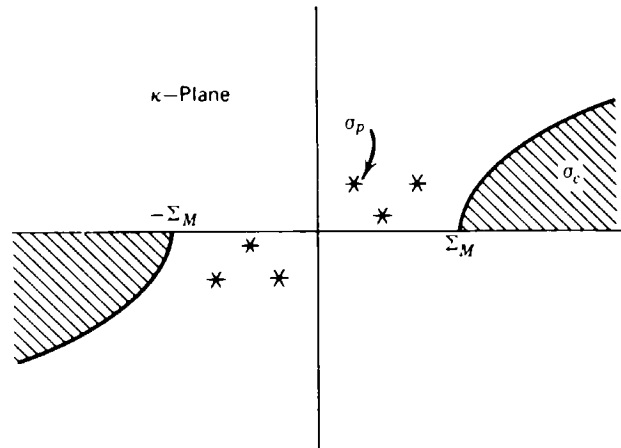


Fig. 5.8 □ Spatial eigenvalue spectrum of the transport operator subjected to an oscillating source, $\exp(i\omega t)$.

Theorem. (“Maximum Frequency Theorem”) For sufficiently large ω or Σ_a , there are no point eigenvalues outside C .

(However now, in contrast to the diffusion length problem, we cannot rule out the possibility of point eigenvalues embedded in the continuous spectrum.)

Further Comments on Asymptotic Relaxation Problems □ We have analyzed three different types of experimental procedure for studying the asymptotic behavior of the neutron distribution in a material: pulsed neutron experiments (PNE), diffusion length experiments (DLE), and neutron wave experiments (NWE). All three experiments are similar in that they seek to measure a fundamental discrete eigenvalue as a function of some experimental parameter: In the NWE, one measures the complex wave number κ versus the source frequency ω ; in the PNE, the time decay constant λ is measured as a function of system size (or B); and in the DLE, the inverse relaxation length κ is measured as a function of absorption concentration.

All three experiments exhibit limiting values of parameters for which a true exponential asymptotic relaxation of the distribution will be present. For example, if system sizes become too small in the PNE, or absorption becomes too large in the DLE, or if source frequency becomes too large in the NWE, the point spectrum will no longer dominate the asymptotic behavior of the neutron distribution. It should be noted that these limiting conditions are actually of the same order of magnitude in all three classes of experiments.

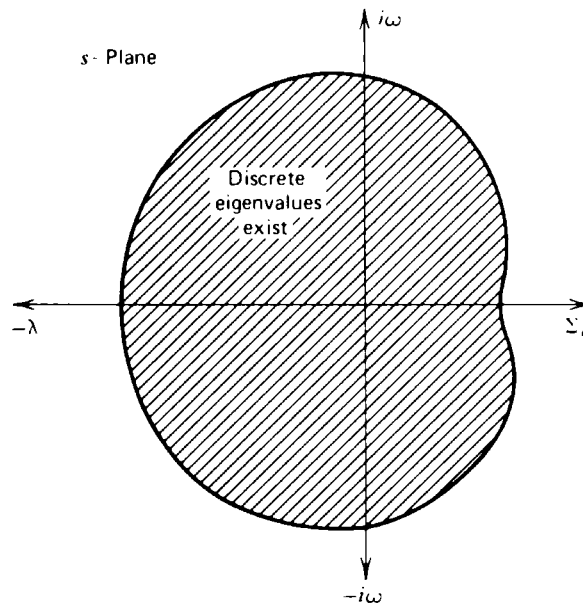


Fig. 5.9 □ Region in which roots to the dispersion law $\Lambda(\kappa, s)$ exist.

From a somewhat different perspective, one can interpret the conditions that determine the point spectrum for each experiment as being a specific representation of a general dispersion law that relates independent and dependent experimental variables. That is, if we recognize that the parameters λ and B in the PNE are related to κ and Σ_a in the DLE and to κ and ω in the NWE, we can define the point eigenvalues by a condition of the form

$$\Lambda(\kappa, s) = 0$$

which relates the two complex variables κ and s . In the s -plane, there will be a region of parameters s for which $\Lambda(\kappa, s)$ may have zeros κ_j (i.e., for which discrete spatial eigenvalues κ_j exist). For s outside this region, no such discrete eigenvalues exist. The maximum frequency (buckling or absorption) theorems occur when the bounding curve R dividing these regions intersects the axes (see Figure 5.9). It is evident that the limiting values of various parameters for each type of experiment can be compared by examining the shape of the curve R . Simple modeled calculations^{37,38} based on separable scattering kernels suggest that R is roughly circular, thus implying that all three experiments are equally restricted by their respective limitations on independent experimental parameters.

The Criticality Eigenvalue Problem □ Perhaps the most important eigenvalue problem in nuclear reactor applications arises in the determination

of the composition and geometry of a system containing fissile material that will sustain a steady-state or critical nuclear fission chain reaction. Since such a process can be identified with a time-independent neutron distribution, we find that one formulation of the criticality problem involves the determination of system parameters that would yield a zero fundamental time eigenvalue (corresponding to an everywhere positive eigenfunction)

$$\begin{aligned} (M - F)\psi_0 &= \left[\mathbf{v} \cdot \nabla + v \Sigma_t - \int d^3v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) \circ - \chi(\mathbf{v}) \int d^3v' v v' \Sigma_f \circ \right] \psi_0 \\ &= \lambda \psi_0 = 0 \end{aligned} \quad (5.20)$$

where we have included the fission operator F in addition to the transport operator, which we have relabeled as M .

However this is an extremely awkward formulation to analyze in practice because it involves determining the time eigenvalues λ_j and adjusting reactor parameters until the smallest of these eigenvalues λ_0 is made to vanish. A more convenient approach involves the insertion of a fictitious eigenvalue k^{-1} in front of the fission term so that Eq. 5.20 can be written as

$$M\psi = \frac{1}{k} F\psi \quad (5.21)$$

One then studies this “criticality eigenvalue problem” for the eigenvalue k^{-1} and adjusts system composition and geometry until the largest k (the smallest eigenvalue k^{-1}) corresponding to an everywhere positive eigenfunction is unity, $k_0 = 1$. This particular formulation presents a number of advantages. For example, the criticality eigenvalue k_0 can be shown to be identical to the *multiplication factor* k , defined as the ratio of the number of neutrons in two successive fission generations. Furthermore, the criticality eigenvalue problem in this form is ideally suited to numerical solution by means of the familiar power iteration (to be more precise, the “inverse” power method)⁹ in which one writes Eq. 5.21 as

$$\psi = \frac{1}{k} M^{-1} F \psi$$

and then iterates as

$$\psi^{n+1} = \frac{1}{k^n} M^{-1} F \psi^n$$

where

$$k^{n+1} = k^n \frac{(F\psi^n, F\psi^{n+1})}{(F\psi^n, F\psi^n)}$$

to obtain the eigenvalue $k^n \rightarrow k_0 = k_{\text{eff}}$ and the corresponding eigenfunction.

On a more theoretical level, there is a paucity of information available concerning the eigenvalue spectrum of the generalized eigenvalue problem represented by Eq. 5.21. Although physical considerations lead us to suspect that there will always exist a unique nonnegative solution to Eq. 5.21 with a corresponding positive eigenvalue k_0 that is larger in modulus than all other eigenvalues, this feature has not been proved in general (although restricted proofs have been provided for the one-speed and multigroup forms of Eq. 5.21, subject to rather stringent continuity assumptions).^{39,40} Very little information is available concerning the higher eigenvalues or the remainder of the eigenvalue spectrum. The importance of the theory of the criticality eigenvalue problem to nuclear reactor applications has stimulated continuing activity on this subject, however, with particular emphasis devoted to providing a more solid foundation for numerical solution methods.

5.1.2 □ Linearized Gas Dynamics⁴¹⁻⁴³ □ We have noted the very close similarity between the mathematical description of neutron transport and the time evolution of a weak disturbance in a rarefied gas. Indeed, within the framework of kinetic theory, neutron transport is actually just the foreign gas problem, whereas conventional gas dynamics involves a single species gas. Both problems are described by the linear Boltzmann equation (but with some significant differences in scattering kernels).

To be more precise, recall (cf. Section 3.2) that if we linearize the Boltzmann equation about an equilibrium distribution and assume finite range (truncated) potentials, we arrive at the linearized Boltzmann equation, which can be written in the form⁴¹

$$\frac{\partial n_1}{\partial t} + \mathbf{v} \cdot \nabla n_1 + v \Sigma n_1 = \int d^3v' v' \Sigma^{\text{LG}}(\mathbf{v}' \rightarrow \mathbf{v}) n_1(\mathbf{r}, \mathbf{v}', t) \quad (5.22)$$

Here the scattering kernel $\Sigma^{\text{LG}}(\mathbf{v}' \rightarrow \mathbf{v})$ characterizing the linearized gas can be defined in terms of the microscopic interaction cross sections for atomic collisions in gases, $\sigma(\mathbf{v}' \rightarrow \mathbf{v})$, as follows:

$$\Sigma^{\text{LG}}(\mathbf{v}' \rightarrow \mathbf{v}) = 2v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) - v' \Sigma_k(\mathbf{v}' \rightarrow \mathbf{v})$$

where

$$v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) = n_0 \int d^3 u' u \sigma(\mathbf{u}' \rightarrow \mathbf{u}) M(|\mathbf{v}' - \mathbf{u}'|)$$

$$v'_1 \Sigma_k(\mathbf{v}'_1 \rightarrow \mathbf{v}) = n_0 M(\mathbf{v}) \int d^3 u' u \sigma(\mathbf{u}' \rightarrow \mathbf{u}), \quad \mathbf{u} = \mathbf{v} - \mathbf{v}_1$$

It is important to note here that in contrast to the neutron transport scattering kernel, $\Sigma^{\text{LG}}(\mathbf{v}' \rightarrow \mathbf{v})$ can assume negative values. This feature has a profound implication for the eigenvalue spectrum of the transport operator characterizing a rarefied gas.

Infinite Medium Time Relaxation □ In analogy with our study of neutron transport, let us consider first the relaxation to equilibrium of a spatially uniform gas of infinite extent, as described by

$$\frac{\partial N}{\partial t} + v \Sigma(v) N(v, t) = \int_0^\infty dv' v' \Sigma(v' \rightarrow v) N(v', t)$$

We can examine the eigenvalue problem generated by seeking separable solutions of the form $N(v, t) = \psi(v) e^{\lambda t}$ to find

$$\left[-v \Sigma(v) + \int_0^\infty dv' v' \Sigma(v' \rightarrow v) \right] \psi_\lambda(v) = \lambda \psi_\lambda(v) \quad (5.23)$$

As in the neutron transport case, we again find both continuous and point spectra in general that depend on the assumed behavior of $v \Sigma(v)$. But now there are some interesting new wrinkles,^{41,44,45} since the form of $v \Sigma(v)$ depends sensitively on the interaction potential. For power law potentials, $V(r) \sim r^{-s}$, one finds that for “hard” potentials (i.e., $s > 4$), $v \Sigma(v)$ increases monotonically; for Maxwell molecules ($s = 4$), $v \Sigma(v) = \nu_0 = \text{constant}$; whereas for “soft” potentials ($s < 4$), $v \Sigma(v)$ decreases (see Figure 5.10).⁴⁵

The location of the continuous spectrum is different for each of these three cases, as shown in Figure 5.11. In particular, only the hard potentials yield a continuous spectrum similar to the neutron transport problem. For Maxwell molecules, the continuous spectrum degenerates to a point at $\lambda = -\nu_0$, but for soft potentials, the continuous spectrum actually comes into the origin.

There are several important differences in the nature of the point spectrum as well. For example, the origin $\lambda = 0$ is now an eigenvalue of twofold degeneracy corresponding to conservation of mass and energy. If we had considered the more general problem in which we allowed the eigenfunctions to be dependent on velocity $\mathbf{v}$ rather than speed v , the

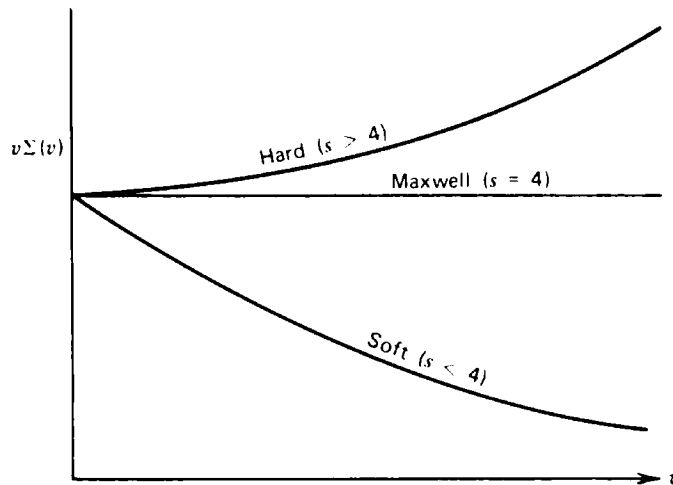


Fig. 5.10 □ Behavior of the collision frequency for various forms of the intermolecular potential in gases.

origin would have been an eigenvalue with fivefold degeneracy corresponding to conservation of momentum as well. In the neutron transport problem in the absence of absorption, there is only a simple eigenvalue at the origin corresponding to conservation of number. This difference arises because of the different mathematical structure of the scattering kernels. In particular, we recall that $\Sigma_s(\mathbf{v}' \rightarrow \mathbf{v})$ is nonnegative for neutron transport, whereas $\Sigma^{LG}(\mathbf{v}' \rightarrow \mathbf{v})$ can assume negative values for the linearized gas problem. Of course, from a physical viewpoint this difference occurs because self-diffusion (e.g., neutron transport) processes only conserve particle number (or mass), but collective transport processes conserve particle mass, momentum, and energy in collisions.

In general there will also be a number of point eigenvalues in the interval $-\lambda^* \leq \lambda \leq 0$. For example, for both hard sphere and Maxwell molecule potentials, there are an infinite number of eigenvalues in this interval of the negative real axis that converge to a limit point at $\lambda = -\lambda^*$.

Sound Wave Propagation □ The spatial relaxation of a disturbance away from a steady-state “source” (the analogue of the neutron diffusion length problem) or the time relaxation of disturbances introduced into a finite volume of gas in a container (the analogue to the pulsed neutron experiment) are of only marginal interest in gas dynamics. Of far more interest are studies of free and forced sound propagation,^{46–48} which examine the properties of plane wave solutions to the transport equation of the form

$$n(\mathbf{r}, \mathbf{v}, t) = \psi(\mathbf{v}) e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)}$$

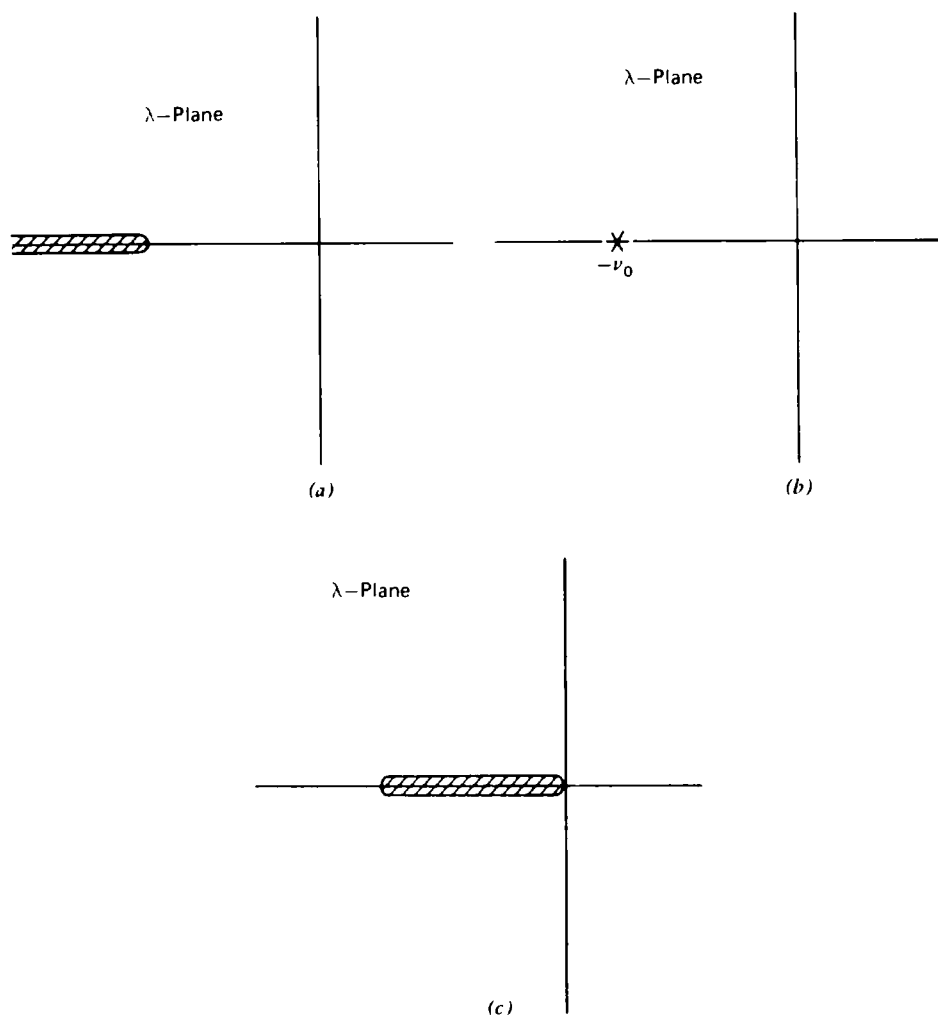


Fig. 5.11 □ Continuous spectra of the infinite medium transport operators characterizing a gas. (a) Hard. (b) Maxwell. (c) Soft.

so that Eq. 5.22 reduces to the form

$$[i\mathbf{k} \cdot \mathbf{v} - i\omega + v\Sigma(v)]\psi(\mathbf{v}) = \int d^3v' v' \Sigma(\mathbf{v}' \rightarrow \mathbf{v}) \psi(\mathbf{v}') \quad (5.24)$$

If we imagine such disturbances as being introduced in the gas by a localized source of fixed frequency ω , we have just the *forced sound wave propagation* problem (the analogue to the neutron wave experiment). If instead we fix $\mathbf{k}$ and determine how the corresponding density disturbance in the gas relaxes in time, we have the *free sound wave propagation* problem (analogous to the pulsed neutron experiment as described by asymptotic

transport theory). Notice that both problems are tractable because of the absence of boundary conditions (i.e., corresponding to infinite medium relaxation problems, in effect). Each problem is an eigenvalue problem in either $\mathbf{k}$ or ω .

i *Free sound wave propagation.*^{46,47} Suppose we first fix $\mathbf{k}$ and regard Eq. 5.24 as an eigenvalue problem for the time relaxation constants characterizing disturbances of wave number $\mathbf{k}$. The continuous spectrum is determined by the condition

$$[i\mathbf{k} \cdot \mathbf{v} - i\omega + v\Sigma(v)] = 0 \quad \text{for all values of } \mathbf{v} \quad (5.25)$$

We align our v_z axis along $\mathbf{k}$ so that Eq. 5.25 becomes

$$\omega = kv\mu - iv\Sigma(v), \quad v \in [0, \infty), \quad \mu \in [-1, +1]$$

Once again we find three cases, depending on the nature of the interatomic potential (see Figure 5.12). The eigenvalues in the point spectrum corresponding to the infinite medium relaxation problem ($k=0$) now move off of the axis for $k>0$ and into the complex plane. In particular, the fivefold degenerate eigenvalue at $\omega=0$ separates into one purely imaginary mode (nonpropagating) and two complex conjugate pairs of propagating modes (again corresponding to the hydrodynamic modes of the gas, i.e., corresponding to conservation of mass, momentum, and energy—see Figure 5.13).

ii *Forced sound wave propagation.*^{47,48} Let us now examine the alternative process in which we fix ω to be real and determine the values of $\mathbf{k}$ for which nontrivial solutions exist to Eq. 5.25. Again we find a continuous spectrum that depends sensitively on the nature of the interaction potential (see Figure 5.14). There are now four discrete eigenvalues, $\pm k_0$ and $\pm k_1$, which emerge from the origin as ω is increased from zero (corresponding to the hydrodynamic modes of the gas). The eigenvalues with smallest imaginary parts correspond to sound waves (i.e., propagating modes), while the second pair is characterized by much larger imaginary parts and damps out rapidly in space (diffusive modes corresponding to thermal conduction).

The similarities between these eigenvalue problems and those representative of neutron transport are quite striking, aside from the richer point spectrum. Once again we find that for sufficiently large k or ω , the point spectrum disappears into the continuous spectrum, although it can be

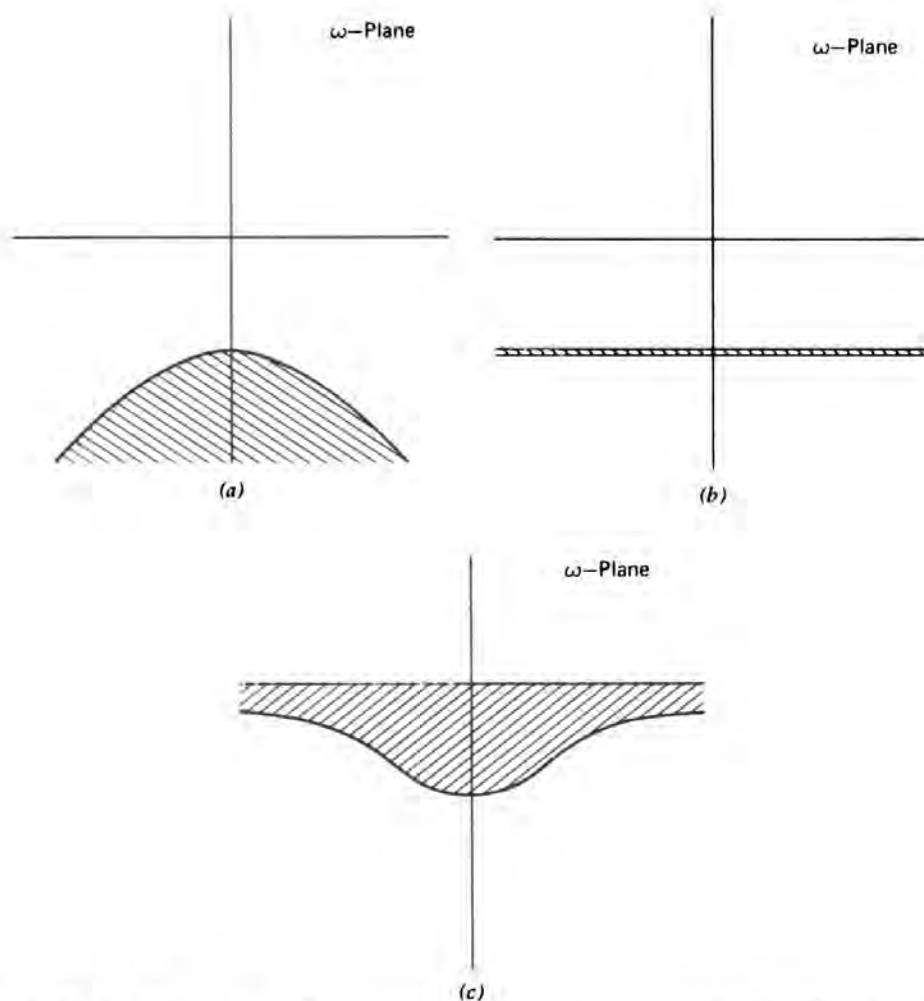


Fig. 5.12 □ Time eigenvalue spectra for free wave propagation problem in gases. (a) Hard. (b) Maxwell. (c) Soft.

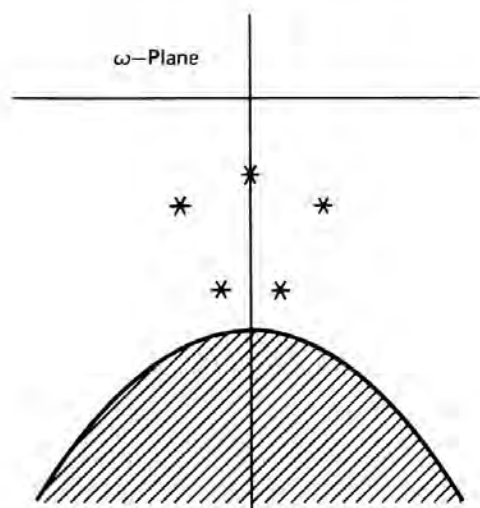


Fig. 5.13 □ Eigenvalue spectrum (including hydrodynamic modes) for free wave propagation in gases.

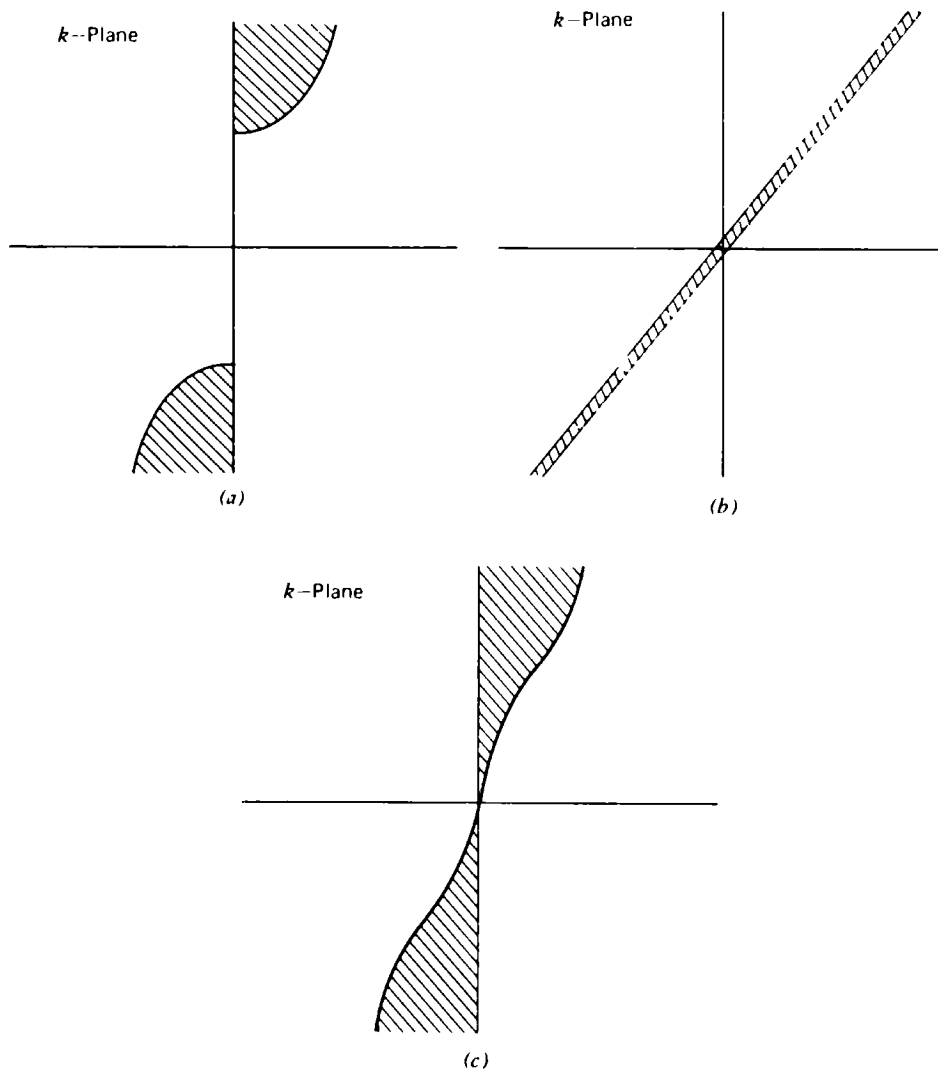


Fig. 5.14 □ Spatial eigenvalue spectra for forced wave propagation in gases. (a) Hard. (b) Maxwell. (c) Soft.

tracked down in modeled problems using analytic continuation procedures^{46,48} (see Figure 5.15).

5.1.3 □ Relaxation Processes in a Plasma □ A wealth of relaxation phenomena of various types arise in plasma physics. We discuss only one of these, electron density oscillations.^{49,50} (Actually, it was this particular topic that led to the original development of the singular eigenfunction methods by Van Kampen.⁵¹)

We simplify the analysis of electron density oscillations by assuming that we have a uniform fixed background of positive ions to provide

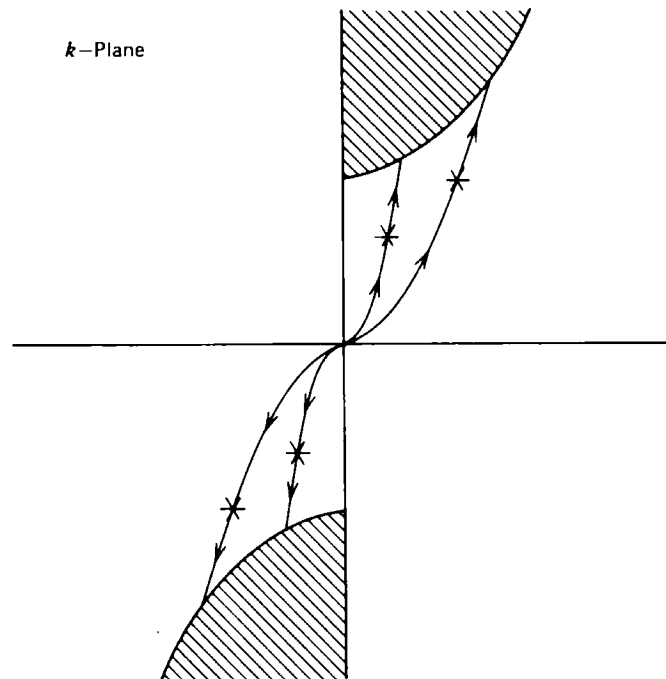


Fig. 5.15 □ Disappearance of point spectrum into continuous spectrum for increasing frequency ω .

macroscopic charge neutrality (at least in equilibrium). Furthermore, we assume that there are no external magnetic fields, and we make the electrostatic approximation that the electric field can be derived from a scalar potential $\mathbf{E} = -\nabla\phi$. Then to a certain level of approximation, the equation describing the electron distribution function $n(\mathbf{r}, \mathbf{v}, t)$ is just the Vlasov equation

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} - \frac{e}{m} \mathbf{E} \cdot \frac{\partial n}{\partial \mathbf{v}} = 0$$

$$\frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{E} = -4\pi e \int d^3v [n(\mathbf{r}, \mathbf{v}, t) - n_0(\mathbf{v})] \quad (5.26)$$

Of course this is a highly nonlinear system, since the self-consistent field term depends itself on the distribution $n(\mathbf{r}, \mathbf{v}, t)$. Therefore we linearize Eq. 5.26 about an equilibrium distribution $n_0(\mathbf{v})$

$$n(\mathbf{r}, \mathbf{v}, t) = n_0(\mathbf{v}) + n_1(\mathbf{r}, \mathbf{v}, t)$$

which we leave unspecified for the present (assuming only that it does not depend on space or time). If we substitute this form into the Vlasov

equation 5.26 and retain only first-order terms in the perturbation $n_1(\mathbf{r}, \mathbf{v}, t)$, we arrive at the linearized Vlasov equation

$$\frac{\partial n_1}{\partial t} + \mathbf{v} \cdot \frac{\partial n_1}{\partial \mathbf{r}} - \frac{e}{m} \mathbf{E}_1 \cdot \frac{\partial n_0}{\partial \mathbf{v}} = 0$$

$$\frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{E}_1 = -4\pi e \int d^3v n_1(\mathbf{r}, \mathbf{v}, t) \quad (5.27)$$

To more easily visualize the relation between this transport equation and the equations encountered in neutron transport or linearized gas dynamics, consider an initial value problem in which all disturbances are characterized by a specified wave vector $\mathbf{k}$

$$n_1(\mathbf{r}, \mathbf{v}, t) = n_1(\mathbf{k}, \mathbf{v}, t) e^{i\mathbf{k} \cdot \mathbf{r}}$$

Then Eq. 5.27 can be written as follows:

$$\frac{\partial n_1}{\partial t} + i\mathbf{k} \cdot \mathbf{v} n_1 - \frac{e}{m} \mathbf{E}_1 \cdot \frac{\partial n_0}{\partial \mathbf{v}} = 0, \quad i\mathbf{k} \cdot \mathbf{E}_1(\mathbf{k}, t) = -4\pi e \int d^3v n_1(\mathbf{k}, \mathbf{v}, t)$$

To simplify this equation, we define our velocity coordinate system along the wave vector $\mathbf{k}$ such that we can integrate out the perpendicular velocity variables to find

$$\frac{\partial n_1}{\partial t} + ikun_1(k, u, t) = \omega_p^2 \frac{i}{k} \left(\frac{dn_0}{du} \right) \int_{-\infty}^{\infty} du' n_1(k, u', t)$$

where $\omega_p^2 = (4\pi e^2 n_0 / m)$ is the plasma frequency. Notice that this is beginning to resemble our earlier linear transport equations (appropriately Fourier transformed in space, of course).

The next step is to solve this equation subject to some initial value, say $n_1(k, u, t) = n_1(k, u, 0)$. Landau⁵⁰ first attacked this problem using Laplace transforms in time. Van Kampen⁵¹ used the “normal mode” approach (singular eigenfunction expansions), which was subsequently extended and rigorized by Case. Since Landau’s approach is the clearest (and the more common), we apply Laplace transforms:

$$\tilde{n}_1(k, u, s) \equiv \int_0^{\infty} dt e^{-st} n_1(k, u, t)$$

to find the transformed Vlasov equation as

$$(s +iku)\tilde{n}_1(k, u, s) = \omega_p^2 \frac{i}{k} \left(\frac{dn_0}{du} \right) \int_{-\infty}^{\infty} du' \tilde{n}_1(k, u', s) + n_1(k, u, 0)$$

We can solve this in the usual fashion to find

$$\int_{-\infty}^{\infty} du \tilde{n}_1(k, u, s) = \frac{\int_{-\infty}^{\infty} du \frac{n_1(k, u, 0)}{s + iku}}{1 - \omega_p^2 \frac{i}{k} \int_{-\infty}^{\infty} du \frac{dn_0/du}{s + iku}} \equiv \frac{\chi(k, s)}{D(k, s)}$$

and also determine the electric field as

$$\tilde{E}_1(k, s) = \frac{4\pi n_0 e i \chi(k, s)}{k D(k, s)}$$

To invert these transformed solutions, we first note that they contain integrals that introduce branch cuts along the imaginary axis in the s -plane (see Figure 5.16). Landau suggested that we analytically continue the definitions of $\chi(k, s)$ and $D(k, s)$ across the cut into the left half-plane. To perform this analytic continuation, we notice that for the Cauchy integral defined in the plane cut along the imaginary axis

$$I(z) = \int_{-\infty}^{\infty} dv \frac{f(v)}{v + iz}, \quad \text{Re}\{z\} > 0$$

we can construct the analytic continuation into the left half-plane as

$$I_{AC}(z) = \int_{-\infty}^{\infty} dv \frac{f(v)}{v + iz} + 2\pi i f(iz), \quad \text{Re}\{z\} < 0$$

(To demonstrate that this is indeed the appropriate analytic continuation, just take the limit as z approaches the imaginary axis using the Plemelj formulas; then use the identity theorem for analytic functions.)

With this analytic continuation, we can deform the inversion path into the left half-plane and pick up the residues from the poles of the transforms. These pole singularities occur at the zeros of $D(k, s)$, that is, at those points s_0 at which

$$D_{AC}(k, s_0) = 1 - \omega_p^2 \frac{i}{k} \int_{-\infty}^{\infty} du \frac{dn_0/du}{s_0 + iku} - 2\pi \frac{\omega_p^2}{k^2} \left(\frac{dn_0}{du} \right)_{is_0/k} = 0$$

When the unperturbed state of the plasma $n_0(v)$ is in thermal equilibrium, we can calculate the form of the dominant poles $s_0 = \pm i\omega_0 - \gamma$ in the small

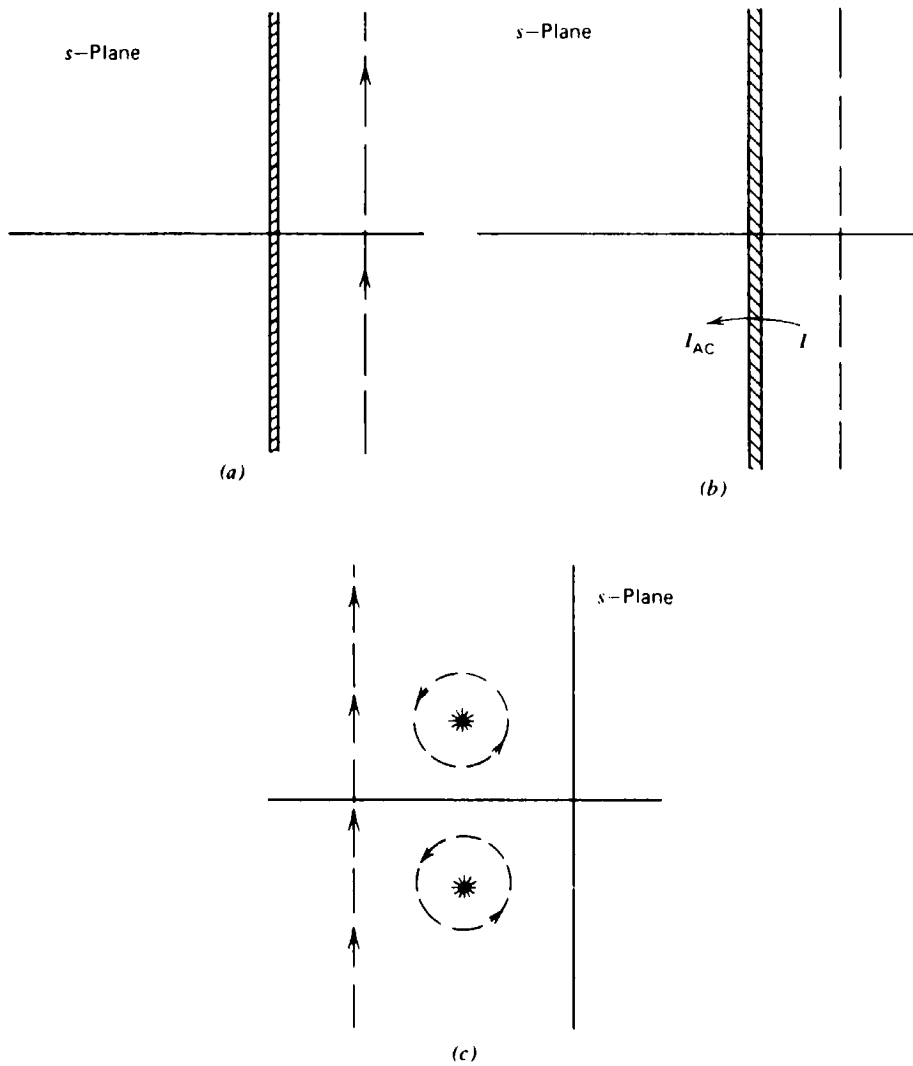


Fig. 5.16 □ Analytic continuation and path deformation for the Landau solution of the Vlasov equation. (a) Original s -plane structure. (b) Analytical continuation. (c) Path deformation.

k limit as

$$\omega_0^2 \sim \omega_p^2 + \left(\frac{3k_B T}{m} \right) k^2$$

$$\gamma = -\omega_p \left(\frac{\pi}{8} \right)^{1/2} e^{-3/2} (k\lambda_D)^{-2} \exp \left[-\frac{1}{2(k\lambda_D)^2} \right]$$

where $\lambda_D = k_B T / ne^2$ is the Debye length. Hence the analytic continuation

into the left half-plane yields a term with damping

$$E_1(k, t) = \sum_j R_j e^{s_j(k)t} + \frac{1}{2\pi i} \int_{-\sigma-i\infty}^{-\sigma+i\infty} ds e^{st} \tilde{E}_1(k, s)$$

and therefore the large time behavior is of the form

$$E_1(k, t) \sim R_0 e^{-\gamma t} \cos(\omega_0 t + \alpha)$$

This damping is referred to as *Landau damping* or phase mixing, and it plays a very important role in plasma physics.⁴⁹

One can continue in this fashion to analyze an enormous variety of other linearized relaxation problems in plasmas. For example, if we apply a static magnetic field, many new complex relaxation phenomena appear. However since these studies would take us too far afield into the discipline plasma physics, and since we have already demonstrated the close similarity between asymptotic solutions of the Vlasov equation and those encountered in neutron transport or gas dynamics, we proceed with the more difficult subject of boundary value problems in transport theory.

5.2 □ GENERAL STUDIES OF BOUNDARY VALUE PROBLEMS □

We have confined our attention thus far in this chapter to asymptotic relaxation problems in transport theory that involve the behavior of the particle distribution at long times or large distances from sources and boundaries. This permitted us to analyze these processes simply by studying the asymptotic form of the particle phase space density $n(\mathbf{r}, \mathbf{v}, t)$, which was governed by the least damped eigenvalue of the transport operator. Hence all we really had to do was classify and determine the eigenvalue spectrum.

In turning to problems in which we are interested in the particle distribution in the neighborhood of sources and boundaries, we find that we must actually construct the solution to a specific boundary value problem. Of course this is extremely difficult, particularly when one attempts to account for a general scattering kernel $\Sigma_s(\mathbf{v}' \rightarrow \mathbf{v})$. If we recall our rather formal analysis of asymptotic relaxation phenomena for this general case, we should not be surprised that direct analytical attempts to confront boundary value problems in which the particle energy dependence is important have experienced only limited success. Indeed, since such problems can be solved quickly and accurately using the sophisticated numerical methods described in Chapter 8, it is not surprising that the development of analytical methods appropriate for solving energy-depen-

dent boundary value problems is a field that is largely ignored in transport theory.

Nevertheless, for completeness we briefly review the attempts that have been made to analyze this class of problem, if only to point out where the principal difficulties arise. We restrict our discussion to time-independent phenomena and usually assume one-dimensional (plane) symmetry. We recall from Chapter 2 that the two most popular approaches to boundary value problems in transport theory are integral transforms and singular eigenfunction expansions. It is not surprising, therefore, that there have been a number of attempts to extend these methods to transport problems in which the particle energy dependence is included. However these efforts have met with very limited success, and they have proved to be capable of yielding explicit solutions only when they employ models of the scattering kernel that reduce the transport equation to a form very similar to that characteristic of one-speed problems.

5.2.1 □ Synthetic Kernel Models □ One of the most popular approaches in neutron transport theory has been to implement the very simple synthetic or separable kernel model¹⁴

$$\Sigma_s(v' \rightarrow v, \mu' \rightarrow \mu) = \left(\frac{\beta}{2} \right) \Sigma_s(v') v M(v) \Sigma_s(v), \quad \beta^{-1} \equiv \int_0^\infty dv v \Sigma_s(v) M(v)$$

to arrive at the transport equation

$$\begin{aligned} \mu v \frac{\partial n}{\partial x} + v \Sigma_t(v) n = \frac{\beta}{2} v M(v) \Sigma_s(v) \int_{-1}^{+1} d\mu' \int_0^\infty dv' v' \Sigma_s(v') n(x, v', \mu') \\ + s(x, \mu, v) \end{aligned} \quad (5.28)$$

This equation is very similar in structure to the one-speed transport equation, particularly if the collision frequency $v \Sigma_t(v)$ can be assumed to be independent of v . Either singular eigenfunction expansions⁵² or integral transform (Wiener-Hopf) methods⁵³ can be carried over from the one-speed theory with little difficulty. A variety of boundary value problems have been treated with this model.

A particularly useful mathematical approximation involves the assumption of constant cross sections $\Sigma_t(v) = \Sigma_t$. However one can also easily handle the case of monotonic cross sections by defining the variable transformations

$$\eta \equiv \frac{\mu}{\Sigma_t(v)}, \quad \psi(x, \eta, v) = v \Sigma_t(v) n(x, \mu, v)$$

so that Eq. 5.28 can be written in the form

$$\eta \frac{\partial \psi}{\partial x} + \psi(x, \eta, v) = \frac{1}{2} \int_0^\infty dv' \int_{-\Sigma_i^{-1}(v')}^{\Sigma_i^{-1}(v')} d\eta' \Sigma_s(v' \rightarrow v) \psi(x, \eta', v')$$

which is very similar to the one-speed transport equation. Mika⁵² has utilized singular eigenfunction methods to solve this equation for a number of the standard problems (e.g., the Milne and two adjacent half-spaces problems). Williams⁵³ has solved similar problems using integral transforms and the Wiener-Hopf technique.

5.2.2 □ BGK Models □ A number of very similar problems have been solved by Cercignani^{19,54} and others in the field of linearized gas dynamics by implementing the BGK collision kernel. When this model is introduced into the linearized Boltzmann equation

$$\mathbf{v} \cdot \frac{\partial \varphi}{\partial \mathbf{r}} = L[\varphi]$$

and this equation is projected onto transverse and longitudinal velocity components [where we will normalize $\mathbf{v} \rightarrow \xi = \mathbf{v}/v_0$, $v_0 = (2n_0 k T_0)^{1/2}$]

$$\begin{aligned} \varphi(x, \xi) = & Y_0(x, \xi_1) + (\xi_2^2 + \xi_3^2 - 1) Y_1(x, \xi_1) \\ & + 2\xi_2 Y_2(x, \xi_1) + 2\xi_3 Y_3(x, \xi_1) + Y_4(x, \xi) \end{aligned}$$

one arrives at a system of transport equations

$$\begin{aligned} \xi_1 \frac{\partial Y_0}{\partial x} + \nu_0 Y_0 = & \frac{\nu_0}{\sqrt{\pi}} \int_{-\infty}^{\infty} d\xi'_1 Y_0(x, \xi'_1) e^{-\xi_1'^2} + \frac{2}{3} \left(\xi_1^2 - \frac{1}{2} \right) \frac{\nu_0}{\sqrt{\pi}} \\ & \times \left[\int_{-\infty}^{\infty} d\xi'_1 \left(\xi_1'^2 - \frac{1}{2} \right) e^{-\xi_1'^2} Y_0(x, \xi'_1) + \int_{-\infty}^{\infty} d\xi'_1 e^{-\xi_1'^2} Y_1(x, \xi'_1) \right] \\ \xi_1 \frac{\partial Y_1}{\partial x} + \nu_0 Y_1 = & \frac{2\nu_0}{3\sqrt{\pi}} \int_{-\infty}^{\infty} d\xi'_1 \left(\xi_1'^2 - \frac{1}{2} \right) e^{-\xi_1'^2} Y_0(x, \xi'_1) \\ & + \frac{2\nu_0}{3\sqrt{\pi}} \int_{-\infty}^{\infty} d\xi'_1 e^{-\xi_1'^2} Y_1(x, \xi'_1) \\ \xi_1 \frac{\partial Y_i}{\partial x} + \nu_0 Y_i = & \frac{\nu_0}{\pi^{3/2}} \int_{-\infty}^{\infty} d\xi'_1 e^{-\xi_1'^2} Y_i(x, \xi'_1), \quad i=2,3 \\ \xi_1 \frac{\partial Y_4}{\partial x} + \nu_0 Y_4 = & 0 \end{aligned}$$

The first two equations are coupled and describe longitudinal processes such as sound wave propagation or thermal conduction. The third equation characterizes transverse processes such as shear flow, and it is decoupled from the rest of the set.

Since the equation characterizing shear flow processes has a form very similar to that of the one-speed transport equation, it is not surprising that this equation has been solved using both integral transform (Wiener-Hopf) and singular eigenfunction methods for a variety of boundary value problems in gas dynamics. The coupling between the longitudinal components Y_0 and Y_1 in the set characterizing thermal processes gives rise to a 2×2 matrix boundary value problem. For reasons that will become apparent in a moment, this feature increases enormously the difficulty of the corresponding boundary value problem in heat transfer. It has been only within the past several years that such problems have begun to yield to exact analytical methods.⁵⁵

5.2.3 □ More General Collision Models □ Consider the general form of the energy-dependent transport equation under the assumptions of plane symmetry and isotropic scattering

$$\mu \frac{\partial \varphi}{\partial x} + \Sigma_t(E) \varphi(x, \mu, E) = \frac{1}{2} \int_{-1}^{+1} d\mu' \int_0^\infty dE' \Sigma_s(E' \rightarrow E) \varphi(x, \mu', E') + s(x, \mu, E) \quad (5.29)$$

Since a solution of this equation in its general form is usually out of the question even for infinite medium problems in which the spatial term vanishes, let us turn instead to approximate methods for treating the energy dependence (discussed in more detail in Chapter 7). The most common schemes include the following:

- i Multigroup energy treatments in which the energy variable is discretized and the integration over energy replaced by a summation over energy groups.
- ii Expansion of the energy dependence of $\varphi(x, \mu, E)$ in a finite set of polynomials

$$\varphi(x, \mu, E) = \sum_{j=1}^N \varphi_j(x, \mu) p_j(E)$$

- iii Approximation of the scattering kernel as a N -term degenerate kernel of the form

$$\Sigma_s(E' \rightarrow E) = \sum_{i,j} a_{ij} p_i(E') q_j(E)$$

All these schemes reduce Eq. 5.29 to a set of N coupled one-speed transport equations. For example, the multigroup approximation leads to

$$\mu \frac{\partial \varphi_g}{\partial x} + \Sigma_{tg} \varphi_g(x, \mu) = \sum_{g'=1}^N \Sigma_{sg' \rightarrow g} \frac{1}{2} \int_{-1}^{+1} d\mu' \varphi_{g'}(x, \mu') + s_g(x, \mu)$$

or in matrix form

$$\mu \frac{\partial}{\partial x} \boldsymbol{\varphi} + \boldsymbol{\Sigma}_t \boldsymbol{\varphi} = \boldsymbol{\Sigma}_s \frac{1}{2} \int_{-1}^{+1} d\mu' \boldsymbol{\varphi}(x, \mu') + \mathbf{s}(x, \mu) \quad (5.30)$$

It is possible to solve these systems of equations for full-range (e.g., infinite medium) boundary value problems. (Indeed, it is possible to solve even the more general Eq. 5.29 formally in terms of operator inverses for full-range problems.⁵⁶) However, as we noted earlier, the study of the more interesting half-range boundary value problems must eventually encounter the difficulties of a Riemann-Hilbert or Wiener-Hopf problem. It is not surprising, therefore, that systems such as Eq. 5.30 lead to *matrix* Riemann-Hilbert problems^{57,58} of the form

$$\Lambda^+(z) X^-(z) - \Lambda^-(z) X^+(z) = 0 \quad (5.31)$$

and to comparable matrix Wiener-Hopf decomposition problems. And, unfortunately, these matrix factorization problems have proved extremely resistant to attempts to construct solutions.⁵⁹⁻⁶¹

Although Mullikin⁵⁹ has been able to demonstrate the existence of the $X^\pm(z)$ matrices and to examine several of their properties, there has been only marginal success (even using recent techniques such as the resolvent integration method) in constructing an explicit representation of these quantities. Although there have been many papers published on the analytical solution of the multigroup transport equation, these efforts usually lead to a set of nonlinear integral equations for the components of the X matrices that must be solved numerically (and require considerably more effort than would a direct discrete ordinates solution of the original transport equation). It has only been very recently that even the simplest of these problems, the two-group case, has been solved explicitly, and then only under the assumption of constant total cross sections, $\Sigma_{t1} = \Sigma_{t2}$.^{55,61}

Case⁶² has noted that it should be possible to solve the half-range problem for several other special cases, including multigroup problems in which only downscattering is considered, and degenerate kernel representations in which the kernel expansion functions satisfy a three-term recursion relation. (It was the latter property that Mika⁶³ utilized in his study of anisotropic scattering.)

However, at least for the moment, the extension of integral transform or singular eigenfunction expansion methods to solve boundary value problems involved with coupled systems of transport equations (e.g., multi-group transport theory or temperature flow problems in rarefied gas dynamics) represents a formidable task that can be attacked more directly using numerical methods.

5.3 □ SUPERHERMAL PARTICLE TRANSPORT □ An extremely important class of transport phenomena involves the slowing down of a fast particle as it moves through a medium. If the energy of the particle is much larger than the thermal energy of the host material, we can ignore the microscopic motion of the particles comprising the host and treat all interactions as if the energetic particle collided with particles which are at rest. In such interactions the energetic particle can only lose energy (upscattering in energy can be ignored). Such “superhermal” particle transport problems arise in a variety of applications such as the slowing down of fission neutrons in a moderator, the transport of energetic charged particles through matter, and the thermalization of energetic particles in gases or plasmas. The simplification of ignoring the motion of the background atoms dramatically changes the mathematical nature of the appropriate form of the transport equation from that we encountered in “thermalization” problems in which the energy of the particles was comparable to the thermal energy of the host medium. In particular, it changes the scattering integral operator from a Fredholm to a Volterra form.²⁴

The neglect of microscopic motion in the host material greatly simplifies the form of the scattering kernel. Indeed, on occasion it even allows for an analytical treatment of the transport process. Furthermore, a new class of approximate collision models can now be introduced which take the form of differential operators in energy (“continuous slowing down” models).

The most dramatic example of superhermal particle transport is provided by the slowing down of very high energy fission neutrons (with initial energies of 10^6 eV $\sim$ 10^7 kT). Because of the importance of this process to fission chain reactor studies, the development of appropriate theories of superhermal particle transport has been most intense in this area. We therefore confine most of the subsequent discussion of this topic to the case of fast neutron transport.

Let us briefly review the behavior of neutron cross sections in the range $1 \text{ eV} \leq E < 10 \text{ MeV}$. In the slowing down range, we can regard the nuclei as essentially free and at rest relative to the incident neutron. The elastic scattering (potential scattering) of neutrons from nuclei depends only weakly on energy and is isotropic in the center of mass system (s -wave scattering) for energies less than several hundred keV. The scattering cross

section for neutron scattering from nuclei of mass number A can then be written as follows:⁶⁴

$$\Sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) = \frac{\Sigma_s(E')}{2\pi(1-\alpha)E'} \delta(\mu_0 - S) \quad \text{if } E \leq E' \leq E/\alpha$$

$$= 0 \quad \text{otherwise}$$

where $\alpha \equiv [(A-1)/(A+1)]^2$, $\mu_0 \equiv \hat{\Omega}' \cdot \hat{\Omega}$, and

$$S \equiv \frac{1}{2} \left[(A+1) \sqrt{\frac{E}{E'}} - (A-1) \sqrt{\frac{E'}{E}} \right]$$

As yet one further alternative representation, it is customary in neutron slowing down studies to introduce a logarithmic energy variable, the neutron *lethargy*, defined by

$$u = \ln \left(\frac{E_0}{E} \right)$$

where E_0 is a reference energy usually chosen as $E_0 = 10$ MeV. Then the elastic scattering kernel in the lethargy variable assumes the form

$$\Sigma_{se}(u' \rightarrow u, \hat{\Omega}' \rightarrow \hat{\Omega}) = \frac{\Sigma_s(u')}{2\pi(1-\alpha)} e^{u'-u} \delta(\mu_0 - S) \quad \text{if } u - \ln \frac{1}{\alpha} \leq u' \leq u$$

We will also find the angle-integrated kernels of use:

$$\Sigma_{se}(E' \rightarrow E) = \frac{\Sigma_s(E')}{(1-\alpha)E'}, \quad E \leq E' \leq E/\alpha$$

$$\Sigma_{se}(u' \rightarrow u) = \frac{\Sigma_s(u')}{(1-\alpha)} e^{u'-u}, \quad u - \ln \frac{1}{\alpha} \leq u' \leq u$$

Let us define the corresponding scattering operators

$$\mathcal{S}_e \circ \equiv \int d\hat{\Omega}' \int_E^{E/\alpha} dE' v' \Sigma_{se}(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \circ$$

and their isotropic counterparts

$$S_e \circ \equiv \int_E^{E/\alpha} dE' v' \Sigma_s(E' \rightarrow E) \circ$$

which will prove useful in our subsequent investigations.

In general, inelastic scattering will also be present and must be considered. In light nuclei the threshold for inelastic scattering is of the order of 1 MeV, whereas for heavy nuclei the threshold may drop as low as 10^4 eV. Although the detailed form of the scattering kernel characterizing inelastic scattering is quite complicated (and is usually available only as a table from nuclear data sets), a very useful model of the kernel makes use of the rather long lifetime of the compound nucleus formed as an intermediate state in an inelastic scattering reaction. This property permits us to assume that the neutron forgets its initial energy and direction of motion during the reaction, suggesting an isotropic scattering kernel of the form

$$\Sigma_{si}(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) = \begin{cases} (4\pi)^{-1} \Sigma_{si}(E') f(E') g(E), & E' > E \\ 0, & E' < E \end{cases} \quad (5.32)$$

where we have also noted that the neutron can only lose energy in such an interaction. It should be noted that although this kernel is separable, it is not a degenerate kernel in the sense of the synthetic kernel used in neutron thermalization theory (cf. Section 5.2.1) because of the condition $E' > E$. Perhaps the most common such model for inelastic scattering is that introduced by Okrent⁶⁵ (which, in turn, is based on the Weisskopf "evaporation model" of the compound nucleus). In this model one takes

$$g(E) = C(E) E e^{-E/T}, \quad [f(E)]^{-1} = \int_0^E dE' g(E')$$

where $C(E)$ is defined such that $C(E) = 1$ for $E > 0.5$ MeV and $C(E) = 15/E$ for $E \leq 0.5$ MeV. One can dream up more sophisticated models that describe neutron energy transfer between discrete energy levels.⁶⁴ In this instance, the transport equation becomes a differential-difference equation in energy.⁶⁶

However in the present discussion we use the general form suggested by Eq. 5.32 augmented with a side condition on $g(E)$ and $f(E)$ that guarantees the preservation of the total cross section

$$[f(E')]^{-1} = \int_0^{E'} dE g(E) \equiv h(E'), \quad \frac{dh}{dE} = g(E)$$

Then we can define the inelastic scattering operator as

$$\mathfrak{S}_i \circ \equiv g(E) \int \frac{d\hat{\Omega}'}{4\pi} \int_E^\infty dE' v' \Sigma_{si}(E') [h(E')]^{-1} \circ \equiv \int \frac{d\hat{\Omega}'}{4\pi} \{ S_i \circ \}$$

We can also use the idea of compound nucleus formation to suggest the analogous form for the fission operator

$$\mathcal{F}_i \circ \equiv \nu \chi(v) \int \frac{d\hat{\Omega}'}{4\pi} \int_0^\infty dE' v' \Sigma_f(E') \circ \equiv \int \frac{d\hat{\Omega}}{4\pi} \{ F \circ \}$$

We are neglecting delayed neutrons by using this form. These can be included in a straightforward manner if necessary, although one must endure a bit of extra algebra.

One of the characteristics of compound nucleus reactions such as inelastic scattering or absorption or fission involves the resonance structure of the cross section energy dependence. The subject of resonance interactions (particularly absorption) is a highly specialized subject whose transport aspects are usually analyzed using collision probability methods (cf. Section 2.1) and rarely are approached by way of direct solution of the transport equation itself. Therefore we usually ignore this aspect of fast neutron cross section behavior.

5.3.1 □ Mathematical Properties of the Fast Neutron Transport Equation

□ We can now write the transport equation describing fast neutrons in operator notation as

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \nabla n + v \Sigma_t n = \mathcal{S}_e n + \mathcal{S}_i n + \mathcal{F} n + s \quad (5.33)$$

Our first task is to establish the mathematical properties of the collision operators $\mathcal{S}_e$, $\mathcal{S}_i$, and $\mathcal{F}$. For reference, we recall that for the case of thermal neutron transport, the scattering operator

$$\mathcal{S} \circ \equiv \int d^3v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) \circ$$

was a completely continuous integral operator (which could be “symmetrized” into a self-adjoint form by suitable variable transformations). A similar analysis of the interaction operators in Eq. 5.33 has been provided by Nicolaenko,⁶⁷ who demonstrates that the elastic scattering operator $\mathcal{S}_e$ has the following properties.

- i It is linear and continuous on the Banach space of continuous functions of energy, $C(E_{th}, E_0)$
- ii It is completely continuous (therefore possessing no continuous spectrum).
- iii It has no eigenvalue spectrum except for the point at infinity.

Actually the empty point spectrum $\sigma_p(S_e)$ might have been anticipated from the theory of integral equations. To demonstrate this, note that the eigenvalue problem $S_e\psi = \lambda\psi$ is of the form

$$\int_E^\infty dE' K(E', E) \psi_\lambda(E') = \lambda \psi_\lambda(E)$$

But this is just a Volterra equation with a bounded kernel, and such integral equations have no nontrivial solutions (i.e., no point eigenvalues). Of course this feature is a consequence of the lack of upscattering, which converts

$$\int_0^\infty dE' K(E', E) \circ \quad \text{Fredholm operator} \quad \text{into} \quad \int_E^\infty dE' K(E', E) \circ \quad \text{Volterra operator}$$

A more physical explanation is as follows. Notice that the existence of eigenvalues, that is, of nontrivial solutions $\psi_\lambda(E)$ to $S_e\psi_\lambda = \lambda\psi_\lambda$ implies physically that the scattering operator S_e is able to “regenerate” or “preserve” the energy spectrum of $\psi_\lambda(E)$. But the absence of upscattering implies that S_e always generates an energy spectrum with a lower average energy (see Figure 5.17). Hence scattering kernels in the fast regime are incapable of maintaining an equilibrium energy spectrum; that is, the corresponding scattering operators have an empty point eigenvalue spectrum.

The inelastic scattering operator S_i has a similar structure and can be shown (i) to be linear and continuous, (ii) to be completely continuous, and (iii) to possess an empty point spectrum except for the point at infinity. The fission operator F is also linear, continuous, and completely continuous. In fact, we can show that F is essentially a projection operator

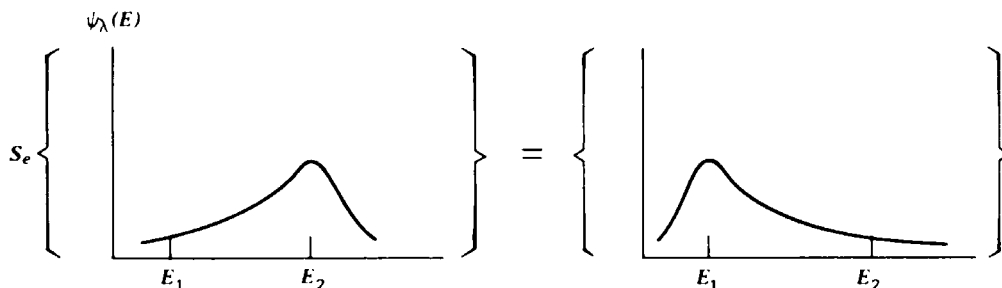


Fig. 5.17 □ Schematic of action of elastic scattering operator on the energy dependence of an eigenfunction.

since

$$F^2 \circ = \nu \chi(E) \int_0^\infty dE' \nu \chi(E') v' \Sigma_f(E') \int_0^\infty dE'' v'' \Sigma_f(E'') \circ \equiv \gamma F \circ$$

But although we can conclude that the residual and continuous spectra of F are empty, it is not obvious that the point spectrum is empty (as we found for the scattering collision operators). In fact, F provides an effective “upscattering” mechanism by way of the fission process that converts low energy neutrons into high energy neutrons (via low energy absorption and the subsequent fission events that yield high energy neutrons). This will “regenerate” the energy spectrum, thereby creating point eigenvalues.

Now we must blend all these operators together into the transport equation (5.33) to study fast neutron transport. In this type of “mixing” of the spectral theory of various operators, there are few general rules (the whole may frequently be greater than the sum of its parts); hence we must consider each case individually as we come to it. We again work in analogy to the procedure followed in studying thermal neutron transport by first studying asymptotic relaxation problems in which we can avoid a detailed treatment of the boundary value problems in energy-dependent transport theory for fast neutrons.

5.3.2 □ Asymptotic Relaxation Processes in Fast Neutron Transport □

To provide a suitable foundation for our further studies, we first consider the very simple problem in which neutrons produced by a time- and space-independent source slow down in an infinite moderating medium characterized by a mass number A . Furthermore, we confine our discussion to the case of elastic scattering that is isotropic in the center of mass system (s -wave scattering). Then the infinite medium “slowing down” equation takes the form (in the lethargy variable):

$$[\Sigma_a(u) + \Sigma_s(u)]\phi(u) = \int_{u-\ln(1/\alpha)}^u du' \Sigma_s(u') \frac{e^{u'-u}}{(1-\alpha)} \phi(u') + S(u) \quad (5.34)$$

One can distinguish between two cases of interest.^{9,10}

i *Proton gas (hydrogen).* $A=1 \Rightarrow \alpha=(A-1)^2/(A+1)^2=0$ so that Eq. 5.34 becomes

$$\Sigma_t(u)\phi(u) = \int_{-\infty}^u du' \Sigma_s(u') e^{u'-u} \phi(u') + S(u)$$

This equation is very easy to solve because it can be converted into a first order differential equation for $\theta(u) \equiv \Sigma_r(u)\phi(u)$

$$\frac{d\theta}{du} + \left[\frac{\Sigma_s(u)}{\Sigma_r(u)} \right] \theta(u) = S(u) + \frac{dS}{du} \quad (5.35)$$

which can be solved for

$$\theta(u) = \exp \left[- \int_{-\infty}^u du' \frac{\Sigma_s(u')}{\Sigma_r(u')} \right] \int_{-\infty}^u du' \left(S(u') + \frac{dS}{du'} \right) \exp \left(\int_{-\infty}^{u'} du'' \frac{\Sigma_s(u'')}{\Sigma_r(u'')} \right)$$

In particular, it should be noted that for large u (or small E), the solution assumes the very simple form (for small absorption)

$$\phi(E) = \phi(u) \left| \frac{du}{dE} \right| \sim \frac{1}{E \Sigma_s(E)} \sim \frac{1}{E}$$

ii *Moderators of mass number $A > 1$.* Now we must solve the more general equation (5.34). This is rather complicated, since the equation analogous to Eq. 5.35 is now a differential-difference equation. For the case of zero absorption, we can apply Laplace transform techniques directly to Eq. 5.34 if we note that it can be written as

$$\theta(u) = \int_0^u du' K(u-u')\theta(u') + S_0\delta(u)$$

where $K(u) = e^{-u}/(1-\alpha)$ for $0 \leq u \leq \ln 1/\alpha$, and $K(u) = 0$ otherwise. But since we have a displacement kernel $K(u'-u)$, this equation is amenable to a Laplace transform in lethargy

$$\tilde{\theta}(s) = \int_0^\infty du e^{-su}\theta(u)$$

The transformed equation can be solved to find

$$\tilde{\theta}(s) = S_0 [1 - \tilde{K}(s)]^{-1}$$

where

$$\tilde{K}(s) = \int_0^\Delta du \frac{e^{-u}e^{-su}}{1-\alpha} = \frac{1 - e^{-\Delta(s+1)}}{(1-\alpha)(s+1)}, \quad \Delta \equiv \ln \frac{1}{\alpha}$$

If we define the zeros of $(1+s)(1-\alpha) - 1 + \exp[-\Delta(s+1)]$ as s_j , we can

invert to find the solution

$$\theta(u) = S_0 \delta(u) + \sum_{j=0}^{\infty} \frac{(1 - e^{-\Delta(s+1)}) e^{s_j u}}{(1 - \alpha) - \Delta e^{-\Delta(s+1)}}$$

Next we consider the more general problem involving time-dependent slowing down in an infinite medium, described by

$$\frac{\partial N}{\partial t} + v \Sigma_t N = S_e N + S_i N + F N + S \quad (5.36)$$

If we Laplace transform in time, this becomes

$$[s + v \Sigma_t(v)] \tilde{N}(v, s) = (S_e + S_i + F) \tilde{N} + \tilde{S} + N(v, 0) \quad (5.37)$$

Again, we consider several special cases.

i *Time-dependent slowing down in a proton gas (hydrogen).* We can safely assume that $\Sigma_s(v) = \text{constant} = \Sigma_s$ in the slowing down range. Furthermore, we take

$$\Sigma_a(v) = \frac{\Sigma_a^0}{v}, \quad S(v, t) = 0, \quad N(v, 0) = N_0 \delta(v - v_0)$$

Then Eq. 5.37 becomes

$$(s + \Sigma_a^0 + v \Sigma_s) \tilde{N} = 2v \Sigma_s \int_v^{\infty} dv' \frac{\tilde{N}(v', s)}{v'} + N_0 \delta(v - v_0) \quad (5.38)$$

We can multiply through by $[s + \Sigma_a^0 + v \Sigma_s]^{-1} v^{-1}$, integrate from v to v_0 , and differentiate with respect to v to find

$$\frac{d\tilde{h}}{dv} = \left(\frac{2\Sigma_s}{s + \Sigma_a^0 + v \Sigma_s} \right) \tilde{h}(v, s), \quad \tilde{h}(v, s) \equiv \int_v^{\infty} dv' \frac{\tilde{N}(v', s)}{v'}$$

But we can integrate this first order differential equation to find

$$\tilde{h}(v, s) = \frac{N_0(s + \Sigma_a^0 + v_0 \Sigma_s)}{v_0(s + \Sigma_a^0 + v \Sigma_s)^2}$$

or finally

$$\tilde{N}(v, s) = \frac{N_0 2(v/v_0) \Sigma_s (s + \Sigma_a^0 + v_0 \Sigma_s)}{(s + \Sigma_a^0 + v \Sigma_s)^3} + \frac{N_0 \delta(v - v_0)}{s + \Sigma_a^0 + v \Sigma_s}$$

Hence we can invert for $v < v_0$ to find

$$N(v, t) = \frac{N_0}{v} (v \Sigma_s t)^2 \left[1 - \frac{v}{v_0} + \frac{2}{(v_0 \Sigma_s t)} \right] e^{-(v \Sigma_s + \Sigma_a^0) t}$$

If we examine the solution for the flux $\phi(v, t) = vN(v, t)$ at speeds far below v_0 ($v/v_0 \ll 1$) and times such that $v_0 \Sigma_s t \gg 1$, we find

$$\phi(v, t) \sim v_0 N_0 (v \Sigma_s t)^2 e^{-v \Sigma_s t} e^{-\Sigma_a^0 t}$$

Notice in particular that this asymptotic behavior is not exponential in time; that is, the slowing down solution never assumes a separable form in v and t for any time. This is explicit evidence of the absence of a point spectrum of S_e . The study of time-dependent slowing down in moderators of mass number $A > 1$ is a bit more complicated, but it has been performed by Marshak.⁶⁴

ii *Time-dependent slowing down in hydrogen in the presence of fission.* If we now include the fission term, we find that Eq. 5.38 becomes

$$\begin{aligned} (s + \Sigma_a^0 + v \Sigma_s) \tilde{N} &= 2v \Sigma_s \int_v^\infty dv' \frac{\tilde{N}(v', s)}{v'} \\ &+ \nu \chi(v) \int_0^\infty dv' v' \Sigma_f(v') \tilde{N}(v', s) + N_0 \delta(v - v_0) \end{aligned}$$

For convenience we assume that $\Sigma_f(v) = \Sigma_f^0/v$, $\Sigma_a(v) = \Sigma_a^0/v$ and take a δ -function fission spectrum $\chi(v) = \delta(v - v_0)$. Then we can solve this equation just as for the previous example to find

$$\phi(v, t) = \phi_{\text{trans}}(v, t) + \frac{\nu \Sigma_f^0 v^2 (\nu \Sigma_f^0 + v_0 \Sigma_s)}{v_0 (\nu \Sigma_f^0 + v \Sigma_s)^3} \exp[-(\Sigma_a^0 - \nu \Sigma_f^0) t]$$

Here we note that $\phi_{\text{trans}}(v, t)$ is nonseparable in v and t as before. However we now find a separable term decaying exponentially in time as $\exp[-(\Sigma_a^0 - \nu \Sigma_f^0) t]$. This term is due to the fission “feedback” or “upscattering” mechanism, which will allow an “equilibrium” energy spectrum—hence an exponential decay. That is, the fission operator F creates a point eigenvalue $\lambda_0 = -(\Sigma_a^0 - \nu \Sigma_f^0)$. Notice also that this exponential term will dominate asymptotically in time, since the slowing down transient term will be decaying in time as $O(\exp[-(\Sigma_a^0 + v \Sigma_s) t])$, hence will damp out much more rapidly than the (v, t) separable term.

The study of spatial relaxation is more complicated, and we defer its discussion until we have developed a more thorough understanding of

energy dependent transport in the fast regime (next section). Suffice it to say that we again expect a general solution of the form

$$N(x, v) \sim N_0(v)e^{-\kappa x} + N_{\text{trans}}(x, v)$$

That is, the solution will contain a space-energy separable term representing the “persistent” mode established by fissions, and a nonseparable transient due to slowing down neutrons (via either elastic or inelastic scattering collisions).

5.3.3 □ Boundary Value Problems in Fast Neutron Transport □ We now turn our attention to a consideration of time-independent fast neutron transport as described by

$$\mu \frac{\partial \varphi}{\partial x} + \Sigma_t(E) \varphi(x, \mu, E) = (\mathcal{S}_e + \mathcal{S}_i + \mathcal{F}) \varphi + s \quad (5.39)$$

subject to various boundary conditions we may place on the flux $\varphi(x, \mu, E)$. We choose to work in one-dimensional plane symmetry for convenience. Recall that our earlier treatment of such energy-dependent transport problems for thermal particles met with little success for general scattering kernels. Although the expressions for the cross sections in the fast regime are a little more tractable (frequently in the form of separable kernels, in fact), the solution of Eq. 5.39 is still beyond reach.

However there is one simplification that we can adopt for fast neutrons, that of constant cross sections $\Sigma(E) = \text{constant}$. Such an assumption, though disastrous in the thermal range, is frequently not too bad in the fast and slowing down range. And, as we will see, such an assumption allows us to reduce the energy-dependent transport equation to an essentially one-speed transport problem that can then be solved by the usual techniques of Chapter 2.

To illustrate, first simplify the transport equation (5.39) by assuming isotropic scattering and measuring x in units of mfp, Σ_t^{-1}

$$\mu \frac{\partial \varphi}{\partial x} + \varphi = \frac{1}{2} \int_{-1}^{+1} d\mu' [S_e + S_i + F] \varphi(x, \mu', E) + s \quad (5.40)$$

Now suppose that we could construct the spectral representation of the operator $J = S_e + S_i + F$, that is, find a complete, orthogonal set of eigenfunctions $\psi_\lambda(E)$ generated by $J\psi_\lambda = \lambda\psi_\lambda$ so that we could expand

$$\varphi(x, \mu, E) = \sum_{\lambda} \varphi_{\lambda}(x, \mu) \psi_{\lambda}(E)$$

(where the summation includes an integration over the continuous spectrum). In a similar fashion we also expand the source term

$$s(x, \mu, E) = \sum_{\lambda} s_{\lambda}(x, \mu) \psi_{\lambda}(E)$$

and substitute these expansions into the transport equation (5.40) to reduce it to a decoupled set of one-speed equations

$$\mu \frac{\partial \varphi_{\lambda}}{\partial x} + \varphi_{\lambda}(x, \mu) = \lambda \frac{c}{2} \int_{-1}^{+1} d\mu' \varphi_{\lambda}(x, \mu') + s_{\lambda}(x, \mu), \quad \lambda \in \sigma(J) \quad (5.41)$$

Hence the assumption of constant cross sections leads to a decoupled set of one-speed problems, which we can then solve using the standard methods. By way of contrast, energy-dependent cross sections $\Sigma_i(E)$ would lead to a coupled set of one-speed problems and eventually to the matrix Riemann-Hilbert or Wiener-Hopf problems. To illustrate this approach, we consider several examples.

Example: Elastic Scattering. The appropriate spectral representation of the elastic scattering operator S_e corresponds to a Laplace transform in the lethargy variable. That is, we rewrite the appropriate form of the transport equation in the lethargy variable as

$$\begin{aligned} \mu \frac{\partial \varphi}{\partial x} + \varphi = c \sum_{n=0}^L \left(\frac{2n+1}{2} \right) P_n(\mu) \int_{-1}^{+1} d\mu' P_n(\mu') \\ \times \int_{u-\Delta}^u du' f_n(u-u') \varphi(x, \mu', u') + s \end{aligned}$$

where we have introduced an expansion of the angular dependence of the scattering kernel in Legendre polynomials. If we now carry out a Laplace transformation with respect to the lethargy variable u , we arrive at

$$\mu \frac{\partial \tilde{\varphi}}{\partial x} + \tilde{\varphi} = c \sum_{n=0}^L \left(\frac{2n+1}{2} \right) \tilde{f}_n(s) P_n(\mu) \int_{-1}^{+1} d\mu' P_n(\mu') \tilde{\varphi}(x, \mu', s) + \tilde{s}$$

But of course this equation is just the one-speed transport equation with anisotropic scattering—except for the complex parameter s . Therefore we can adapt the work of Mika⁶³ to find the appropriate eigenfunction expansion. Following Mika's work, McInerney⁶⁸ has solved several of the standard boundary value problems (including an inversion of the Laplace transform) for hydrogenous media.

Example: Inelastic Scattering. Now the equation of interest is

$$\mu \frac{\partial \varphi}{\partial x} + \varphi = \frac{c}{2} \int_{-1}^{+1} d\mu' g(E) \int_E^\infty dE' [h(E')]^{-1} \varphi(x, \mu', E') + s \quad (5.42)$$

Nicolaenko⁶⁷ has developed an integral transform appropriate for this equation by studying the spectrum of the inelastic scattering operator S_i . To this end, he defines the transform (which is closely related to the Mellin transform)

$$\tilde{\varphi}(x, \mu, \lambda) \equiv \int_0^\infty dE [h(E)]^{\lambda-1} \varphi(x, \mu, E) \equiv \mathfrak{M}[\varphi]$$

The inverse transform is given by

$$\varphi(x, \mu, E) = \frac{g(E)}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} d\lambda [h(E)]^{-\lambda} \tilde{\varphi}(x, \mu, \lambda) \equiv \mathfrak{M}^{-1}[\tilde{\varphi}]$$

We can apply this transform to Eq. 5.42 by multiplying through by $h(E)^{\lambda-1}$ and integrating over E , noting that

$$\int_0^\infty dE g(E) [h(E)]^{\lambda-1} \int_E^\infty dE' [h(E')]^{-1} \varphi(x, \mu, E') = \frac{1}{\lambda} \tilde{\varphi}(x, \mu, \lambda)$$

to find the transformed equation

$$\mu \frac{\partial \tilde{\varphi}}{\partial x} + \tilde{\varphi} = \frac{c}{\lambda 2} \int_{-1}^{+1} d\mu' \tilde{\varphi}(x, \mu', \lambda) + \tilde{s}$$

Hence this transform pair has performed the desired task of reducing the energy-dependent transport equation to the usual one-speed form (with a parameter λ), which can now be managed with the standard techniques. After solving the usual boundary value problems, one can invert the integral transform.

Example: Fast Neutron Transport Including Fission. In the absence of fission, both the elastic and inelastic scattering operators generate only a continuous eigenvalue spectrum, or in transform language, the energy dependence may be transformed out by an appropriate integral transform. For elastic scattering, a Laplace transform in lethargy was applied, whereas for inelastic scattering, a generalized Mellin transform in energy was appropriate. The addition of the fission operator creates a discrete eigenvalue of the combined operator $T = S + F$ at the point $\lambda_0 = c_s + c_f$. Therefore a corresponding discrete eigenfunction must be added to the

appropriate integral transform to obtain the correct eigenfunction expansion in energy (to achieve a complete set of eigenfunctions).

Consider, for example, the interaction of the fission term with elastic scattering by defining

$$T_1 \circ \equiv S_e \circ + F \circ \equiv c_e \int_{-\infty}^u du' g(u-u') \circ + c_f \chi(u) \int_{-\infty}^{\infty} du' \circ$$

and the associated eigenvalue problem

$$T_1 \varphi_\lambda(u) = \lambda \varphi_\lambda(u)$$

Now suppose we Fourier transform in lethargy, using

$$\tilde{\varphi}(k) \equiv \int_{-\infty}^{\infty} du e^{-iku} \varphi(u)$$

to transform the eigenvalue equation

$$c_e \int_{-\infty}^u du' g(u-u') \varphi_\lambda(u') + c_f \chi(u) \int_{-\infty}^{\infty} du' \varphi_\lambda(u') = \lambda \varphi_\lambda(u)$$

into

$$c_e \tilde{g}(k) \tilde{\varphi}_\lambda(k) + c_f \tilde{\chi}(k) \int_{-\infty}^{\infty} du \varphi_\lambda(u) = \lambda \tilde{\varphi}_\lambda \quad (5.43)$$

There are two cases that must be considered separately.

i Suppose

$$\tilde{\varphi}_\lambda(0) = \int_{-\infty}^{\infty} du \varphi_\lambda(u) \neq 0$$

Then we can solve Eq. 5.43 for all k as

$$\tilde{\varphi}_\lambda(k) = \frac{c_f \tilde{\chi}(k) \varphi_\lambda(0)}{\lambda - c_e \tilde{g}(k)}$$

or, in particular, for $k=0$,

$$\tilde{\varphi}_\lambda(0) = \frac{c_f \tilde{\varphi}_\lambda(0)}{\lambda - c_e}$$

which implies that $\lambda_0 = c_e + c_f$. Hence in this case we have a discrete

eigenvalue λ_0 and a corresponding eigenfunction

$$\tilde{\varphi}_0(k) = \frac{c_f \tilde{\chi}(k)}{c_f + c_e [1 - \tilde{g}(k)]}$$

ii Suppose

$$\tilde{\varphi}_\lambda(0) = \int_{-\infty}^{\infty} du \varphi_\lambda(u) = 0$$

Now we find

$$c_e \tilde{g}(k) \tilde{\varphi}_\lambda(k) = \lambda \tilde{\varphi}_\lambda(k)$$

But this is just the slowing down eigenvalue problem, which possesses only a continuous spectrum

$$\lambda = c_e \tilde{g}(k_0), \quad k_0 \neq 0$$

and corresponding eigenfunctions

$$\tilde{\varphi}_\lambda(k) = \delta(k - k_0) \quad [\varphi_\lambda(u) = (2\pi)^{-1} e^{ik_0 u}]$$

Hence we find that Eq. 5.43 has a single point eigenvalue λ_0 characteristic of fission regeneration and a continuous spectrum characteristic of neutron slowing down. Using the properties of Fourier transforms, we can prove that the corresponding eigenfunctions are complete, thus justifying the eigenfunction expansion for a problem with combined elastic scattering slowing down and fission as

$$\phi(u) = a_0 \varphi_0(u) + \frac{1}{2\pi} \int_{-\infty}^{\infty} dk_0 A(k_0) e^{ik_0 u}$$

where the expansion coefficients are given by

$$a_0 = \int_{-\infty}^{\infty} du \phi(u)$$

$$A(k_0) = \int_{-\infty}^{\infty} dk_0 [\phi(u) - a_0 \varphi_0(u)] e^{ik_0 u}$$

A very similar analysis can be performed for the interaction of fission and inelastic scattering.

In conclusion then, by using the assumptions of constant cross sections and isotropic scattering, one can always reduce the energy-dependent

transport equation to equivalent one-speed problems by subtracting out the space-energy separable fission modes, then using the appropriate integral transform ("eigenfunction expansion") on the remaining slowing down equation (Laplace transform for elastic scattering and generalized Mellin transforms for inelastic scattering). The remaining one-speed problems can be solved, and the general solution can be formally reconstructed.⁶⁶ Unfortunately, the inversions of the Laplace or $\mathfrak{M}$ transforms are usually quite difficult, although asymptotic information can frequently be obtained. Anisotropic scattering can also be handled in principle, although only with considerable complications in the necessary manipulations.

We have also noted that discrete energy level models of inelastic scattering can lead to differential-difference equations⁶⁶ that can be solved for certain simple transport problems (e.g., infinite medium, time-dependent slowing down).

It is important that we stress once again the difficulty of solving boundary value problems in energy-dependent transport theory, even when simplified models of collision processes are implemented. The analysis of such problems invariably forces one to adopt either approximate methods (Chapter 7) or numerical methods (Chapter 8) for solving the relevant transport equation.

□ PROBLEMS □

5.1 Determine the time relaxation parameter λ_0 characterizing the decay of the asymptotic mode of a neutron pulse in a sphere of nonmultiplying material. Use a one-speed diffusion theory description. In particular, sketch the behavior of λ_0 as a function of the radius of the sphere.

5.2 Demonstrate that the dispersion function $\Lambda(s)$ characterizing the infinite medium transport equation within the synthetic kernel model (cf. Section 5.1.1) has only a single zero, $-\lambda_0$. Furthermore, verify that for a $1/v$ absorption cross section of the form $\Sigma_a(v) = \Sigma_a^0/v$, one finds that $\lambda_0 = \Sigma_a^0$.

5.3 Sketch the completeness theorem and proof for the time eigenfunctions characterizing the infinite medium transport operator in the synthetic kernel model approximation.

5.4 Repeat the analysis of the pulsed neutron experiment under the asymptotic transport theory approximation using a modified synthetic kernel that includes a component to simulate elastic, coherent scattering (cf. Section 3.1.1). This calculation would describe the decay of the neutron pulse in crystalline materials such as graphite or beryllium.

5.5 Study the spatial eigenvalue problem (5.19) by employing a synthetic kernel model. In particular, identify the point eigenvalue spectrum.

5.6 Consider the neutron wave propagation problem in the one-speed approximation. Demonstrate that for sufficiently large source frequencies ω , there will be no discrete relaxation modes κ_j . Sketch how you might extend this result to the energy-dependent case.

5.7 Verify the small k expansions of the least damped roots of the analytically continued plasma dielectric function $D_{AC}(k, s)$, assuming that the unperturbed distribution function is that characterizing thermal equilibrium.

5.8 Perform the decomposition of the BGK equation into longitudinal and transverse components.

5.9 Determine the neutron flux that is established in an infinite, hydrogenous medium by a monoenergetic, uniform source emitting neutrons at energy E_0 . (Ignore neutron absorption processes.)

5.10 Demonstrate that the asymptotic energy dependence of the flux in an infinite nonabsorbing medium behaves as $\phi(E) \sim 1/\Sigma_s E$.

5.11 One can define the slowing down density $q(\mathbf{r}, E, t)$ as the rate at which particles slow down past the energy E per unit volume. Write down a mathematical expression for this quantity in terms of the flux $\phi(\mathbf{r}, E, t)$ and the scattering kernel $\Sigma_s(E' \rightarrow E)$.

5.12 Show that the neutron continuity equation can be written quite generally in terms of the slowing down density $q(\mathbf{r}, E, t)$ as

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{J} + \Sigma_a(E) \phi(\mathbf{r}, E, t) = \frac{\partial q}{\partial E} + S(\mathbf{r}, E, t)$$

5.13 Develop the infinite medium slowing down equation in hydrogenous moderators using the lethargy variable. Verify that this can be rewritten as a pair of coupled ordinary differential equations:

$$\Sigma_a(u) \phi(u) = - \frac{dq}{du} + S(u)$$

$$\frac{dq}{du} + q(u) = \Sigma_s(u) \phi(u)$$

Solve these equations for the flux $\phi(u)$ resulting from a monoenergetic source emitting neutrons at lethargy $u=0$.

5.14 Solve for the time-dependent flux in an infinite hydrogenous moderator containing fissioning nuclei. Be particularly careful to identify the asymptotic term.

5.15 Determine the eigenfunctions and eigenvalues of the operator $S_i + F$ (use the $\mathfrak{M}$ transform in energy E).

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Nonlinear Transport Processes

Nonlinear effects can become quite important in transport phenomena. Nonlinearities arise in random walk or self-diffusion problems when the transport process significantly perturbs the background medium. Examples include photon energy deposition in radiative transfer processes and the heat produced by neutron-induced nuclear fission reactions. Nonlinearities become significant in collective phenomena when the particle distribution is sufficiently far from equilibrium that the usual linearization approximations no longer apply. We are primarily concerned with the latter situation. In these problems the nonlinearities enter by way of the collision or particle interaction term (e.g., the Boltzmann, Fokker-Planck, or self-consistent field or Vlasov term). Typical problems of interest include the propagation of shock waves in gases and plasmas, thermal energy transport in the presence of very strong temperature gradients, and, of course, turbulence at both the macroscopic fluid level and the microscopic phase space level (in plasmas).

Most of the analytical methods used to analyze boundary value problems in transport theory such as integral transforms or eigenfunction expansions are restricted to linear equations. Furthermore, the fundamental mathematical theory of nonlinear transport equations is in a rather primitive state compared to the theory of linear or linearized transport equations. Therefore it is not surprising that there has been only limited development of methods capable of dealing with nonlinear transport problems.

We discuss three such methods: (i) the method of moments, which attempts to develop a set of nonlinear continuum equations by taking velocity moments of the transport equation, (ii) perturbation or iteration methods, which utilize the integral form of the transport equation, and (iii) direct numerical solutions of the nonlinear transport equation. As in most areas of nonlinear analysis, the success of each approach depends sensitively on the type of problem of interest, and very few general rules apply.

Before discussing these methods, it is useful to comment briefly on the physical significance of nonlinear transport processes. Such nonlinearities arise because of interactions among particles. To illustrate this almost obvious, yet highly nontrivial feature, recall for a moment the general form

of the transport equation

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial n}{\partial \mathbf{v}} = \left(\frac{\partial n}{\partial t} \right)_{\text{coll}}$$

If the range of interparticle forces is short (e.g., neutral gases or liquids), the dominant nonlinearity appears through the collision term $(\partial n / \partial t)_{\text{coll}}$. For the purposes of our immediate discussion, we regard $(\partial n / \partial t)_{\text{coll}}$ as the Boltzmann collision term

$$\left(\frac{\partial n}{\partial t} \right)_{\text{coll}} = J(n, n) = \int d^3 v_1 \int d\hat{\Omega} |\mathbf{v} - \mathbf{v}_1| \sigma(|\mathbf{v} - \mathbf{v}_1|, \theta) (n' n'_1 - n n_1)$$

which exhibits a quadratic nonlinearity. This discussion, however, would apply as well to other collision models such as the nonlinear Fokker-Planck-Landau term.

If the interparticle forces are of long range, then the “self-consistent field” term, $\mathbf{F}/m \cdot (\partial n / \partial \mathbf{v})$, provides the dominant nonlinear interaction. In particular, for an electron plasma in the electrostatic approximation, we recall $\mathbf{F} \rightarrow q\mathbf{E}$, where the electric field is given by Poisson’s equation

$$\frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{E} = 4\pi q \int d^3 v (n - n_0)$$

An important feature of nonlinear transport processes should be noted at this point. Suppose we were to totally ignore all particle interactions. Then the transport equation would look trivially linear

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} = 0 \quad (6.1)$$

but the corresponding hydrodynamics equations would still exhibit an apparently nonlinear structure:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 \\ \rho \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{u} &= -\nabla \cdot \mathbf{P} \\ \rho c_v \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \theta &= -\nabla \cdot \mathbf{q} - \mathbf{P} : \Lambda \end{aligned} \quad (6.2)$$

Where is the contradiction? The apparent nonlinear structure of the hydrodynamics equations (6.2) characterizing inviscid flow arises because

we have chosen the “incorrect” hydrodynamic variables to represent the continuum equations resulting from Eq. 6.1. If we had chosen instead the variables

$$\rho \equiv \int d^3v mn(\mathbf{r}, \mathbf{v}, t), \quad \mathbf{J} \equiv \int d^3v m\mathbf{v}n(\mathbf{r}, \mathbf{v}, t)$$

$$\Pi \equiv \int d^3v m\mathbf{v}\mathbf{v}n(\mathbf{r}, \mathbf{v}, t)$$

$$\mathcal{E} \equiv \int d^3v \frac{1}{2} mv^2 n(\mathbf{r}, \mathbf{v}, t)$$

$$\mathbf{Q} \equiv \int d^3v \mathbf{v} \frac{1}{2} mv^2 n(\mathbf{r}, \mathbf{v}, t)$$

we would have arrived at the linear set of continuum equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0$$

$$\frac{\partial \mathbf{J}}{\partial t} + \nabla \cdot \Pi = 0$$

$$\frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot \mathbf{Q} = 0$$

Thus we are immediately tempted to question the traditional choice of hydrodynamic variables $\rho, \mathbf{u}, \theta$ (which are obviously related to $\rho, \mathbf{J}$, and $\mathcal{E}$ by $\mathbf{J} = \rho \mathbf{u}$ and $\mathcal{E} = 3\rho\theta/2$), since these lead to the nonlinear hydrodynamic equations (6.2). Since both sets of conservation equations are incomplete in the sense that they contain too many unknowns (e.g., $\mathbf{P}$ and $\mathbf{q}$ or Π and $\mathbf{Q}$), it would seem more neutral to work with the linear variables.

The choice of the more traditional hydrodynamic variables $(\rho, \mathbf{u}, \theta)$ is motivated by the recognition that when we can in fact close the set, that is, when the system is close to local thermodynamic equilibrium, the distribution function becomes a time-independent functional of $\rho, \mathbf{u}, \theta$, not $\rho, \mathbf{J}$, and $\mathcal{E}$. And, of course, it is the presence of collisions that forces the phase space density $n(\mathbf{r}, \mathbf{v}, t)$ into the form $n(\mathbf{r}, \mathbf{v} | \rho, \mathbf{u}, \theta)$.

Thus it may make sense to avoid the choice of the traditional hydrodynamic variables for the problems in which the system is very far from local thermodynamic equilibrium (e.g., free molecular flow problems in which we totally ignore collisions). More generally, however, one must face the fact that the nonlinear continuum description is the appropriate macroscopic description. But this is not surprising, since we know that all the

demons hidden in the nonlinear structure of the hydrodynamic equations (e.g., turbulence) correspond to the observed properties of fluids.¹⁻³

6.1 □ THE METHOD OF MOMENTS □ The method of moments⁴⁻⁷ is one of the most popular approaches to analyzing nonlinear problems in kinetic theory. In this scheme one first assumes a functional form for the phase space density $n(\mathbf{r}, \mathbf{v}, t)$ that depends on unknown hydrodynamiclike variables. These variables are defined as velocity space moments of $n(\mathbf{r}, \mathbf{v}, t)$. One then obtains equations for these unknowns by taking velocity moments of the transport equation. In general, the continuum equations resulting from this approach are of a form quite different from the conventional hydrodynamics equations.

To illustrate, let us first develop the Maxwell moment or transfer equations characterizing arbitrary functions of velocity $\psi_i(\mathbf{v})$, by multiplying the transport equation by these functions and integrating over velocity to find

$$\frac{\partial}{\partial t} \int d^3v \psi_i n + \frac{\partial}{\partial \mathbf{r}} \cdot \int d^3v \mathbf{v} \psi_i n + \frac{\mathbf{F}}{m} \cdot \int d^3v \psi_i \frac{\partial n}{\partial \mathbf{v}} = \int d^3v \psi_i J(n, n) \quad (6.3)$$

If we restrict ourselves to transport problems described by the Boltzmann equation (for the moment), the collision term $C[\psi_i]$ can be explicitly written as

$$C[\psi_i] \equiv \int d^3v \psi_i J(n, n) = \int d^3v \int d^3v_1 \int d\hat{\Omega} |\mathbf{v} - \mathbf{v}_1| \sigma n n_1 [\psi_i(\mathbf{v}') - \psi_i(\mathbf{v})]$$

Of course, if the moment functions ψ_i formed a complete set, the corresponding infinite set of moment equations would be formally equivalent to the original transport equation. However in the method we describe, the idea is to first assume a specific form for the particle phase space density $n(\mathbf{r}, \mathbf{v}, t)$ that depends on N of these moments, then use the N corresponding moment equations to generate a set of partial differential equations in $\mathbf{r}$ and t for these quantities.

The choices of the form of the phase space density $n(\mathbf{r}, \mathbf{v}, t)$ and the moment functions $\psi_i(\mathbf{v})$ are quite arbitrary. A variety of choices has been proposed for various problems of interest. In fact, we have already seen one example of this approach in the Grad 13-moment method. Here, the phase space density was chosen to be a Maxwell-Boltzmann distribution multiplied by a set of three-dimensional Hermite polynomials $H_n(\mathbf{v})$

$$n(\mathbf{r}, \mathbf{v}, t) = n_0(\mathbf{v}) \sum_{n=0}^{N-1} \Psi_n(\mathbf{r}, t) H_n(\mathbf{v})$$

In this case one chooses $N=2$ so that the corresponding moments can be identified as the hydrodynamic variables ρ , u_i , T , p_{ij} , and q_i . The corresponding Maxwell moment equations then yield a generalization of the hydrodynamic equations for these variables.

This particular choice of distribution would not be expected to be appropriate for highly nonequilibrium flows in which $n(\mathbf{r}, \mathbf{v}, t)$ is strongly anisotropic. Therefore the most successful applications of moments methods to nonlinear problems assume a form for the distribution that allows discontinuities in velocity space to more nearly approximate the known behavior for free streaming (large Knudsen number, $\text{Kn} = mfp/L \gg 1$). The most famous examples of this approach are the bimodal distribution functions used by Mott-Smith⁸ to describe the propagation of strong shock waves and by Lees⁹ to analyze a variety of highly nonequilibrium flow processes in gas dynamics. We briefly summarize each of these approaches.

6.1.1 □ The Mott-Smith Theory of Strong Shock Wave Propagation □

Perhaps the classic nonlinear problem in kinetic theory involves the propagation of a shock wave.¹⁰⁻¹² When a large disturbance is suddenly introduced into a gas (say by a rapid, local deposition of energy, or by the rupture of a diaphragm maintaining a pressure differential in the gas), this disturbance will propagate into the adjacent gas with the local speed of sound c_s . But since $c_s \sim \rho^{1/2}$, a large disturbance will steepen into a shock wave propagating faster than the speed of sound in the ambient gas ahead of the shock.

From a mathematical point of view, a shock wave can be defined as any abrupt transition that propagates through the gas, causing a change of state, while (at least on the average) stationary in time in its rest frame. Indeed, the Euler equations for an ideal fluid predict that this shock will be a true discontinuity in ρ , $\mathbf{u}$, and θ propagating through the gas. In fact, however, dissipative processes such as viscosity and thermal conduction yield a finite shock thickness.

It is customary to characterize the strength of a shock wave by its Mach number M , defined as the ratio of the propagation speed of the shock to the speed of sound in the ambient gas ahead of the shock. The hydrodynamic (Navier-Stokes) theory of shock waves is limited to Mach numbers of less than $M \sim 1.2$.^{13,14} For stronger shocks, a more sophisticated kinetic theory treatment is required.¹⁵

To be more specific, consider a one-dimensional shock propagating from left to right with a speed D (see Figure 6.1). In the ambient gas ahead of the shock, let us specify the state of the gas by the variables $\rho = \rho_0$, $p = p_0$, and $\mathbf{u} = \mathbf{u}_0 = 0$. We could have chosen to work with the set ρ , θ , and $\mathbf{u}$, but

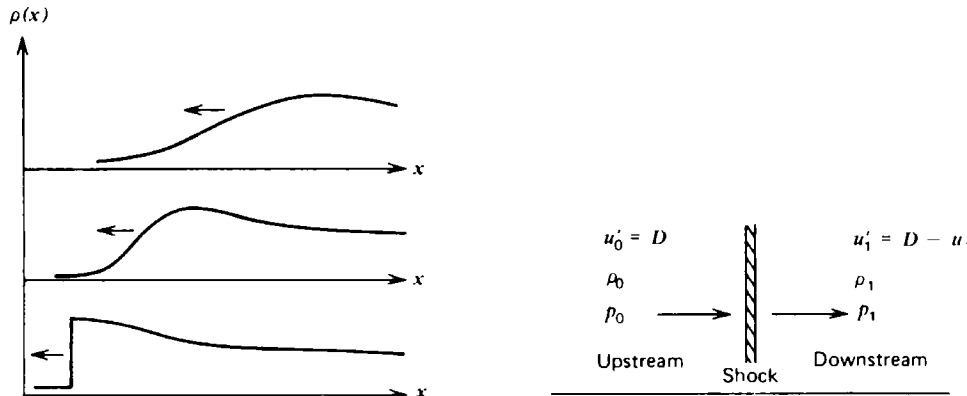


Fig. 6.1 □ Steepening of a density perturbation into a shock wave and the coordinate system moving with the shock.

the use of pressure is somewhat more convenient for this problem. Our goal is the determination of the state of the gas behind the shock as described by the values ρ_1 , p_1 , and u_1 . This analysis is most conveniently accomplished in a coordinate frame moving with the shock (Figure 6.1). In this frame, the gas appears to decelerate from a speed $u'_0 = D$ to a speed $u' = D - u_1$ as it passes through the shock. We refer to these regions as the “upstream” and “downstream” regions of the gas, respectively.

We can determine the downstream variables in terms of the upstream variables without recourse to kinetic theory because only conservation laws are required. To this end, consider the conservation equations for the gas written as

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) &= 0 \\ \frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(p + \rho u^2) &= 0 \\ \frac{\partial}{\partial t}\left(\rho e + \frac{\rho u^2}{2}\right) + \frac{\partial}{\partial x}\left(\rho u\left(e + \frac{u^2}{2} + \frac{p}{\rho}\right)\right) &= 0\end{aligned}$$

where e is the internal energy (i.e., $e = c_p \theta$) for the gas. For a steady state problem, we can ignore time derivatives and integrate the conservation equations across the shock to find the relations

$$\begin{aligned}\text{Mass conservation} & \quad \rho_1 u_1 = \rho_0 u_0 \\ \text{Momentum conservation} & \quad p_1 + \rho_1 u_1^2 = p_0 + \rho_0 u_0^2 \\ \text{Energy conservation} & \quad e_1 + \frac{p_1}{\rho_1} + \frac{u_1^2}{2} = e_0 + \frac{p_0}{\rho_0} + \frac{u_0^2}{2}\end{aligned}\quad (6.4)$$

These equations are known as the *Rankine-Hugoniot relations*^{10,11} for the shock. We have identified the specific enthalpy $h = e + p/\rho$. Note in particular that the equation of state will determine h as a function of ρ and p . Hence we have three equations for six unknowns, ρ_0, u_0, p_0 and ρ_1, u_1, p_1 .

In most shock wave problems one is given the ambient gas density ρ_0 and pressure p_0 . The “strength” of the shock wave is specified in terms of either p_1 or $u_0 - u_1 = D$. We can then use the Rankine-Hugoniot relations to determine the other three variables. That is, the thermodynamic state of the gas on either side of the shock will be completely determined.

By way of example, consider an ideal monatomic gas for which

$$h = c_p \theta = \left(\frac{\gamma}{\gamma - 1} \right) \frac{p}{\rho}$$

We can solve the Rankine-Hugoniot equations for this case to find

$$u_0^2 = \frac{1}{2\rho_0} [(\gamma - 1)p_0 + (\gamma + 1)p_1]$$

$$u_1^2 = \frac{1}{2\rho_0} \left[\frac{[(\gamma + 1)p_0 + (\gamma - 1)p_1]^2}{(\gamma - 1)p_0 + (\gamma + 1)p_1} \right]$$

To determine the spatial variation of $\rho(x)$, $p(x)$, and $u(x)$ across the shock, that is, to determine the shock structure, one must solve the appropriate form of the Boltzmann equation

$$v_x \frac{\partial n}{\partial x} = J(n, n)$$

subject to the boundary conditions that the phase space density approach the appropriate upstream and downstream equilibrium distributions

$$\begin{aligned} \text{i} \quad & n(x \rightarrow \infty, \mathbf{v}) \rightarrow n_0(\mathbf{v}; \rho_1, p_1, u_1) \\ \text{ii} \quad & n(x \rightarrow -\infty, \mathbf{v}) \rightarrow n_0(\mathbf{v}; \rho_0, p_0, u_0) \end{aligned}$$

where

$$n_0(\mathbf{v}; \rho, p, u) \equiv \left(\frac{\rho}{m} \right) \left(\frac{m}{2\pi\theta} \right)^{3/2} \exp \left(- \frac{m|\mathbf{v} - \mathbf{u}|^2}{2\theta} \right)$$

Since a direct solution of the Boltzmann equation is formidable, Mott-Smith⁸ argued that for large Mach numbers the shock is thin and therefore might be adequately modeled as two interpenetrating streams of particles,

with each stream corresponding to either upstream or downstream conditions. That is, he sought $n(x, \mathbf{v})$ as a bimodal distribution

$$n(x, \mathbf{v}) = N_0 f_0(u_0, \theta_0) + N_1 f_0(u_1, \theta_1)$$

where

$$f_0(\mathbf{v}; u, \theta) = \left(\frac{m}{2\pi\theta} \right)^{3/2} \exp \left\{ -\frac{m}{2\theta} [(v_x - u)^2 + v_y^2 + v_z^2] \right\}$$

Here N_0, u_0, T_0 and N_1, u_1, T_1 are unknown functions of position, but they are required to satisfy the boundary conditions such as

$$\begin{aligned} N_0(x \rightarrow -\infty) &= n_0, & N_1(x \rightarrow -\infty) &= 0 \\ N_0(x \rightarrow \infty) &= 0, & N_1(x \rightarrow \infty) &= n_0 \end{aligned}$$

One imposes the normalization condition

$$N_0(x) + N_1(x) = n_0(x)$$

for all x . The conservation equations are used as further constraints on the unknowns

$$\begin{aligned} N_0 u_0 + N_1 u_1 &= n_0 u_0 \\ N_0(\theta_0 + m u_0^2) + N_1(\theta_1 + m u_1^2) &= p_0 + \rho_0 u_0^2 \\ N_0 u_0 \left(\frac{5}{2} \theta_0 + \frac{1}{2} m u_0^2 \right) + N_1 u_1 \left(\frac{5}{2} \theta_1 + \frac{1}{2} m u_1^2 \right) &= \rho_0 u_0 \left(h_0 + \frac{1}{2} u_0^2 \right) \end{aligned} \quad (6.5)$$

One final condition is required to complete the determination of the unknowns. Mott-Smith demanded that the bimodal distribution satisfy the Maxwell moment equation (6.3). The choice of weighting function $\psi_i(\mathbf{v})$ is arbitrary and must be motivated by physical considerations. Mott-Smith examined both the choices of $\psi_i = v_x^2$ and $\psi_i = v_x^3$. For example, using $\psi_i = v_x^2$ for a Maxwell molecule gas along with the assumed form of the distribution function, he found that the equation of transfer which augments the conservation equations becomes

$$\begin{aligned} \frac{d}{dx} \left[N_0 u_0 \left(\frac{3\theta_0}{m} + u_0^2 \right) + N_1 u_1 \left(\frac{3\theta_1}{m} + u_1^2 \right) \right] \\ = -\frac{1}{m\lambda_0} \left(\frac{\pi\theta_0}{2m} \right)^{1/2} \frac{u_0}{u} \left[p_0 + \rho_0 u_0^2 - \rho_0 u_0 u - (N_0 \theta_0 + N_1 \theta_1) \right] \end{aligned}$$

where λ_0 is the upstream mean free path. We can use the conservation equations (6.4) to simplify this to

$$A \frac{k_0}{u_0} \frac{du}{dx} = - \left(1 - \frac{u}{u_0} \right) \left(\frac{u}{u_0} - \frac{u_1}{u_0} \right)$$

where

$$A \equiv \left(\frac{2}{\pi} \right)^{1/2} \frac{u_1}{u_0} \left[\left(1 - 2 \frac{u_1}{u_0} \right) \frac{u_0}{(\theta_0/m)^{1/2}} + \frac{3}{u_0} \left(\frac{\theta_0}{m} \right)^{1/2} \right]$$

Then integrating yields the local velocity $u(x)$ as

$$\frac{u - u_1}{u_0 - u_1} = \left\{ 1 + \exp \left[\left(1 - \frac{u_1}{u_0} \right) \frac{x}{A \lambda_0} \right] \right\}^{-1}$$

This shock structure agrees quite closely with direct numerical solutions of the Boltzmann equation for very strong shocks ($M > 5$). For shocks of intermediate strength, the bimodal approximation loses its validity, and alternative approaches must be used.

We note in passing that a variety of other methods have been utilized to study the kinetic theory of strong shock waves. Of particular note was the classic work of Liepman et al.,¹⁵ who directly solved the integral equations characterizing a shock wave within the BGK collision model (cf. Section 6.2). A number of authors have applied Monte Carlo methods to analyze shock wave propagation.¹⁶

These methods have also been extended to study shock waves in plasmas.¹⁷⁻²⁰ However the analysis becomes considerably more complicated because now one must consider two fluids (electrons and ions) that can interact by both short-range Coulomb collisions and long-range self-consistent fields. The key parameter that determines the nature of the shock is the ratio of the Debye length to the downstream mfp . If $\lambda_D / mfp \ll 1$, the electric fields can be neglected to first order and the plasma can be treated as a single fluid, although with two characteristic temperatures, since the electron-ion equilibrium time may be rather long in high temperature plasmas. Then the appropriate hydrodynamics equations become

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) &= 0 \\ \rho \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} \right) &= - \frac{1}{m} \frac{\partial}{\partial x} [\rho(\theta_i + \theta_e)] + \frac{\partial}{\partial x} [(\mu_i + \mu_e) \frac{\partial u}{\partial x}] \\ \frac{\partial \theta_i}{\partial t} + u \frac{\partial \theta_i}{\partial x} &= - \frac{2}{3} \theta_i \frac{\partial u}{\partial x} + \frac{2}{3} \frac{m_i}{\rho} \mu_i \left(\frac{\partial u}{\partial x} \right)^2 + \frac{2}{3} \frac{m_i}{\rho} \frac{\partial}{\partial x} k_i \frac{\partial \theta_i}{\partial x} + \frac{1}{\tau_{ei}} (\theta_e - \theta_i) \\ \frac{\partial \theta_e}{\partial t} + u \frac{\partial \theta_e}{\partial x} &= - \frac{2}{3} \theta_e \frac{\partial u}{\partial x} + \frac{2}{3} \frac{m_e}{\rho} \mu_e \left(\frac{\partial u}{\partial x} \right)^2 + \frac{2}{3} \frac{m_e}{\rho} \frac{\partial}{\partial x} k_e \frac{\partial \theta_e}{\partial x} + \frac{1}{\tau_{ei}} (\theta_i - \theta_e) \end{aligned}$$

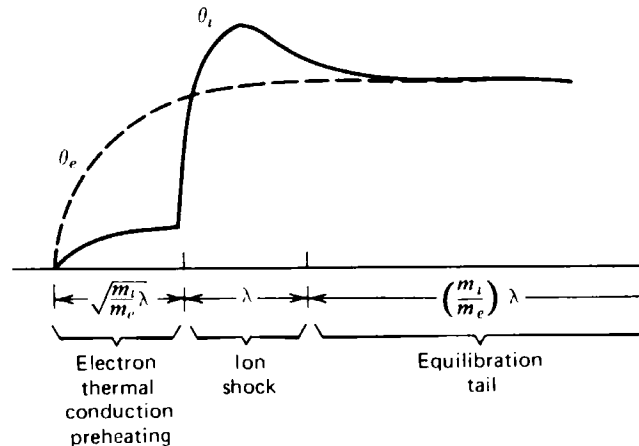


Fig. 6.2 □ The multistructured nature of a plasma shock wave.

One usually assumes that the ions carry the momentum of the shock, $\mu_i(\partial u/\partial x) \gg \mu_e(\partial u/\partial x)$ while the electrons carry thermal energy, $k_e(\partial \theta_e/\partial x) \gg k_i(\partial \theta_i/\partial x)$. These considerations result in a multistructured shock in which electron thermal conduction carries energy ahead of the shock causing a precursor “foot” in the ion temperature (see Figure 6.2).

The existence of the many alternative interaction length scales and the occurrence of shock waves thinner than a collisional *mfp* (due to electric field effects) make it more imperative to use kinetic theory for plasma shock waves than for gas shock waves.²⁰ The analysis of such turbulent shocks is quite involved, since there is no generally accepted transport equation characterizing the distribution of a turbulent plasma. Several modeled kinetic or transport equations have been proposed (e.g., the quasilinear kinetic equation developed in Section 6.3) in which an average of the Vlasov equation over the fluctuating fields introduces a pseudocollision term.²⁰ Many of the usual techniques (e.g., Mott-Smith’s method) can be utilized to analyze these equations.

6.1.2 □ Lees’s Method □ An alternative method of moments has been developed by Lees⁹ and applied with considerable success to a variety of problems in gas dynamics. To illustrate this approach, consider heat flow²¹ between two parallel plates maintained at surface temperatures T_0 and T_L , respectively (see Figure 6.3). The appropriate form of the Boltzmann equation is

$$v_x \frac{\partial n}{\partial x} = J(n, n)$$

Once again we seek a distribution function in a bimodal form

$$n(x, \mathbf{v}) = n_+(x, \mathbf{v}) + n_-(x, \mathbf{v})$$

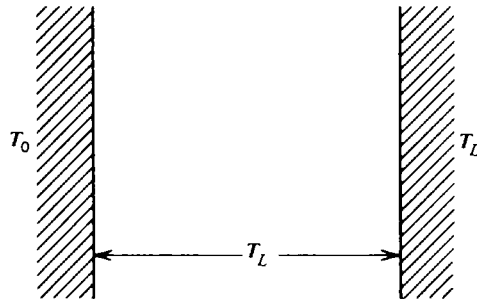


Fig. 6.3 □ Heat flow in a gas between two parallel plates.

except now the $n_{\pm}(x, \mathbf{v})$ are one-sided Maxwell-Boltzmann distributions:

$$n_{\pm}(x, \mathbf{v}) = \frac{2n_{\pm}(x)}{\pi^{3/2}u_{\pm}^3(x)} \exp\left[-\left(\frac{v_x^2 + v_y^2 + v_z^2}{u_{\pm}^2(x)}\right)\right], \quad v_x \gtrless 0$$

$$= 0, \quad v_x \lessgtr 0$$

and represent flows in the positive or negative x -direction. Since there are four unknowns, $n_{\pm}(x)$ and $u_{\pm}(x)$, we need four moment equations. These can be chosen as

$$\frac{d}{dx} mn \overline{v_x} = \rho u_x = 0$$

$$\frac{d}{dx} mn \overline{v_x^2} = \frac{d}{dx} P_{xx} = 0$$

$$\frac{d}{dx} mn \frac{1}{2} \overline{v_x v^2} = \frac{d}{dx} q_x = 0$$

$$\frac{d}{dx} mn \overline{v_x^2 v^2} = mC[v_x v^2]$$

Note here that the first three equations correspond to conservation laws since m , mv_x , and $mv^2/2$ are collisional invariants. In addition, one can apply the boundary condition of zero mass flow

$$\rho \overline{v_x} = m \int d^3v v_x n(x, \mathbf{v}) = 0, \quad x = 0, L$$

and diffuse reflection

$$u_+(0) = \left(\frac{2kT_0}{m}\right)^{1/2}$$

$$u_-(L) = \left(\frac{2kT_L}{m}\right)^{1/2}$$

This set of equations can be solved for both Maxwell molecule and hard sphere potentials.²¹ The Lees's moments method has proved quite successful in describing both time-independent and transient rarefied gas flows.²²

6.1.3 □ Some Final Comments on Moments Methods □ The essential feature of the moments method involves postulating a trial form of distribution function with free parameters, which are determined by weighted integrals of the transport equation. This scheme is very similar to the variational or weighted-residual methods (sometimes known as synthesis methods) described in the next chapter. And like these methods, it suffers from a considerable degree of arbitrariness in the choice of the appropriate moment or weighting functions. There is also usually some ambiguity in specifying boundary conditions appropriate to the moment equations (somewhat reminiscent of the Marshak and Mark prescriptions for choosing boundary conditions for the P_N equations).

Finally we should note that the moment equations take the form of a complicated system of nonlinear partial differential equations. The analysis and solution of these equations (usually by way of numerical methods) is itself a challenging (and usually frustrating) problem.²³

6.2 □ INTEGRAL EQUATION METHODS □ Several of the more popular approaches to nonlinear problems attempt to represent them as a perturbation from either continuum flow or free molecular flow. On the simplest level one can develop a first collision theory that bypasses the transport equation entirely. Rather, one simply considers the change in the distribution function due to first collision encounters between freely streaming particles and particles reflected from boundaries.²⁴ One can develop a collision iteration procedure in this fashion by integrating the integrodifferential form of the transport equation along its characteristics. But this scheme, known as the *Knudsen iteration* method, experiences serious convergence difficulties.

A somewhat more sophisticated approach would be to develop a collision iteration method using the integral form of the transport equation similar to that discussed in Section 2.2 but allowing for the nonlinear collision term. To be more specific, one can integrate the steady-state form of the transport equation to find

$$n = n_0 + F[n]$$

Then one can use this equation as the basis for an iteration scheme

$$n^{(n)} = n_0^{(n-1)} + F[n^{(n-1)}]$$

Willis²⁵ has developed this approach using the free molecular flow solution as the zeroth iterate.

A related approach attempts to linearize the transport equation about the free streaming form of the distribution function. Then classical methods of linear analysis can be applied to solve the resulting equation.²⁶

Unfortunately, more sophisticated studies of the Boltzmann equation based on perturbation expansions in the inverse Knudsen number $\text{Kn} = mfp/L$ have shown that these attempts will invariably encounter difficulties because the zeroth-order solution, free streaming, is singular. That is, all such approaches are in effect encountering a singular perturbation problem in the large Kn limit.²³ One must allow for a nonanalytic behavior in Knudsen number to achieve a successful expansion about the free molecular flow limit.^{27,28}

One can approach this problem from the other extreme by attempting to develop interaction schemes based on continuum flow as a zeroth order solution. An excellent example here is the analysis of shock wave structure by Liepmann, Narashima, and Chahine.¹⁵ These authors integrated the BGK form of the transport equation characterizing a plane shock wave

$$v_x \frac{dn}{dx} = \nu(n_0 - n)$$

subject to the boundary conditions

$$n(-\infty, \mathbf{v}) = n_{10} \equiv n_1 \left(\frac{m}{2\pi\theta_1} \right)^{3/2} \exp \left[-\frac{m(\mathbf{v} - \mathbf{u}_1)^2}{2\theta_1} \right]$$

$$n(+\infty, \mathbf{v}) = n_{20} \equiv n_2 \left(\frac{m}{2\pi\theta_2} \right)^{3/2} \exp \left[-\frac{m(\mathbf{v} - \mathbf{u}_2)^2}{2\theta_2} \right]$$

to obtain equations of the form

$$n(x, v_x \geq 0) = \int_{-\infty}^x dx' \nu_0 n_0(x', \mathbf{v}) v_x^{-1} \exp \left[-\int_{x'}^x dx'' \nu_0 n(x'', \mathbf{v}) v_x^{-1} \right] \quad (6.6)$$

Then by taking the appropriate velocity moments, one can obtain a set of three nonlinear integral equations for the unknown hydrodynamic variables $n(x)$, $u(x)$, and $T(x)$.

An iterative procedure can be used to solve these equations numerically. First substitute the zeroth order estimate $n_0 = n_0^{(0)} = \text{continuum limit}$ into Eq. 6.6 to calculate a first estimate of $n = n^{(1)}$. This can be used to determine $n(x)$, $u(x)$, and $T(x)$, then calculate a new $n_0^{(1)}$, and so on.

Liepmann et al. used the Navier-Stokes solution to provide a first guess of $n^{(0)}$, $u^{(0)}$, and $T^{(0)}$ to begin this iterative process, with excellent results.

6.3 □ QUASILINEAR THEORY OF PLASMA DYNAMICS □ A somewhat different approach that includes nonlinear transport effects to lowest order is utilized in plasma physics to describe the time evolution of a weakly unstable Vlasov plasma.²⁹⁻³¹ To illustrate this approach, we reconsider a simple one-component plasma model as described by the Vlasov equation

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{r}} + \frac{q}{m} \mathbf{E} \cdot \frac{\partial n}{\partial \mathbf{v}} = 0$$

$$\frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{E} = 4\pi q \int d^3v (n - n_0)$$

In our earlier studies of this problem, we linearized the Vlasov equation about a stationary distribution $n_0(\mathbf{v})$

$$n(\mathbf{r}, \mathbf{v}, t) = n_0(\mathbf{v}) + n_1(\mathbf{r}, \mathbf{v}, t)$$

We then demonstrated that the linearized Vlasov equation could be solved using Fourier-Laplace transform techniques to find

$$n_1(\mathbf{k}, \mathbf{v}, t) = \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} ds e^{st} \left\{ \frac{n(k, \mathbf{v}, 0)}{s + i\mathbf{k} \cdot \mathbf{v}} - \frac{\frac{q^2}{m} \frac{\partial n_0}{\partial \mathbf{v}} \cdot \mathbf{k} \frac{4\pi}{k^2} \int du \frac{N_0(u)}{s + i|k|u}}{(s + i\mathbf{k} \cdot \mathbf{v}) D(k, is)} \right\} \quad (6.7)$$

where

$$N_0(u) \equiv \int d^3v n_0(\mathbf{v}) \delta\left(u - \frac{\mathbf{k} \cdot \mathbf{v}}{|\mathbf{k}|}\right)$$

It is usually assumed that the long time behavior of $n_1(\mathbf{k}, \mathbf{v}, t)$ is determined by the zeros of $D(k, is)$ with largest real parts. If we denote these zeros by ω_j ,

$$D(k, \omega_j) = 1 - \frac{\omega_p^2}{k^2} \int du \frac{\partial N_0 / \partial u}{u - \omega_j / |\mathbf{k}|} = 0$$

we find the asymptotic solution for long times as

$$n_1(\mathbf{k}, \mathbf{v}, t) \sim \sum_j \left[\frac{q^2}{m} \frac{\partial n_0}{\partial \mathbf{v}} \cdot \mathbf{k} \right] \frac{4\pi}{k^2} \left[\frac{\partial D}{\partial s} \Big|_{i\omega_j} \right]^{-1} \left[\int du \frac{N_0(u)}{\omega_j - ku} \right] e^{-i\omega_j t} \quad (6.8)$$

Of course we must assume the appropriate analyticity properties of $N_0(u)$ and $n_0(\mathbf{v})$ to allow analytic continuation and contour deformation to pick up the contribution from these poles (see Figure 6.4).

The location of the mode frequencies (their stability or instability) depends on the detailed properties of the zeroth order distribution function. Of course if the plasma is unstable, that is, if modes occur with $s_j = i\omega_j$ in the right half s -plane, our linear theory will no longer be valid. For sufficiently weak instabilities we can extend the theory slightly to account for mildly nonlinear effects. That is, we can study the time evolution of mild instabilities.

To pursue this, let us return for a moment to the nonlinear Vlasov equation. Suppose that at time $t=0$, $n(\mathbf{v}, 0)$ is a stationary solution of the Vlasov equation but is Landau unstable in the sense that several of the poles s_j lie in the right half s -plane. In the linear theory we would find

$$n(\mathbf{r}, \mathbf{v}, t) = n(\mathbf{v}, 0) + \frac{1}{(2\pi)^3} \int d^3k e^{i\mathbf{k} \cdot \mathbf{x}} n_1(\mathbf{k}, \mathbf{v}, t)$$

Suppose we redefine the average phase space density for a spatially uniform plasma in analogy to this even for the more general nonlinear case

$$n_0(\mathbf{v}, t) \equiv \frac{1}{V} \int d^3r n(\mathbf{r}, \mathbf{v}, t) \equiv \langle n(t) \rangle \quad (6.9)$$

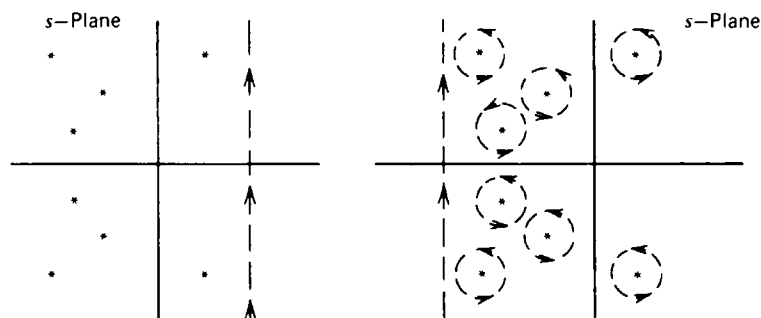


Fig. 6.4 □ Deformation of Laplace inversion contour to pick up contributions from unstable modes of plasma.

In developing a nonlinear theory we will assume that $n_0(\mathbf{v}, t)$ changes slowly with time. That is, the formal definition of Eq. 6.9 of $n_0(\mathbf{v}, t) = \langle n(\mathbf{r}, \mathbf{v}, t) \rangle$ allows a unique separation of the rapidly fluctuating components $n(\mathbf{k}, \mathbf{v}, t) \exp(i\mathbf{k} \cdot \mathbf{r})$ from the slowly varying $n_0(\mathbf{v}, t)$, which takes place as the instability increases the amplitude of the unstable plasma waves.

To implement this formal definition, we proceed as follows by writing

$$\begin{aligned} n(\mathbf{r}, \mathbf{v}, t) &= \langle n \rangle + n_1 = n_0 + n_1 \\ \mathbf{E}(\mathbf{r}, t) &= \langle \mathbf{E} \rangle^0 + \mathbf{E}_1 = \mathbf{E}_1 \end{aligned} \quad (6.10)$$

Next we spatially average the Vlasov equation

$$\frac{\partial}{\partial t} \langle n \rangle + \mathbf{v} \cdot \left\langle \frac{\partial n}{\partial \mathbf{r}} \right\rangle^0 + \frac{q}{m} \frac{\partial}{\partial \mathbf{v}} \cdot [\langle \mathbf{E}_1 \rangle^0 n_0 + \langle \mathbf{E}_1 n_1 \rangle] = 0$$

to find

$$\frac{\partial n_0}{\partial t} = - \frac{q}{m} \frac{\partial}{\partial \mathbf{v}} \cdot \langle \mathbf{E}_1 n_1 \rangle \quad (6.11)$$

Notice here that if the perturbations E_1 and n_1 are regarded as small, then the time rate of change of n_0 is second order in the perturbation.

We now substitute Eq. 6.10 into the Vlasov equation and subtract Eq. 6.11 to find

$$\begin{aligned} \frac{\partial n_1}{\partial t} + \mathbf{v} \cdot \frac{\partial n_1}{\partial \mathbf{r}} + \frac{q}{m} \mathbf{E}_1 \cdot \frac{\partial n_0}{\partial \mathbf{v}} &= - \frac{q}{m} \frac{\partial}{\partial \mathbf{v}} \cdot [\mathbf{E}_1 n_1 - \langle \mathbf{E}_1 n_1 \rangle] \\ \frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{E}_1 &= 4\pi q \int d^3v n_1 \end{aligned} \quad (6.12)$$

Thus far in our analysis we have made no approximations. However we now will assume the following:

- i That the second order term $[\mathbf{E}_1 n_1 - \langle \mathbf{E}_1 n_1 \rangle]$ can be ignored (this is known as the *quasilinear* approximation).
- ii That we can assume $n_1(\mathbf{k}, \mathbf{v}, t)$ varies sufficiently rapidly in time compared to $n_0(t)$ that in solving Eq. 6.12 for $n_1(t)$, we can ignore the time dependence of $n_0(t)$ ("freeze" it) and solve only for the long time behavior of $n_1(t)$ (this is known as the *adiabatic* approximation).

Notice that under these assumptions, Eq. 6.12 becomes just the usual

linearized Vlasov equation

$$\frac{\partial n_1}{\partial t} + \mathbf{v} \cdot \frac{\partial n_1}{\partial \mathbf{r}} + \frac{q}{m} \mathbf{E}_1 \cdot \frac{\partial n_0}{\partial \mathbf{v}} = 0$$

$$\frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{E}_1 = 4\pi q \int d^3v n_1 \quad (6.13)$$

Therefore we can use our earlier solution to this equation in the long time limit to write

$$n_1(\mathbf{k}, \mathbf{v}, t) \sim -\frac{q}{m} \frac{\mathbf{E}(\mathbf{k}, t) \cdot (\partial n_0 / \partial \mathbf{v})}{i(\mathbf{k} \cdot \mathbf{v} - \omega_0)}, \quad \mathbf{E}(\mathbf{k}, t) \equiv E(\mathbf{k}, 0) e^{-i\omega_0 t}$$

where $\omega_0(k)$ is the most unstable mode of $D(k, \omega_0) = 0$,

$$\omega_0(k) = \omega_r(k) + i\gamma_0(k), \quad \gamma_0(k) > 0$$

If we now utilize this to calculate

$$\langle \mathbf{E}_1 n_1 \rangle = \frac{1}{V} \int \frac{d^3k}{(2\pi)^3} \mathbf{E}(-\mathbf{k}, t) n_1(\mathbf{k}, \mathbf{v}, t)$$

we can find that the equation for $n_0(t)$ takes the form

$$\frac{\partial n_0}{\partial t} = \frac{\partial}{\partial \mathbf{v}} \cdot \left(\frac{q}{m} \right)^2 \frac{1}{V} \int \frac{d^3k}{(2\pi)^3} \mathbf{E}(-\mathbf{k}, t) \frac{1}{i(\mathbf{k} \cdot \mathbf{v} - \omega_0)} \mathbf{E}(\mathbf{k}, t) \cdot \frac{\partial}{\partial \mathbf{v}} n_0(t) \quad (6.14)$$

To proceed further, we define the “spectral energy density” of the electrostatic fields as

$$\mathcal{E}_k(t) \equiv \frac{1}{V} \frac{1}{(2\pi)^3} \frac{\mathbf{E}(-\mathbf{k}, t) \cdot \mathbf{E}(\mathbf{k}, t)}{8\pi}$$

Here it should be noted that $\mathcal{E}_k(t)$ evolves in time in a very simple fashion

$$\mathcal{E}_k(t) = \mathcal{E}_k(0) e^{2\gamma_0 t}$$

Therefore the quasilinear approximation results in a diffusion-like equation in velocity space of the form

$$\frac{\partial n_0}{\partial t} = \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{D}(\mathbf{v}, t) \cdot \frac{\partial}{\partial \mathbf{v}} n_0(\mathbf{v}, t) \quad (6.15)$$

where the quasilinear diffusion coefficient is given by

$$D(\mathbf{v}, t) = \left(\frac{q}{m} \right)^2 \int d^3k \frac{\mathbf{k}\mathbf{k}}{|\mathbf{k}|^2} \frac{\mathcal{E}_k(t)}{i(\mathbf{k} \cdot \mathbf{v} - \omega_0)}$$

while the field spectral density is given by

$$\frac{\partial \mathcal{E}_k}{\partial t} = 2\gamma_0(k, t)\mathcal{E}_k(t)$$

The quasilinear kinetic equation has been applied to analyze the time evolution of a variety of weak instabilities in plasma physics.²⁹⁻³¹ It also applies (although in a somewhat different context) to describe the phenomenon of weak plasma turbulence.^{32,33}

Several attempts have been made to generalize quasilinear theory. For example, one could utilize perturbation methods to include the contribution from the term $[\mathbf{E}_1 n_1 - \langle \mathbf{E}_1 n_1 \rangle]$, which gives rise to so-called mode-mode coupling contributions.³⁴ Considerable effort has been directed toward extending this theory to the description of strongly turbulent plasmas in which the wave energy is comparable to the particle kinetic energy. To lowest order, such generalizations yield a damping contribution to the unstable mode frequency $\omega_0(t)$ because of fluctuation effects. This result, referred to as *resonance broadening theory*,^{35,36} has been developed from a variety of different perspectives and is essentially a renormalization approach very similar to that used in statistical mechanics to account for the renormalization of transport coefficients due to nonlinear mode-mode coupling interactions.

□ PROBLEMS □

- 6.1** Integrate the steady-state hydrodynamics equations across a shock wave to obtain the Rankine-Hugoniot relations.
- 6.2** Solve the Rankine-Hugoniot relations to determine the upstream and downstream flow velocities u_0 and u_1 .
- 6.3** Determine the maximum compression one can achieve across a plane shock wave in an ideal gas.
- 6.4** Verify the form of the Maxwell moment equation for $\psi_i = v_x^2$.
- 6.5** Derive the form of the integral equations characterizing the BGK model of a shock wave.
- 6.6** Demonstrate that the quasilinear kinetic equation conserves particle number and momentum but not kinetic energy.

6.7 Demonstrate explicitly that the quasilinear kinetic equation *plus* the equation for the field spectral density $\mathcal{E}_k$ conserve energy.

6.8 How would you expect the structure of the quasilinear kinetic equation to change if the plasma were to become “Landau stable”—that is, all roots of $D(k,s)$ would lie in the left half s -plane?

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Approximate Methods in Transport Theory

The mathematical description of transport processes can become extremely complex. We have noted that the transport equation characterizing such processes is usually far too complicated to allow a direct analytical solution for any but simple, modeled problems (e.g., simplified geometries or scattering kernels). Therefore it is not surprising that transport theory represents a fertile field for application of many of the standard approximation methods used in mathematical physics. Of particular interest are the techniques such as perturbation or variational methods that make use of the solutions to simple problems to estimate features of the solutions to more complex problems. There are also several more specialized techniques such as multigroup methods or degenerate kernel expansions, which can be used to generate approximate solutions to transport problems.

However several complications appear in applying the more familiar versions of perturbation theory or the calculus of variations to transport problems. Foremost among these is the unfortunate fact that the operators that arise in transport equations are not self-adjoint. Furthermore, we have noted that transport operators usually possess a continuous eigenvalue spectrum. These features demand that the more popular methods,^{1,2} which were developed for the treatment of self-adjoint operators characterized by a point eigenvalue spectrum, must be extended considerably. The non-self-adjoint nature of transport problems also frequently destroys one's confidence that the approximation technique will yield meaningful results. This is particularly significant for variational methods. Finally, the techniques considered here are usually restricted to linear transport problems.

7.1 □ PERTURBATION METHODS □ We frequently encounter situations in which a complicated transport problem possesses features that are quite similar to a far simpler problem for which exact solutions can be obtained. That is, the complexity in such problems can be represented mathematically as a small perturbation on the transport equation characterizing a far simpler problem. For these problems we can use familiar methods from perturbation theory to obtain first order estimates of integral quantities such as eigenvalues or reaction rates in terms of the

solution to the unperturbed problem. For example, in nuclear reactor calculations one is frequently obliged to estimate the effects of a small change in the reactor core composition or geometry on the multiplication factor k_{eff} (the criticality eigenvalue). If these changes or perturbations are sufficiently small, it is not necessary to repeat the criticality calculation for the new core configuration; rather, the calculated flux for the unperturbed core can be used to make simple estimates of the change in k_{eff} . Similar problems arise in a variety of other transport phenomena.

Our primary concern is with the application of perturbation theory to the analysis of eigenvalue problems involving the linear (or linearized) transport operator. Such methods can also be applied to inhomogeneous problems involving sources (e.g., to estimate the perturbation in the response of a neutron detector due to the introduction of a small amount of absorption in a subcritical assembly).

Traditional perturbation methods also have been extended considerably to allow the estimation of nonlinear functionals or local properties of the particle density itself. Furthermore, a variety of higher order perturbation theories have been developed and applied. A particularly intense activity involving such generalized perturbation methods has been stimulated by transport problems arising in the field of nuclear reactor analysis.³

7.1.1 □ Application of Perturbation Theory to Eigenvalue Problems □

The basic approach to eigenvalue problems is quite simple. Consider the “unperturbed” eigenvalue problem

$$L\psi_j = \lambda_j\psi_j \quad (7.1)$$

(which, presumably, we have solved for the unperturbed eigenvalues λ_j and eigenfunctions ψ_j). If L is not a self-adjoint operator—and it generally is *not* for transport problems—we must also assume that we can determine the eigenvalues and eigenfunctions of the adjoint operator $L^\dagger$:

$$L^\dagger\psi_j^\dagger = \lambda_j^*\psi_j^\dagger \quad (7.2)$$

Here we will assume that the point spectrum of $L^\dagger$ is merely the complex conjugate of the point spectrum of L , and that we have denoted conjugate pairs of eigenvalues with the same index j . (This is usually the case in transport problems, since as noted in Section 5.1, these operators do not possess a residual spectrum.)

We now consider the eigenvalue problem characterizing an operator L' which is perturbed from L by a “small” amount δL :

$$L'\psi'_j = \lambda'_j\psi'_j \quad (7.3)$$

where

$$L' \equiv L + \delta L, \quad \|\delta L\| \ll \|L\|$$

If we define the corresponding perturbations in the eigenvalues and eigenfunctions by

$$\lambda'_j = \lambda_j + \delta\lambda_j, \quad \psi'_j = \psi_j + \delta\psi_j$$

our goal is to obtain a simple estimate of the perturbation $\delta\lambda_j$ caused by δL . To proceed, take the inner product of the perturbed eigenvalue problem (7.3) with the unperturbed adjoint eigenfunction $\psi_j^\dagger$:

$$(\psi_j^\dagger, (L + \delta L)\psi'_j) = \lambda'_j (\psi_j^\dagger, \psi'_j) \quad (7.4)$$

But note that from the definition of the adjoint operator

$$(\psi_j^\dagger, L\psi'_j) = (L^\dagger\psi_j^\dagger, \psi'_j)$$

Furthermore, if we utilize Eq. 7.2, we find

$$(L^\dagger\psi_j^\dagger, \psi'_j) = (\lambda_j^* \psi_j^\dagger, \psi'_j) = \lambda_j (\psi_j^\dagger, \psi'_j)$$

Thus we can return to Eq. 7.4 to find

$$(\lambda'_j - \lambda_j)(\psi_j^\dagger, \psi'_j) = (\psi_j^\dagger, \delta L\psi'_j)$$

or

$$\delta\lambda_j = \frac{(\psi_j^\dagger, \delta L\psi'_j)}{(\psi_j^\dagger, \psi'_j)} \quad (7.5)$$

Thus far we have made no approximation. Our expression Eq. 7.5 for the perturbation $\delta\lambda_j$ is exact. But it is also very formal, since it involves the perturbed eigenfunction ψ'_j . But if the perturbation δL is small, presumably $\delta\psi_j$ is similarly small, and we can approximate ψ'_j by the unperturbed eigenfunction ψ_j . To be more precise, we can write Eq. 7.5 as follows:

$$\delta\lambda_j = \frac{(\psi_j^\dagger, \delta L\psi_j)}{(\psi_j^\dagger, \psi_j)} + \frac{(\psi_j^\dagger, \delta L\delta\psi_j)}{(\psi_j^\dagger, \psi_j)} - \frac{(\psi_j^\dagger, \delta L\psi_j)(\psi_j^\dagger, \delta\psi_j)}{(\psi_j^\dagger, \psi_j)^2} + \dots$$

If we retain only terms to first order in the perturbation (i.e., *first order*

perturbation theory), we find

$$\delta\lambda_j \cong \frac{(\psi_j^\dagger, \delta L \psi_j)}{(\psi_j^\dagger, \psi_j)}$$

Hence, using only the unperturbed eigenfunction and its adjoint, we can calculate the first order perturbation $\delta\lambda_j$ in the eigenvalue λ_j .

One can develop expressions for the first order perturbation in the eigenfunction $\delta\psi_j$, as well as extensions of the calculation to higher order by employing expansions in the unperturbed eigenfunctions ψ_j .^{1,2} Although these topics are of great importance in quantum mechanics, they find limited application in transport theory because of the complexity of the eigenfunctions (e.g., continuous spectrum and singular eigenfunctions). Although we will discuss higher order methods that utilize variational calculus, we avoid a discussion of higher order applications of the more familiar perturbation methods ("Rayleigh-Schrödinger" perturbation theory).

The original expression (7.5) is occasionally used as the basis for an efficient scheme to calculate the effect of perturbations on integral quantities such as eigenvalues even when a direct solution of the perturbed problem for ψ'_j is available.

7.1.2 □ The Adjoint Transport Equation □ It is immediately apparent that the adjoint operator and its eigenfunctions play a very important role in the perturbation theory of non-self-adjoint operators. Hence our first task is to derive the form of the adjoint to the transport operator:

$$L \equiv \mathbf{v} \cdot \nabla \circ + v \Sigma_t(v) \circ - \int d^3v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) \circ \quad (7.6)$$

Of course, if we are going to consider eigenvalue problems such as

$$L\psi_\lambda = \lambda\psi_\lambda$$

or inhomogeneous problems such as

$$Ln = s$$

we must include boundary conditions. For convenience we choose free surface boundary conditions:

$$n(\mathbf{R}_s, \mathbf{v}) = 0, \quad \hat{\mathbf{e}}_s \cdot \mathbf{v} < 0$$

That is, we define the domain of the transport operator $\mathfrak{D}(L)$ by

$$\mathfrak{D}(L) \equiv \left\{ f(\mathbf{r}, \mathbf{v}) : f \text{ continuous in } \mathbf{r}, \text{ integrable in } \mathbf{v}, \right. \\ \left. f(\mathbf{R}_s, \mathbf{v}) = 0, \hat{\mathbf{e}}_s \cdot \mathbf{v} < 0 \right\}$$

Next, if we are to define the operator adjoint to L by

$$(L^\dagger g, f) = (g, Lf) \quad (7.7)$$

we must define the inner product (g, f) . We choose to define this as follows:

$$(g, f) \equiv \int d^3r \int d^3v g^*(\mathbf{r}, \mathbf{v}) f(\mathbf{r}, \mathbf{v})$$

To construct $L^\dagger$, we proceed to examine each component in the definition of Eq. 7.6. We begin by noting immediately that since $v\Sigma_t(v)$ is real,

$$v\Sigma_t^\dagger \circ = v\Sigma_t \circ$$

Next, if we interchange orders of integration over $\mathbf{v}$ and $\mathbf{v}'$, we find

$$(g, \mathfrak{S}f) = \int d^3r \int d^3v g^*(\mathbf{r}, \mathbf{v}) \int d^3v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) f(\mathbf{r}, \mathbf{v}') \\ = \int d^3r \int d^3v' \int d^3v v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) g^*(\mathbf{r}, \mathbf{v}) f(\mathbf{r}, \mathbf{v}')$$

If we now relabel $\mathbf{v} \rightleftharpoons \mathbf{v}'$, we can identify

$$\mathfrak{S}^\dagger \circ \equiv \int d^3v' v' \Sigma_s(\mathbf{v} \rightarrow \mathbf{v}') \circ$$

Finally, we examine

$$(g, \mathbf{v} \cdot \nabla f) = \int d^3r \int d^3v g^*(\mathbf{r}, \mathbf{v}) \mathbf{v} \cdot \nabla f \\ = \int_S d^2r \int d^3v (\mathbf{v} \cdot \hat{\mathbf{e}}_s) g^*(\mathbf{R}_s, \mathbf{v}) f(\mathbf{R}_s, \mathbf{v}) + \int d^3r \int d^3v (-\mathbf{v} \cdot \nabla g)^* f$$

where we have used Gauss's law. If we note that the free surface boundary condition $f(\mathbf{R}_s, \mathbf{v}) = 0$ for $\hat{\mathbf{e}}_s \cdot \mathbf{v} < 0$ eliminates the surface integral (the "con-junct"²) for inward directions, it is apparent that by demanding that

$g(\mathbf{R}_s, \mathbf{v})$ vanish for $\hat{\mathbf{e}}_s \cdot \mathbf{v} > 0$, we can eliminate this term entirely and identify

$$\mathbf{v} \cdot \nabla^\dagger \circ = -\mathbf{v} \cdot \nabla \circ$$

Hence we have now derived the adjoint transport operator $L^\dagger$ along with adjoint boundary conditions which appear as a restriction on the domain $\mathfrak{D}(L)$:

$$L^\dagger \circ = -\mathbf{v} \cdot \nabla \circ + v \Sigma_t(v) \circ - \int d^3v' v \Sigma_s(\mathbf{v} \rightarrow \mathbf{v}') \circ$$

where

$$\mathfrak{D}(L^\dagger) \equiv \mathfrak{D}^\dagger = \left\{ \begin{array}{l} g(\mathbf{r}, \mathbf{v}) : g \text{ continuous in } \mathbf{r}, \text{ integrable in } \mathbf{v} \\ g(\mathbf{R}_s, \mathbf{v}) = 0, \hat{\mathbf{e}}_s \cdot \mathbf{v} > 0 \end{array} \right\}$$

Since the domain of $L^\dagger$ involves different boundary conditions, it is common to denote functions in this domain with a dagger, that is, $g^\dagger(\mathbf{r}, \mathbf{v})$, and to refer to them as “adjoint” solutions.

As a simple example, suppose we restrict ourselves to one-speed transport theory for which

$$\mathcal{L} \circ \equiv \hat{\Omega} \cdot \nabla \circ + \Sigma_t \circ - c \Sigma_t \int d\hat{\Omega}' f(\hat{\Omega}' \cdot \hat{\Omega}) \circ$$

$$\mathcal{L}^\dagger \circ \equiv -\hat{\Omega} \cdot \nabla \circ + \Sigma_t \circ - c \Sigma_t \int d\hat{\Omega}' f(\hat{\Omega} \cdot \hat{\Omega}') \circ$$

These operators can be augmented by the boundary conditions:

$$\varphi(\mathbf{R}_s, \hat{\Omega}) = 0, \quad \hat{\mathbf{e}}_s \cdot \hat{\Omega} < 0$$

$$\varphi^\dagger(\mathbf{R}_s, \hat{\Omega}) = 0, \quad \hat{\mathbf{e}}_s \cdot \hat{\Omega} > 0$$

Now since $f(\hat{\Omega}' \cdot \hat{\Omega}) = f(\hat{\Omega} \cdot \hat{\Omega}')$, we find that if we consider both the direct and the adjoint problems

$$\mathcal{L}\varphi = s, \quad \mathcal{L}^\dagger\varphi^\dagger = s$$

the adjoint flux $\varphi^\dagger$ is related quite simply to φ by

$$\varphi^\dagger(\mathbf{r}, \hat{\Omega}) = \varphi(\mathbf{r}, -\hat{\Omega})$$

Note in particular that the adjoint angle-integrated flux is identical to the

direct flux

$$\phi^\dagger(\mathbf{r}) = \int d\hat{\Omega} \varphi^\dagger(\mathbf{r}, \hat{\Omega}) = \int d\hat{\Omega} \varphi(\mathbf{r}, -\hat{\Omega}) = \phi(\mathbf{r})$$

But we might have expected this, since we recall that the integral transport equation (in one-speed theory),

$$\phi(\mathbf{r}) = \int d^3r' \frac{e^{-\Sigma_t|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|^2} [c\Sigma_t\phi(\mathbf{r}') + S(\mathbf{r}')]]$$

has a symmetric kernel and therefore is self-adjoint.

In this sense, we find that the streaming operator $\hat{\Omega} \cdot \nabla$ is “almost” self-adjoint. The energy dependence of the transport equation can also be symmetrized in many instances to yield a self-adjoint problem (e.g., gas dynamics, plasma dynamics, and thermal neutron diffusion). In fact, almost the only inherently non-self-adjoint class of transport problems involves the slowing down of superthermal particles, a prime example being the moderation of fast fission neutrons in a nuclear reactor. In these problems, there is an intrinsic lack of symmetry because of the physical nature of the transport process (i.e., particles will only lose energy in collision events), therefore we would expect the non-self-adjoint character of the transport equation to play a very significant role in their mathematical analysis.

In summary then, we have shown that the integrodifferential form of the transport operator L is not only non-self-adjoint (actually “formally non-self-adjoint”), $L^\dagger \neq L$, but, moreover, has corresponding non-self-adjoint boundary conditions such that $\mathcal{D}^\dagger \neq \mathcal{D}$. Although this feature complicates somewhat the application of the standard approximation techniques of mathematical physics (perturbation or variational methods), it does allow for a rather interesting physical interpretation of the adjoint transport equation.^{4,5}

To illustrate this feature, suppose we consider the inhomogeneous (time-independent) transport equation

$$Ln = s, \quad n(\mathbf{R}_s, \mathbf{v}) = 0, \quad \hat{\mathbf{e}}_s \cdot \mathbf{v} < 0 \quad (7.8)$$

and its adjoint

$$L^\dagger n^\dagger = s^\dagger, \quad n^\dagger(\mathbf{R}_s, \mathbf{v}) = 0, \quad \hat{\mathbf{e}}_s \cdot \mathbf{v} > 0 \quad (7.9)$$

where the source term $s^\dagger(\mathbf{r}, \mathbf{v})$ that appears in the adjoint problem is perfectly arbitrary. If we now multiply Eq. 7.8 by $n^\dagger(\mathbf{r}, \mathbf{v})$, Eq. 7.9 by $n(\mathbf{r}, \mathbf{v})$,

integrate over $\mathbf{r}$ and $\mathbf{v}$, and subtract the resulting equations, we find that

$$(n^\dagger, s) = (s^\dagger, n) \quad (7.10)$$

(where we have used the definition Eq. 7.6 of the adjoint operator $L^\dagger$). This relation holds for arbitrary sources $s(\mathbf{r}, \mathbf{v})$ and $s^\dagger(\mathbf{r}, \mathbf{v})$. In particular, it holds for the case in which we choose

$$s(\mathbf{r}, \mathbf{v}) = \delta(\mathbf{r} - \mathbf{r}_0) \delta(\mathbf{v} - \mathbf{v}_0)$$

$$s^\dagger(\mathbf{r}, \mathbf{v}) = v \Sigma_d(\mathbf{r}, \mathbf{v})$$

where $\Sigma_d(\mathbf{r}, \mathbf{v})$ is the cross section characterizing a particle detector. Hence Eq. 7.10 becomes

$$n^\dagger(\mathbf{r}_0, \mathbf{v}_0) = \int d^3r \int d^3v v \Sigma_d(\mathbf{r}, \mathbf{v}) n(\mathbf{r}, \mathbf{v})$$

But the right-hand side of this equation is just the response of the detector to the particle density produced by a unit point source at position $\mathbf{r}_0$ emitting particles with velocity $\mathbf{v}_0$. In this sense, then the adjoint solution $n^\dagger(\mathbf{r}_0, \mathbf{v}_0)$ can be interpreted as a measure of the “importance” of particles emitted at $(\mathbf{r}_0, \mathbf{v}_0)$ in contributing to the detector response. This explains why the adjoint boundary conditions demand that $n^\dagger(\mathbf{r}, \mathbf{v})$ vanish for outward directions on a free surface, since obviously any such source particles could not contribute to the detector response. One occasionally encounters a reference to the adjoint solution $n^\dagger(\mathbf{r}, \mathbf{v})$ as the *particle importance* or *importance function*.^{4,5}

7.1.3 □ Specific Applications of Perturbation Theory to Transport Problems □

Time-Eigenvalue Problems □ We noted in Chapter 5 that the relaxation parameters governing the time decay of the phase space density $n(\mathbf{r}, \mathbf{v}, t)$ are determined by an eigenvalue problem of the form

$$L\psi_\lambda = \left[\mathbf{v} \cdot \nabla + v \Sigma_t(v) - \int d^3v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) \right] \psi_\lambda(\mathbf{v}) = \lambda \psi_\lambda$$

Our first application of perturbation theory is to determine the change in the fundamental eigenvalue due to a small perturbation in the cross

sections governing particle interactions:⁶

$$\begin{aligned}\Sigma'_t(\mathbf{r}, v) &= \Sigma_t(\mathbf{r}, v) + \delta \Sigma_t(\mathbf{r}, v) \\ \Sigma'_s(\mathbf{r}, \mathbf{v}' \rightarrow \mathbf{v}) &= \Sigma_s(\mathbf{r}, \mathbf{v}' \rightarrow \mathbf{v}) + \delta \Sigma_s(\mathbf{r}, \mathbf{v}' \rightarrow \mathbf{v})\end{aligned}$$

If we note that the corresponding perturbation in the transport operator is

$$\delta L \equiv \delta \Sigma_t(\mathbf{r}, v) \circ - \int d^3 v' v' \delta \Sigma_s(\mathbf{r}, \mathbf{v}' \rightarrow \mathbf{v}) \circ$$

we can immediately apply our general first-order perturbation result to find

$$\delta \lambda = \frac{(\psi_\lambda^\dagger, \delta \Sigma_t \psi_\lambda)}{(\psi_\lambda^\dagger, \psi_\lambda)} - \frac{\left(\psi_\lambda^\dagger, \int d^3 v' v' \delta \Sigma_s(\mathbf{r}, \mathbf{v}' \rightarrow \mathbf{v}) \psi_\lambda(\mathbf{v}') \right)}{(\psi_\lambda^\dagger, \psi_\lambda)}$$

As a specific application, consider the time eigenvalue problem characterizing a spherical geometry as described by the one-speed transport operator

$$\mathcal{L} \circ \equiv \hat{\Omega} \cdot \nabla \circ + \Sigma_t \circ - \Sigma_s \int d\hat{\Omega}' f(\hat{\Omega}' \cdot \hat{\Omega}) \circ$$

We recall that for this problem, $\varphi^\dagger(\mathbf{r}, \hat{\Omega}) = \varphi(\mathbf{r}, -\hat{\Omega})$. Now suppose that we first perturb only the absorption cross section

$$\Sigma'_a(\mathbf{r}) = \Sigma_a(\mathbf{r}) + \delta \Sigma_a(\mathbf{r})$$

Then the perturbation in the time eigenvalue is given by

$$\delta \lambda = \frac{\int d^3 r \int d\hat{\Omega} \varphi(\mathbf{r}, -\hat{\Omega}) \delta \Sigma_a(\mathbf{r}) \varphi(\mathbf{r}, \hat{\Omega})}{\int d^3 r \int d\hat{\Omega} \varphi(\mathbf{r}, -\hat{\Omega}) \varphi(\mathbf{r}, \hat{\Omega})}$$

On the surface of the sphere, $\varphi(\mathbf{R}_s, \hat{\Omega}) \varphi(\mathbf{R}_s, -\hat{\Omega}) = 0$ because of the boundary conditions. Hence any absorption introduced near the surface will cause only a small increase in the decay constant λ . However absorption introduced near the center of the sphere will give a relatively large change $\delta \lambda$, since the angular flux is maximum there (see Figure 7.1).

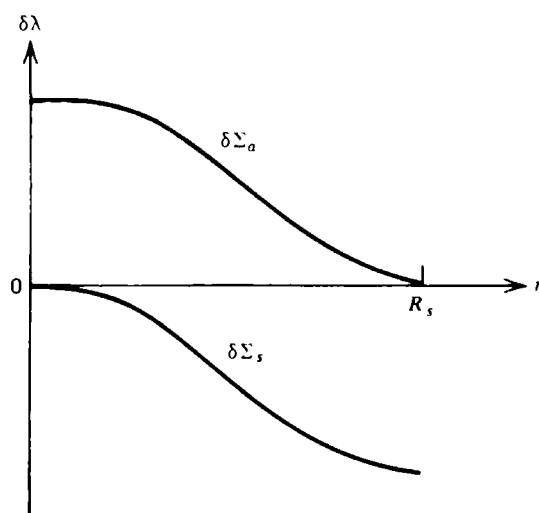


Fig. 7.1 □ Perturbation in time eigenvalue as a function of position of localized perturbation in absorption or scattering cross section.

If we had perturbed the scattering cross section instead, say by adding a small isotropic increment

$$\delta \Sigma_s(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega}) = \frac{\delta \Sigma_s(\mathbf{r})}{4\pi}$$

then

$$\delta \lambda = \frac{\int d^3r \int d\hat{\Omega} \varphi(\mathbf{r}, -\hat{\Omega}) \delta \Sigma_s(\mathbf{r}) \varphi(\mathbf{r}, \hat{\Omega})}{\int d^3r \int d\hat{\Omega} \varphi(\mathbf{r}, -\hat{\Omega}) \varphi(\mathbf{r}, \hat{\Omega})} - \frac{\int d^3r \phi^2(\mathbf{r}) \delta \Sigma_s(\mathbf{r}) / 4\pi}{\int d^3r \int d\hat{\Omega} \varphi(\mathbf{r}, -\hat{\Omega}) \varphi(\mathbf{r}, \hat{\Omega})} \quad (7.11)$$

Now at the center of the sphere, the flux is essentially isotropic, $\varphi(\mathbf{r}, \hat{\Omega}) \sim (4\pi)^{-1} \phi(\mathbf{r})$. From the form of Eq. 7.11 we can see that the two terms will cancel. Hence a change in the scattering cross section at the center of the sphere produces very little change in λ . However near the surface, the first term vanishes (because of boundary conditions), and a net decrease in λ occurs.

Criticality Eigenvalue Problem □ A closely related application of perturbation theory involves the criticality eigenvalue problem characteristic of fission chain reaction systems. Suppose we have determined the critical composition and geometry of a nuclear assembly. Frequently we speculate

about just how the criticality of the system would be affected if we were to make a small change in the assembly—for example, in a control rod position or by a slight modification of the fuel concentration. Of course we could re-solve the criticality problem for this new system. However if the change or perturbation in the new system is small, we can use perturbation theory to determine the desired information concerning the new system (e.g., k_{eff}) directly in terms of the solutions we have already obtained for the original assembly.⁷

Many calculations involved in nuclear reactor analysis can be analyzed merely by studying the effects of perturbations on a known result. For example, to measure the reactivity worth of a control rod material, one can insert it into a critical assembly, then measure the change in reactivity of the perturbed system. Perturbation theory can be used to study the effects of fuel burnup or poison concentration in a critical reactor. Frequently, complicated geometries or cross section behavior (e.g., resonances) can be reexpressed as a perturbation from a much simpler problem. And, in fact, perturbation theory can be used to study the sensitivity of a criticality calculation to uncertainties in cross section data (which always exist) and, on occasion, to adjust such cross section data to yield better agreement with experiment.

The unperturbed criticality eigenvalue problem can be written as

$$\hat{\Omega} \cdot \nabla \varphi + \Sigma_t \varphi - \int d\hat{\Omega}' \int_0^\infty dE' \Sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \varphi = \frac{1}{k} \frac{\chi}{4\pi} \int d\hat{\Omega}' \int dE' \nu \Sigma_f \varphi$$

or in an obvious operator notation

$$M\varphi = \frac{1}{k} F\varphi \quad (7.12)$$

Since M and F are not self-adjoint operators, we must also consider the adjoint unperturbed problem

$$M^\dagger \varphi^\dagger = \frac{1}{k} F^\dagger \varphi^\dagger$$

Here we have noted that the fundamental eigenvalue that is of most interest is real, so that $k^\dagger = k^* = k$. We now consider the effect of perturbations in either the transport or fission operators

$$M' = M + \delta M, \quad F' = F + \delta F$$

on the criticality eigenvalue k . Aside from the minor complication that we now have a generalized eigenvalue problem in the sense that operators

appear on both sides of Eq. 7.12, the derivation of a first order expression for the perturbation in the eigenvalue is quite similar to that used for the more traditional form of an eigenvalue problem, $L\psi = \lambda\psi$. In particular, if we define the *reactivity* ρ of the system by

$$\rho = \frac{k-1}{k}$$

we can easily show that the reactivity change $\Delta\rho = \rho' - \rho$ induced by perturbations δM and δF is given to first order by

$$\Delta\rho = \frac{(\varphi^\dagger, (\delta F - \delta M)\varphi)}{(\varphi^\dagger, F\varphi)}$$

For example, if we imagine perturbing the system absorption and fission cross sections such that

$$\Sigma'_a = \Sigma_a + \delta\Sigma_a, \quad \Sigma'_f = \Sigma_f + \delta\Sigma_f$$

then we find the corresponding reactivity change is given by

$$\Delta\rho = \frac{(\varphi^\dagger, (4\pi)^{-1} \chi \int d\hat{\Omega}' \int dE' \nu \delta\Sigma_f \varphi)}{(\varphi^\dagger, F\varphi)} - \frac{(\varphi^\dagger, \delta\Sigma_a \varphi)}{(\varphi^\dagger, F\varphi)}$$

Once again this result is consistent with physical intuition, since an increase in Σ_a causes a decrease in reactivity, whereas an increase in Σ_f causes a corresponding increase in ρ .

One must be very careful in applying these formulas in practice. The validity of perturbation theory rests on the assumption of *small* perturbations—in a *local* sense. That is, these first order formulas would not be valid for a strongly absorbing control rod, since the resulting perturbation in the flux in the local vicinity of the rod would be quite large.

Further Developments □ Certainly the most extensive application of perturbation methods to transport theory has occurred in the analysis of fission chain reacting systems. Indeed, first order perturbation estimates of integral parameters such as reactor core reactivity are used routinely in reactor analysis and design and are commonly implemented in a variety of the more popular computer codes. Such methods allow for a cheap and rapid estimate of the reactivity effects of small, local perturbations. They can also be used to provide an exact expression for the effect of an

alteration in reactor composition or geometry on reactivity if a direct solution of the perturbed problem is available.

Therefore it is not surprising that the most significant efforts to extend the conventional first order theory have also occurred in this field.³ These extensions have branched out into several directions. There has been considerable effort directed at developing methods for estimating the effect of perturbations on the flux (or adjoint flux). Such methods extend well beyond the familiar first order expansions in the unperturbed eigenfunctions used in quantum mechanics. For example, when the perturbation is localized, a detailed solution for the perturbed flux in the region of interest can be coupled to the global solution to the unperturbed problem.⁸ One can also develop equations directly for the difference between the perturbed and unperturbed solutions $\delta\varphi = \varphi' - \varphi$.⁹

Yet another area of active investigation has involved the development of higher order perturbation theories, so-called generalized perturbation theories, in which the perturbations in the solution are taken into account to yield a second or higher order estimate of integral quantities. Frequently variational methods can be used to develop such second order theories¹⁰ (see Section 7.2.3). Or traditional first order methods can be applied to the alternative integral form of the transport equation, since this equation is already of higher order in perturbations in the cross sections.¹¹ We avoid a discussion of these generalized perturbation theories and refer the interested reader to several comprehensive review articles.^{3,12}

7.2 □ VARIATIONAL METHODS □ As we have seen, the complexity of the transport equation either limits its practical utility to extremely simple situations (one speed, one dimension) or necessitates the use of elaborate numerical schemes to generate a solution. However there is one very powerful and elegant technique of mathematical physics that occasionally can be used to attack realistic problems directly: the calculus of variations. This theory can be applied to transport problems in several ways:¹³⁻¹⁷

- i Variational principles can be used to express in a compact and elegant manner the mathematical content of a given physical problem.
- ii They can be used to estimate “gross aspects” of the solution to a given equation (e.g., an eigenvalue or a weighted average of a solution).
- iii Variational principles can be used to derive simple, approximate equations in a consistent fashion by suitably restricting the class of

trial functions considered. (In fact, this is the most effective manner in which to derive numerical schemes such as the multigroup or discrete ordinate equations.)

Of course the application of variational methods to problems in transport theory requires several modifications of the standard theories. As we have noted, the transport operator is non-self-adjoint. Furthermore, to derive the standard numerical schemes using variational principles, one must consider trial functions that are discontinuous (e.g., step functions in space, angle, or energy). But the extension of the standard variational principles to non-self-adjoint operators and discontinuous trial functions has been accomplished. Before considering these topics, let us quickly review the standard theory of the calculus of variations.

7.2.1 □ A Review of the Calculus of Variations^{2,13} □ What is a *variational principle*? Depending on your point of view, a variational principle can be regarded as either (i) the characterization of a function (usually the solution to some problem of interest) as the stationary point of an appropriate functional, or (ii) a characterization of a number associated with the problem as the stationary value of an appropriate functional. Here we recall that a functional is a mathematical operation that converts a function into a scalar, for example

$$F[q] = \int_a^b dx q(x) \quad \text{and} \quad F[q] = q(a)$$

The collection of functions for which the functional F is defined is referred to as the domain of F , $\mathcal{D}(F)$.

We can perform many of the same operations on functionals that we are accustomed to applying to functions. For example, we define the directional derivative of a function $f(\mathbf{r})$ in a direction specified by a unit vector $\hat{h}$ by

$$(\hat{h} \cdot \nabla) f(\mathbf{r}) = \lim_{\epsilon \rightarrow 0} \frac{f(\mathbf{r} + \epsilon \hat{h}) - f(\mathbf{r})}{\epsilon}$$

In a similar fashion, consider a functional F defined on a domain of functions $\mathcal{D}(F)$. Then if $q(x)$ and $h(x)$ are functions in $\mathcal{D}(F)$, we can define the *weak derivative* of F at the “point” $q(x)$ in “direction” $h(x)$ as

$$\delta F[q, h] = \lim_{\epsilon \rightarrow 0} \frac{F[q + \epsilon h] - F[q]}{\epsilon} \quad (7.13)$$

Notice that this derivative of a functional depends on the function $h(x)$, just as the directional derivative depends on the unit vector $\hat{h}$. Furthermore, note that we can express the weak derivative in terms of an ordinary derivative as

$$\delta F[q, h] = \left. \frac{d}{d\epsilon} F[q + \epsilon h] \right|_{\epsilon=0}$$

We refer to $\delta F[q, h]$ as the *first variation* of F and to h as the *variation* in q .

If at some point $\bar{q}(x)$ the first variation $\delta F[\bar{q}, h]$ is zero for *all* variations $h \in \mathcal{D}$, we say that the functional $F[q]$ is *stationary* at the point $\bar{q}$. In this sense

$$\delta F[\bar{q}, h] = 0 \quad \text{for all } h \in \mathcal{D} \quad (7.14)$$

is the *variational principle characterizing the function* $\bar{q}(x)$. Usually $\bar{q}(x)$ is also given as the solution of some kind of equation

$$f(\bar{q}(x), x) = 0 \quad (7.15)$$

Hence the variational principle (7.14) can be regarded as just an alternative specification of the solution $\bar{q}(x)$ of Eq. 7.15.

But several questions immediately arise.

Question 1. What does $\delta F[\bar{q}, h] = 0$ imply about $F[\bar{q}]$?

In analogy with ordinary derivatives, we might expect $F[\bar{q}]$ to be an *extremum* point of $F[q]$, that is, $F[q]$ would attain a relative maximum or minimum value at $\bar{q}$. But this may not be the case. In fact, $\bar{q}$ usually is an inflection point or saddle point of $F[q]$.

Question 2. Does the variational principle (7.14) imply an equation such as Eq. 7.15 for $\bar{q}(x)$?

The answer to this question is yes. One usually can obtain this equation using integration by parts. Consider as an example the functional

$$F[q] = \int_a^b dx L[q(x), q'(x), x], \quad q'(x) \equiv \frac{dq}{dx}$$

Let us now take the first variation of $F[q, h]$ and set it equal to zero to find the stationary point $\bar{q}(x)$:

$$\delta F[\bar{q}, h] = \int_a^b dx \{ L_{\bar{q}}[\bar{q}, \bar{q}', x] h(x) + L_{\bar{q}'}[\bar{q}, \bar{q}', x] h'(x) \} = 0, \quad L_{\bar{q}} \equiv \frac{\partial L}{\partial \bar{q}}$$

If we integrate by parts, we find

$$\int_a^b dx \left\{ L_{\bar{q}} - \frac{d}{dx} L_{\bar{q}'} \right\} h(x) + h(b) L_{\bar{q}}[\bar{q}(b), \bar{q}'(b), b] - h(a) L_{\bar{q}}[\bar{q}(a), \bar{q}'(a), a] = 0 \quad (7.16)$$

But we must remember that $h(x)$ is an arbitrary function. Hence Eq. 7.16 can be satisfied only if we require

$$\frac{\partial L}{\partial \bar{q}} - \frac{d}{dx} \left(\frac{\partial L}{\partial \bar{q}'} \right) = 0 \quad (7.17)$$

subject to boundary conditions

$$L_{\bar{q}'}[\bar{q}(b), \bar{q}'(b), b] = 0, \quad L_{\bar{q}}[\bar{q}(a), \bar{q}'(a), a] = 0$$

[This makes use of what Courant and Hilbert² refer to as the “fundamental lemma” of the calculus of variations: If $\int_a^b dx \eta(x) \psi(x) = 0$, where $\psi(x) \in C$, for all $\eta(x) \in C^{(2)}$ for which $\eta(a) = \eta(b) = 0$, then $\psi(x) \equiv 0$.] Equation 7.17 is known as the *Euler* or *Euler-Lagrange equation*, and L is sometimes referred to as the “Lagrangian” in analogy to classical mechanics.

The mere fact that a function $\bar{q}(x)$ satisfies the Euler equation does not necessarily mean that $F[q]$ has an extremum value at $\bar{q}(x)$. The Euler equation is only a necessary, not a sufficient condition for $\bar{q}(x)$ to be an extremum point. In fact, it is very difficult in general to obtain necessary and sufficient conditions for a function $\bar{q}(x)$ to be an extremum point of a functional $F[q]$. There is no general theorem to even guarantee the existence of such an extremum function. Hence we will be primarily concerned with necessary conditions for the existence of stationary or extremum points (such as the Euler equations).

One can easily develop generalizations of the Euler equations for various other functionals. For example, if $F[q]$ involves higher order derivatives

$$F[q] = \int_a^b dx L[q, q', q'', \dots, q^{[n]}, x]$$

the corresponding Euler equation takes the form

$$\frac{\partial L}{\partial \bar{q}} - \frac{d}{dx} \left(\frac{\partial L}{\partial \bar{q}'} \right) + \dots + (-1)^n \frac{d^n}{dx^n} \left(\frac{\partial L}{\partial \bar{q}^{[n]}} \right) = 0$$

If the functional depends on several functions,

$$F[q_1, q_2, \dots, q_n] = \int_a^b dx L[q_1, \dots, q_n; q'_1, \dots, q'_n; x]$$

then setting the first variation equal to zero generates a set of Euler equations:

$$\begin{aligned} \frac{\partial L}{\partial \bar{q}_1} - \frac{d}{dx} \left(\frac{\partial L}{\partial \bar{q}'_1} \right) &= 0 \\ \vdots & \\ \frac{\partial L}{\partial \bar{q}_n} - \frac{d}{dx} \left(\frac{\partial L}{\partial \bar{q}'_n} \right) &= 0 \end{aligned}$$

We can also consider higher order variations. For example, a necessary condition for a functional $F[q]$ to be a minimum at $\bar{q}$ is given by “Legendre’s condition”: if $\bar{q}(x)$ makes $F[q]$ a minimum, then

$$\delta^2 F = \frac{\epsilon^2}{2} \frac{d^2}{d\epsilon^2} F[\bar{q} + \epsilon h] \Big|_{\epsilon=0} \geq 0$$

Here, $\delta^2 F$ is referred to as the *second variation* of F .

Question 3. How do we determine the variational principle that corresponds to a given Euler equation?

This is perhaps the least satisfying facet of the calculus of variations. There are usually many variational principles that correspond to the same equation (i.e., have the same Euler equation). Although all these variational principles possess the same stationary point $\bar{q}(x)$ (by definition), some functionals may be more appropriate for the study of $\bar{q}(x)$ than others (e.g., within the context of a given approximation scheme). Hence the choice of a proper variational principle for a given problem is usually a matter of trial and error—plus a dash of black magic.

Before we consider several explicit applications of variational methods in transport theory, let us mention quickly a very useful calculational tool. Recall that we have defined the weak derivative or first variation of a functional with respect to a given variation $h(x)$ by Eq. 7.13. But suppose we were to choose $h(x)$ to be a Dirac δ -function, $h(x) = \delta(x - x')$. Then the corresponding first variation could be identified as a *functional derivative*:

$$\frac{\delta F}{\delta q} \equiv \lim_{\epsilon \rightarrow 0} \frac{F[q + \epsilon \delta] - F[q]}{\epsilon} \quad (7.18)$$

In particular, if our functional is of the form

$$F[q] = \int dx' L[q, x']$$

Table 7.1 □ A Brief Table of the More Useful Functional Derivatives

$F[q]$	$\frac{\delta F}{\delta q}$
$\int dx \Sigma(x)q(x)$	$\Sigma(x)$
$\int dx \Sigma(x)q^n(x)$	$n\Sigma(x)q^{n-1}(x)$
C	0
$q(x_0)$	$\delta(x - x_0)$
$\left. \frac{dq}{dx} \right _{x_0}$	$\delta'(x - x_0)$
$f(x, y)q(x)$	$f(x, y)\delta(x - x')$

the functional derivative yields

$$\frac{\delta F}{\delta q} = \int dx' \left(\frac{\partial L}{\partial q} \right) \delta(x - x') = \frac{\partial L}{\partial q}$$

Table 7.1 lists a few of the more useful functional derivatives.

Some Examples of Variational Principles □

i *Sturm-Liouville equations*. For the important class of self-adjoint second order differential equations, the usual variational principle chosen is

$$F[\varphi] = \int_a^b dx \left\{ p(x) \left(\frac{d\varphi}{dx} \right)^2 + q(x) [\varphi(x)]^2 + 2f(x)\varphi(x) \right\}$$

Then, if we seek the stationary point $\bar{\varphi}(x)$, demanding $h(a) = h(b) = 0$ for convenience, we find that

$$\delta F[\bar{\varphi}, h] = 2 \int_a^b dx \left\{ - \frac{d}{dx} \left(p \frac{d\bar{\varphi}}{dx} \right) + q\bar{\varphi} + f \right\} h(x) = 0$$

implies the Euler equation

$$- \frac{d}{dx} \left[p(x) \frac{d\bar{\varphi}}{dx} \right] + q(x)\bar{\varphi}(x) + f(x) = 0$$

which, of course, is just the usual form of the Sturm-Liouville equation.

ii *Fredholm integral equations with symmetric kernels.* The analogous variational principle for self-adjoint integral equations [i.e., integral equations with symmetric kernels $K(x, x') = K(x', x)$] is

$$F[\varphi] = \int_a^b dx \left\{ [\varphi(x)]^2 - \varphi(x) \int_a^b dx' K(x, x') \varphi(x') - 2f(x)\varphi(x) \right\} \quad (7.19)$$

Then we find that

$$\delta F[\bar{\varphi}, h] = 2 \int_a^b dx \left\{ \bar{\varphi}(x) - \int_a^b dx' K(x, x') \bar{\varphi}(x') - f(x) \right\} h(x) = 0$$

yields the Euler equation

$$\bar{\varphi}(x) = \int_a^b dx' K(x, x') \bar{\varphi}(x') + f(x)$$

iii *Eigenvalue problems.* Consider the general eigenvalue problem

$$L\psi_\lambda = \lambda\psi_\lambda$$

where L is a linear operator. Note that if we take the inner product of this equation with the adjoint eigenfunction $\psi_\lambda^\dagger$ defined by

$$L^\dagger \psi_\lambda^\dagger = \lambda^* \psi_\lambda^\dagger$$

we find

$$(\psi_\lambda^\dagger, L\psi_\lambda) = \lambda(\psi_\lambda^\dagger, \psi_\lambda)$$

This suggests a variational principle for the eigenvalue problem

$$F[\varphi^\dagger, \varphi] = \frac{(\varphi^\dagger, L\varphi)}{(\varphi^\dagger, \varphi)} \quad (7.20)$$

We immediately find that setting the first variation equal to zero, $\delta F[\bar{\varphi}^\dagger, h^\dagger; \bar{\varphi}, h] = 0$, implies the Euler equations

$$L\bar{\varphi} = \lambda\bar{\varphi} \quad \text{and} \quad L^\dagger \bar{\varphi}^\dagger = \lambda^* \bar{\varphi}^\dagger$$

This variational principle, sometimes referred to as the *Ritz principle*, is not

only an elegant formulation of the eigenvalue problem, but it is also of considerable use in estimating the eigenvalues themselves. For notice that if we set $\varphi = \psi_\lambda$, then

$$F[\varphi^\dagger, \psi_\lambda] = \frac{(\varphi^\dagger, L\psi_\lambda)}{(\varphi^\dagger, \psi_\lambda)} = \lambda$$

Hence we find that the stationary value of $F[\varphi^\dagger, \varphi]$ is just the eigenvalue λ . If we choose instead approximate “trial functions”

$$\varphi = \psi_\lambda + \delta\psi_\lambda \quad \varphi^\dagger = \psi_\lambda^\dagger + \delta\psi_\lambda^\dagger$$

we find that the error in the estimate of the eigenvalue λ is just

$$\delta\lambda = \frac{(\delta\psi^\dagger, L\delta\psi) - \lambda(\delta\psi^\dagger, \delta\psi)}{(\varphi^\dagger, \varphi)}$$

That is, a first order error in the trial functions leads to a second order error in the estimate of the eigenvalue λ .

If L is a self-adjoint operator, we can actually determine the sign of the error $\delta\lambda$. For in that case, we can expand the trial function in a complete set of eigenfunctions

$$\varphi(x) = \sum_n a_n \psi_n(x)$$

to find

$$\delta\lambda = \frac{(\varphi, L\varphi)}{(\varphi, \varphi)} = \frac{\sum_n (\lambda_n - \lambda) |a_n|^2}{\sum_n |a_n|^2}$$

Since the λ_n are real, our estimate of the lowest eigenvalue λ_0 will always be such that $\delta\lambda \geq 0$. That is, *any* trial function $\varphi(x)$ will yield an estimate $\lambda \geq \lambda_0$. Similarly for the largest eigenvalue, we find that the variational principle (7.20) yields $\delta\lambda \leq 0$.

We can actually use the variational principle (7.20) to generate all the eigenvalues and eigenfunctions of a self-adjoint operator.

Theorem. The function ψ_1 which minimizes $F[\varphi] = (\varphi, L\varphi)/(\varphi, \varphi)$ is an eigenfunction of the self-adjoint operator L . This minimum value of $F[\varphi]$ is the corresponding eigenvalue λ_1 . If we were to impose the additional

condition that $(\varphi, \psi_1) = 0$, we would find that $\varphi \rightarrow \psi_2$. Hence we can successively construct the eigenfunctions and eigenvalues of L by demanding the auxiliary condition $(\varphi, \psi_j) = 0, j = 1, 2, \dots, n-1$ to determine ψ_n and λ_n .

Proof. See Courant and Hilbert.²

Notice that these remarks hold only for self-adjoint operators. In the more general case of non-self-adjoint operators, the λ_n are no longer real, and we can no longer conclude that the stationary point of $F[\varphi^\dagger, \varphi]$ will be a relative maximum or minimum. (In fact, in the general case it will be a saddle point.) This restricts the usefulness of variational principles to provide bounds on the eigenvalues of non-self-adjoint operators (such as the transport operator, unfortunately). Hence to obtain reliable eigenvalues for non-self-adjoint operators, one must use rather accurate trial functions.

iv *Inhomogeneous problems.* We can always write the equations describing a linear system as an inhomogeneous operator equation

$$H\phi = f$$

(In the homogeneous case, $f=0$, and we can take $H \rightarrow L - \lambda$.) Frequently we are less interested in the solution ϕ to this equation than in some weighted average of ϕ , which we can formally write as an inner product (g, ϕ) . (Here the weighting f might be, e.g., a detector response cross section.) Hence it would be desirable to find a variational principle for this average (g, ϕ) so that we could use crude approximate trial functions to obtain accurate estimates of (g, ϕ) . Such a principle was suggested by Roussopoulos.¹⁸ Consider the adjoint problem with a source term g

$$H^\dagger \phi^\dagger = g$$

Then the *Roussopoulos variational principle* is based on the functional

$$F[\varphi^\dagger, \varphi] = (g, \varphi) + (\varphi^\dagger, f) - (\varphi^\dagger, H\varphi)$$

Notice that if either $\varphi = \phi$ or $\varphi^\dagger = \phi^\dagger$ then

$$F[\phi^\dagger, \phi] = (\phi^\dagger, f) = (g, \phi)$$

We can calculate the total variation as

$$\delta F = -(\delta \phi^\dagger, H\delta \phi)$$

Thus $F[\varphi^\dagger, \varphi]$ has the desired property of variational principles: first order

errors in the trial functions produce only second order errors in the quantity of interest—namely, (g, ϕ) .¹⁹ It is easily verified that the Euler equations corresponding to $F[\varphi^\dagger, \varphi]$ are just

$$H\phi = f \quad \text{and} \quad H^\dagger \phi^\dagger = g$$

The Roussopoulos principle includes many other variational principles as special cases:

(a) If $H = H^\dagger, g = f, \phi^\dagger = \phi$, then

$$F \rightarrow F_1[\varphi] = 2(f, \varphi) - (\varphi, H\varphi)$$

(b) If $H = H^\dagger, H \rightarrow L - \lambda$, then

$$F \rightarrow F_2[\varphi] = \frac{(\varphi, L\varphi)}{(\varphi, \varphi)}$$

(c) If we choose trial functions $\varphi = c\phi$ and $\varphi^\dagger = c^\dagger \phi^\dagger$, we find

$$F[\varphi^\dagger, \varphi] = c(g, \varphi) + c^\dagger(\varphi^\dagger, f) - cc^\dagger(\varphi^\dagger, H\varphi) \quad (7.21)$$

Hence $\delta F = 0$ implies that

$$c = \frac{(\phi^\dagger, f)}{(\phi^\dagger, H\phi)} \quad \text{and} \quad c^\dagger = \frac{(g, \phi)}{(\phi^\dagger, H\phi)}$$

If we substitute these back into the functional Eq. 7.21, we find an alternative principle first proposed by Schwinger²⁰

$$F \rightarrow F_3[\varphi^\dagger, \varphi] = \frac{(\varphi^\dagger, f)(g, \varphi)}{(\varphi^\dagger, H\varphi)}$$

These are just several representative examples of some of the variational principles which have proven useful in transport theory. We discuss later how such principles are applied.

The Rayleigh-Ritz Method □ Thus far we have discussed various “indirect” methods for determining the stationary point of a functional (i.e., by determining the corresponding Euler equation for the functional). There are more direct methods for determining the function $\bar{q}(x)$ that yields a functional $F[q]$ stationary. One such method useful for self-adjoint problems is the *Rayleigh-Ritz* method.² The essential idea is to construct a

“minimizing sequence” of functions $\varphi_1, \varphi_2, \dots, \varphi_n$ such that

$$F[\varphi_n] = d_n \geq d \quad \text{and} \quad \lim_{n \rightarrow \infty} F[\varphi_n] = d$$

In particular, Ritz suggested picking a complete set of functions $\{u_n(x)\}$, then choosing as the minimizing sequence, trial functions of the form

$$\varphi_n = c_1 u_1 + c_2 u_2 + \dots + c_n u_n$$

To determine the c_n 's, we just apply $\delta F = 0$, which yields a system of equations

$$\frac{\partial F}{\partial c_k} = 0, \quad k = 1, 2, \dots, n$$

These will determine the c_n 's, hence the φ_n 's. Then by taking

$$\lim_{n \rightarrow \infty} F[\varphi_n] = F[\bar{\varphi}] = d$$

we can find the stationary value of $F[\varphi]$. (Here one can usually prove that $d_n \rightarrow d$, but not that $\varphi_n \rightarrow \bar{\varphi}$.)

Table 7.2 □ The Common Variational Principles Used in Transport Theory

Functional	Parameter	Euler Equation
$F[\varphi] = \int dx L[\varphi, \varphi', x]$	—	$\frac{\partial L}{\partial \varphi} - \frac{d}{dx} \left(\frac{\partial L}{\partial \varphi'} \right) = 0$
$F[\varphi] = \frac{(\varphi, L\varphi)}{(\varphi, \varphi)}$	λ	$L\psi_\lambda = \lambda\psi_\lambda, L = L^\dagger$
$F[\varphi^\dagger, \varphi] = \frac{(\varphi^\dagger, L\varphi)}{(\varphi^\dagger, \varphi)}$	λ	$L\psi_\lambda = \lambda\psi_\lambda$ $L^\dagger\psi_\lambda^\dagger = \lambda^*\psi_\lambda^\dagger$
$F[\varphi^\dagger, \varphi] = \frac{(\varphi^\dagger, M\varphi)}{(\varphi^\dagger, F\varphi)}$	λ	$M\psi_\lambda = \lambda F\psi_\lambda$ $M^\dagger\psi_\lambda^\dagger = \lambda^* F^\dagger\psi_\lambda^\dagger$
$F[\varphi^\dagger, \varphi] = (g, \varphi) + (\varphi^\dagger, f) - (\varphi^\dagger, H\varphi)$	(g, ϕ)	$H\phi = f$ $H^\dagger\phi^\dagger = g^\dagger$
$F[\varphi] = 2(\varphi, f) - (\varphi, H\varphi)$	(f, ϕ)	$H\phi = f, H = H^\dagger$

A variation of this scheme is to choose a trial function $\varphi(a_1, a_2, \dots, a_n, x)$ dependent on n arbitrary parameters $a_1, \dots, a_n$ (which may themselves be functions). Then substituting this trial function into $F[\varphi]$ and taking the variation with respect to $a_1, \dots, a_n$ yields a set of equations $\partial F / \partial a_k = 0$, $k = 1, \dots, n$ that determines the a_n 's, hence the "best" trial function of the form $\varphi(a_1, \dots, a_n, x)$.

Table 7.2 summarizes the more popular variational principles utilized in transport theory applications.

7.2.2 □ Applications of Variational Principles in Transport Theory □

We now demonstrate with a few relatively simple examples two of the principal ways in which the calculus of variations can be applied to transport theory calculations: (i) using variational principles to estimate "gross aspects" of the solution to the problem of interest, and (ii) using variational principles to derive in a consistent fashion approximations to a problem too difficult to solve by a direct attack.²¹ We make no attempt to explain in detail why a particular functional is chosen to attack a given problem. As we noted earlier, the choosing of an appropriate functional can be a rather ambiguous procedure.

Calculation of Integral Quantities □ Frequently we are interested only in rather gross features of the solution to a given problem. For example, we might be concerned with eigenvalues such as the time or spatial eigenvalues of the transport operator or the criticality eigenvalue characterizing a nuclear system. Or our interest might be with a weighted average of the particle density such as a detector response. The essential scheme is to characterize such quantities (which are just numbers) as the stationary value of an appropriate functional. In doing so, we are able to obtain an expression for these quantities that is remarkably insensitive to any errors made in the solution itself. Indeed, we find that first order errors in the solution result in only second order errors in the value of the functional (which, of course, is the quantity we wish to calculate).

i *Variational estimates of eigenvalues.* Recall that the variational principle (the Ritz principle) for the eigenvalue problem $L\psi_\lambda = \lambda\psi_\lambda$ takes the form

$$F[\varphi^\dagger, \varphi] = \frac{(\varphi^\dagger, L\varphi)}{(\varphi^\dagger, \varphi)} \quad (7.22)$$

That is, the Euler equations for this functional are just

$$L\psi_\lambda = \lambda\psi_\lambda \quad \text{and} \quad L^\dagger\psi_\lambda^\dagger = \lambda^*\psi_\lambda^\dagger$$

But it is of particular interest that for *either* $\varphi^\dagger = \psi_\lambda^\dagger$ or $\varphi = \psi_\lambda$, the functional assumes the stationary value

$$F[\psi_\lambda^\dagger, \varphi] = F[\varphi^\dagger, \psi_\lambda] = \lambda$$

Of course, we do not know these eigenfunctions ψ_λ or $\psi_\lambda^\dagger$, otherwise we could calculate λ directly. Instead, the best we can usually do is to make a guess or estimate of these eigenfunctions, that is, insert so-called trial functions into the functional. Suppose these trial functions φ and $\varphi^\dagger$ are in error by the respective amounts $\delta\psi_\lambda$ and $\delta\psi_\lambda^\dagger$:

$$\varphi = \psi_\lambda + \delta\psi_\lambda \quad \text{and} \quad \varphi^\dagger = \psi_\lambda^\dagger + \delta\psi_\lambda^\dagger$$

Inserting these guesses into our functional, we find that the resultant error in the eigenvalue estimate is

$$\delta\lambda = \frac{(\delta\psi_\lambda^\dagger, L\psi_\lambda) - \lambda(\delta\psi_\lambda^\dagger, \delta\psi_\lambda)}{(\varphi^\dagger, \varphi)}$$

Hence, as advertised, a first order error in the trial functions leads to a second order error in the estimate of the eigenvalue. This remarkable insensitivity of the functional can be used to great advantage in generating rather accurate estimates of the eigenvalues of the problem of interest from quite crude guesses of the eigenfunction and its adjoint.

Example. Suppose we attempt to determine that value of $c \equiv (\nu\Sigma_f + \Sigma_s)/\Sigma_t$ for which a slab of multiplying material of width $2a$ will be critical, as described by one-speed transport theory under the assumption of isotropic scattering.⁶ Then the integral form of the transport equation for this problem is just

$$\phi(x) = \frac{c\Sigma_t}{2} \int_{-a}^a dx' E_1(\Sigma_t|x-x'|)\phi(x') \quad (7.23)$$

We can write this as an eigenvalue problem of the form

$$K\phi = \frac{1}{c}\phi$$

where K is the integral operator $K \circ \equiv (\Sigma_t/2) \int_{-a}^a dx' E_1(\Sigma_t|x-x'|) \circ$. Hence we can directly adapt the Ritz functional Eq. 7.22 to write

$$F[\varphi] = \frac{(\varphi^\dagger, K\varphi)}{(\varphi^\dagger, \varphi)} \quad (7.24)$$

But since the kernel of Eq. 7.23 is symmetric, we can identify K as a self-adjoint operator so that the functional Eq. 7.24 becomes

$$F[\varphi] = \frac{\frac{1}{2} \Sigma_t \int_{-a}^a dx \int_{-a}^a dx' E_1(\Sigma_t|x-x'|) \varphi(x) \varphi(x')}{\int_{-a}^a dx \varphi^2(x)} \rightarrow \frac{1}{c} \quad (7.25)$$

Now by making crude estimates of the critical flux shape [e.g., $\varphi(x)=1$ or $\varphi(x)=\cos \pi x/2a$], we can utilize Eq. 7.25 to make rather accurate estimates for the critical value of c .

ii *Estimate of integral quantities.* Suppose we wish to calculate a weighted integral of the solution such as

$$R \equiv \int d^3r \int d^3v v \Sigma_d(\mathbf{r}, v) n(\mathbf{r}, v)$$

where $\Sigma_d(\mathbf{r}, v)$ might be a detector cross section. Here $n(\mathbf{r}, v)$ is the solution to the transport equation:

$$\mathbf{v} \cdot \nabla n + v \Sigma_t(\mathbf{r}, v) n(\mathbf{r}, v) - \int d^3v' v' \Sigma_s(\mathbf{v}' \rightarrow \mathbf{v}) n(\mathbf{r}, v') = s(\mathbf{r}, v)$$

subject to boundary conditions such as $n(\mathbf{R}_s, v) = 0$, $\hat{\mathbf{e}}_s \cdot \mathbf{v} < 0$. We can rewrite this problem in a more abstract notation by noting that

$$R = (v \Sigma_d, n)$$

where

$$(f, g) \equiv \int d^3r \int d^3v f^*(\mathbf{r}, v) g(\mathbf{r}, v)$$

while n is the solution of the inhomogeneous problem: $Ln = s$, where L is the transport operator. But we have already considered the appropriate variational principle for this problem, just the principle based on the

Roussopoulos functional

$$F[\varphi^\dagger, \varphi] = (v\Sigma_d, \varphi) + (\varphi^\dagger, s) - (\varphi^\dagger, L\varphi)$$

The Euler equations generated by this principle are just

$$Ln = s \quad \text{and} \quad L^\dagger n^\dagger = v\Sigma_d$$

and for either $\varphi = n$ or $\varphi^\dagger = n^\dagger$,

$$F[\varphi^\dagger, n] = F[n^\dagger, \varphi] = (v\Sigma_d, n) = R$$

Hence we need only insert our guessed form of trial function to calculate an estimate of R .

This principle has been used to calculate a variety of quantities of interest in transport theory. The usual trick in such calculations is to manipulate the problem of interest into the form suitable for application of the Roussopoulos principle. We illustrate with perhaps the most famous application of variational methods in transport theory.

Example. The Extrapolated Endpoint for the Milne Problem. In this application, we wish to obtain a stationary functional for the extrapolated endpoint z_0 characterizing the particle density in the neighborhood of a free surface (see Figure 7.2).²² It is most convenient to work with the integral transport equation (in dimensionless form)

$$\phi(x) = \frac{1}{2} \int_0^\infty dx' E_1(|x - x'|) \phi(x'), \quad 0 \leq x < \infty \quad (7.26)$$

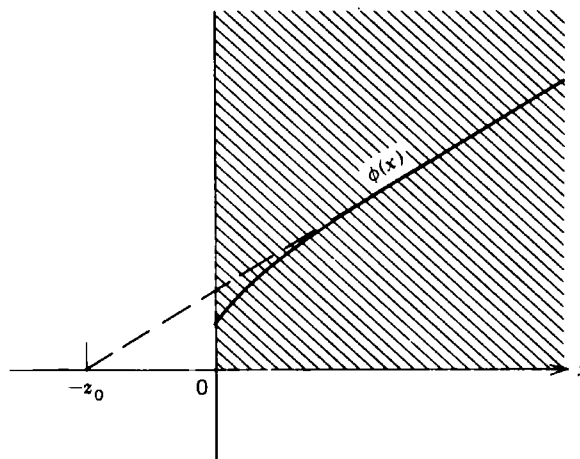


Fig. 7.2 □ Extrapolated endpoint z_0 for the Milne problem.

We confine ourselves to the case of pure scattering, $c = 1$, for convenience. Recall now that we defined the extrapolated endpoint z_0 as that value of $x < 0$ for which the asymptotic flux distribution deep within the medium extrapolated to zero. But how do we obtain a functional with a stationary value z_0 ? This takes a bit of manipulation. First recall that the asymptotic behavior of $\phi(x)$ for $c = 1$ is

$$\phi(x) \sim x \quad \text{as} \quad x \rightarrow \infty$$

Suppose we subtract out this linear behavior by defining a function $\theta(x)$ such that

$$\phi(x) = x + \theta(x) \quad (7.27)$$

Here it is evident that $\theta(x)$ approaches a constant as $x \rightarrow \infty$. In fact, from Figure 7.2 we can identify this limiting value as just the extrapolated endpoint itself:

$$\lim_{x \rightarrow \infty} \theta(x) = z_0$$

We use this fact to derive a functional for $z_0 = \theta(\infty)$. First substitute Eq. 7.27 into the integral equation (7.26) to arrive at a new equation for $\theta(x)$

$$\theta(x) = \frac{1}{2} \int_0^\infty dx' E_1(|x - x'|) \theta(x') + \frac{1}{2} E_3(x) \quad (7.28)$$

Notice that if we take the limit $x \rightarrow \infty$ of this equation, we find

$$\theta(\infty) = \frac{3}{2} \int_0^\infty dx E_3(x) \theta(x) + \frac{3}{8} \quad (7.29)$$

Now we can use these equations to construct a variational principle for $z_0 = \theta(\infty)$. Here we need only recall that our variational principle for a Fredholm equation such as Eq. 7.29 was given by Eq. 7.19. Hence we can use this functional to write

$$J[\varphi] = \frac{\int_0^\infty dx \left\{ [\varphi(x)]^2 - \frac{1}{2} \varphi(x) \int_0^\infty dx' E_1(|x - x'|) \varphi(x') \right\}}{\left[\frac{1}{2} \int_0^\infty dx E_3(x) \varphi(x) \right]^2} \quad (7.30)$$

But if $\varphi = \theta(x)$, then from Eq. 7.28 we find

$$J[\theta] = \left[\frac{1}{2} \int_0^\infty dx E_3(x) \theta(x) \right]^{-1} = \left[\frac{4}{3} \theta(\infty) - 1 \right]^{-1}$$

Therefore we can use Eqs. 7.29 and 7.30 to find the desired variational estimate

$$F[\varphi] = \frac{3}{8} + \frac{3}{4} \frac{\left[\int_0^\infty dx E_3(x) \varphi(x) \right]^2}{\int_0^\infty dx \varphi(x) \left[\varphi(x) - \frac{1}{2} \int_0^\infty dx' E_1(|x-x'|) \varphi(x') \right]} \rightarrow z_0$$

This is a remarkably accurate expression for z_0 . Even the crudest approximate trial function $\varphi(x)=1$ yields an estimate of $z_0 = \frac{3}{8} + \frac{1}{3} = 0.7083$, which should be compared to the exact value of $z_0 = 0.7104\dots$. This scheme was generalized to the energy-dependent Milne problem by Nelkin²³ in 1960 and has been extended to several other boundary value problems by Williams.²⁴

Variational principles can also be applied to estimate the values of nonlinear functionals of the solutions to linear equations²⁵ (e.g., reaction rate ratios) or functionals of the solutions to nonlinear equations²⁶ (e.g., the Boltzmann equation).

iii *Variational derivation of approximate equations.* An alternative application of variational methods in transport theory involves the use of the functional to derive approximate sets of equations—that is, we use the functional as a “Lagrangian” to generate approximate sets of “Euler equations.” In this regard, consider again the Roussopoulos functional

$$F[\varphi^\dagger, \varphi] = (s^\dagger, \varphi) + (\varphi^\dagger, s) - (\varphi^\dagger, L\varphi)$$

with the associated Euler equations

$$L\phi = s \quad \text{and} \quad L^\dagger\phi^\dagger = s^\dagger$$

That is, if the functional F is made stationary with respect to *all* variations in φ and $\varphi^\dagger$, the corresponding Euler equations must yield the exact values of ϕ and $\phi^\dagger$.

Suppose, however, that we do not let φ and $\varphi^\dagger$ vary in an arbitrary fashion, but rather we make F stationary with respect to a *limited* class of variations. Then the resultant Euler equations will be only approximate, and their solution will be only the “best” form of the trial functions for this restricted class. (“Best” here is really a meaningful concept only for self-adjoint problems.)

Example. By way of example, consider the one-speed transport equation (assuming isotropic scattering and sources)

$$\mu \frac{\partial \phi}{\partial x} + \Sigma_t \phi(x, \mu) - \frac{c \Sigma_t}{2} \int_{-1}^{+1} d\mu' \phi(x, \mu') = \frac{1}{2} S(x)$$

and its adjoint

$$-\mu \frac{\partial \phi^\dagger}{\partial x} + \Sigma_t \phi^\dagger(x, \mu) - \frac{c \Sigma_t}{2} \int_{-1}^{+1} d\mu' \phi^\dagger(x, \mu') = \frac{1}{2} S^\dagger(x)$$

The corresponding Roussopoulos functional for this problem is

$$F[\varphi^\dagger, \varphi] = \int dx \int_{-1}^{+1} d\mu \left[\frac{1}{2} \varphi^\dagger S + \frac{1}{2} S^\dagger \varphi - \varphi^\dagger \mu \frac{\partial \varphi}{\partial x} - \varphi^\dagger \Sigma_t \varphi + \varphi^\dagger \frac{c \Sigma_t}{2} \int_{-1}^{+1} d\mu' \varphi(x, \mu') \right] \quad (7.31)$$

Now suppose we compute the variation of F with respect to the restricted class of all functions that have linear anisotropy only:

$$\varphi(x, \mu) = \frac{1}{2} \phi_0(x) + \frac{3}{2} \mu \phi_1(x), \quad \varphi^\dagger(x, \mu) = \frac{1}{2} \phi_0^\dagger(x) + \frac{3}{2} \mu \phi_1^\dagger(x)$$

where $\phi_0(x)$, $\phi_0^\dagger(x)$, $\phi_1(x)$, and $\phi_1^\dagger(x)$ are arbitrary functions of x . Then if we substitute these trial functions into Eq. 7.31 and integrate over angle, we find an approximate or “reduced” functional

$$\begin{aligned} F[\varphi^\dagger, \varphi] &\rightarrow F_R[\phi_0^\dagger, \phi_1^\dagger; \phi_0, \phi_1] \\ &= \frac{1}{2} \int dx \left[\phi_0^\dagger S + S^\dagger \phi_0 - 3c \Sigma_t \phi_1^\dagger \phi_1 - (1-c) \Sigma_t \phi_0^\dagger \phi_0 \right. \\ &\quad \left. - \phi_1^\dagger \frac{d\phi_0}{dx} - \phi_0^\dagger \frac{d\phi_1}{dx} \right] \end{aligned}$$

If we calculate $\delta F_R = 0$, we find the corresponding approximate Euler equations

$$\begin{aligned} \frac{d\phi_1}{dx} + (1-c) \Sigma_t \phi_0 &= S \\ \frac{d\phi_0}{dx} + 3 \Sigma_t \phi_1 &= 0 \end{aligned}$$

and

$$-\frac{d\phi_1^\dagger}{dx} + (1-c)\Sigma_t\phi_0^\dagger = S^\dagger$$

$$-\frac{d\phi_0^\dagger}{dx} + 3\Sigma_t\phi_1^\dagger = 0$$

But if we identify $\phi_0(x) = \phi(x)$ and $\phi_1(x) = J(x)$, then we find that these equations are just the P_1 equations and their adjoint. Hence the variational principle has implied that the “best” approximation to the solution of the transport equation subject to the limitation of only a linear dependence on angle is just the solution of the P_1 equations. In this sense then, we have utilized a variational principle to generate a systematic approximation to the transport equation.^{21,27} Such a procedure has been utilized to approximate energy,²⁸⁻³⁰ space,^{31,32} and time,³³ as well as the angle dependence of the solution. The application of a variational principle as an approximate Lagrangian can also be used to derive the boundary conditions most appropriate for a given approximation to the transport equation.

7.2.3 □ Some Additional Topics □

Error Estimates □ For self-adjoint variational principles, we can easily estimate both the magnitude and sign of the error in a variational estimate. For example, consider the Roussopoulos principle for a self-adjoint inhomogeneous problem $L\phi = s$. The appropriate functional is then

$$F[\varphi] = 2(\varphi, s) - (\varphi, L\varphi)$$

If we calculate the first variation, we find

$$\delta F[\varphi, \delta\varphi] = 2(\delta\varphi, s - L\varphi)$$

We can continue on in this fashion to calculate the second variation as

$$\delta^2 F = -\frac{1}{2}(\delta\varphi, L\delta\varphi)$$

But notice that this implies that if L is a positive definite operator, then $\delta^2 F \leq 0$. But this implies that the stationary value of the functional will be a minimum

$$F[\varphi] \geq F[\phi]$$

For non-self-adjoint problems we must utilize the functional

$$F[\varphi^\dagger, \varphi] = (s^\dagger, \varphi) + (\varphi^\dagger, s) - (\varphi^\dagger, L\varphi)$$

Then we find that

$$\delta^2 F = -\frac{1}{2}(\delta\varphi^\dagger, L\delta\varphi) \stackrel{?}{\geq} 0$$

and it is evident that even for a positive definite operator L , one cannot characterize the second variation by a fixed sign, since it depends on *both* $\delta\varphi$ and $\delta\varphi^\dagger$. Hence the stationary point is not necessarily an extremum.

Therefore a non-self-adjoint variational principle will not necessarily select out of a given subset of trial functions the “best” solution—at least in the sense of minimizing the error in the estimate of the value of the functional. Indeed, this feature has inhibited a wider application of variational methods to the non-self-adjoint problems commonly encountered in transport theory. It can lead to anomalous failures of variationally derived approximate methods. Such failures are compounded by the absence of adequate error estimates. These difficulties are particularly annoying when they arise in numerical (computer based) attempts to solve the transport equation.³⁴

It should be noted, however, that we can always convert a non-self-adjoint problem into an equivalent self-adjoint problem, but this will be accompanied by a rather stiff price. To illustrate, consider

$$L\phi = s \quad \text{and} \quad L^\dagger\phi^\dagger = s^\dagger \quad (7.32)$$

We now define “symmetric” and “antisymmetric” combinations of these operators and the corresponding solutions:

$$\begin{aligned} L_s &= \frac{1}{2}(L + L^\dagger), & L_a &= \frac{1}{2}(L - L^\dagger), & s_s &= \frac{1}{2}(s + s^\dagger), \\ s_a &= \frac{1}{2}(s - s^\dagger), & \phi_s &= \frac{1}{2}(\phi + \phi^\dagger), & \phi_a &= \frac{1}{2}(\phi - \phi^\dagger) \end{aligned}$$

so that we can write Eq. 7.32 as follows:

$$\begin{aligned} L_s\phi_s + L_a\phi_a &= s_s \\ L_a\phi_s + L_s\phi_a &= s_a \end{aligned} \quad (7.33)$$

Now *suppose* that we can invert the operator L_s . Then we could solve for

$$\phi_a = L_s^{-1}(s_a - L_a\phi_s)$$

and substitute this back into Eq. 7.33 to find a new problem

$$B\phi_s \equiv (L_s - L_a L_s^{-1} L_a)\phi_s = s_s - L_a L_s^{-1} s_a \equiv Q$$

In particular we find that the new operator B is now self-adjoint

$$B^\dagger = L_s - L_a L_s^{-1} L_a = B$$

and therefore we can use the self-adjoint form of the Roussopoulos functional

$$F[\varphi] = 2(Q, \varphi) - (\varphi, B\varphi)$$

But, of course, the price we must pay for this “symmetrization” is the inversion of L_s .

A closely related approach is to rewrite Eq. 7.33 as a matrix problem

$$\begin{pmatrix} L_s & L_a \\ L_a & L_s \end{pmatrix} \begin{pmatrix} \phi_s \\ \phi_a \end{pmatrix} = \begin{pmatrix} s_s \\ s_a \end{pmatrix}$$

It should be apparent that this matrix problem is now in a self-adjoint form.

Example. One instance in which this symmetrization can be carried out arises in one-speed transport theory under the assumption of isotropic scattering. Then we recall

$$L\phi = \hat{\Omega} \cdot \nabla \phi + \Sigma_t \phi - \frac{\Sigma_s}{4\pi} \int d\hat{\Omega}' \phi(\mathbf{r}, \hat{\Omega}') = s$$

$$L^\dagger \phi^\dagger = -\hat{\Omega} \cdot \nabla \phi^\dagger + \Sigma_t \phi^\dagger - \frac{\Sigma_s}{4\pi} \int d\hat{\Omega}' \phi^\dagger(\mathbf{r}, \hat{\Omega}') = s^\dagger$$

In this case it is apparent that

$$L_s = \Sigma_t \circ - \frac{\Sigma_s}{4\pi} \int d\hat{\Omega}' \circ$$

$$L_a = \hat{\Omega} \cdot \nabla \circ$$

In particular, we should note that L_s involves only the angular variable, whereas L_a involves only the non-self-adjoint spatial operator. We can explicitly invert the symmetric component to find

$$L_s^{-1} = \frac{1}{\Sigma_t} \circ + \frac{\Sigma_s}{\Sigma_a \Sigma_t} \frac{1}{4\pi} \int d\hat{\Omega}' \circ$$

Therefore the B operator takes the form of a second order differential operator

$$B\varphi = -\hat{\Omega} \cdot \nabla \left[\frac{1}{\Sigma_t} \circ + \frac{\Sigma_s}{\Sigma_a \Sigma_t} \frac{1}{4\pi} \int d\hat{\Omega}' \circ \right] \hat{\Omega} \cdot \nabla \varphi + \Sigma_t \varphi - \frac{\Sigma_s}{4\pi} \int d\hat{\Omega}' \varphi = s$$

This symmetrized form of the transport equation has been used by a number of investigators as the basis for a self-adjoint variational principle for developing approximate transport methods.³⁵

This approach becomes quite cumbersome if anisotropic scattering is allowed. Then one must expand the scattering

$$\Sigma_s(\hat{\Omega}' \cdot \hat{\Omega}) = \sum_{l=0}^N \left(\frac{2l+1}{4\pi} \right) \Sigma_l P_l(\hat{\Omega}' \cdot \hat{\Omega})$$

and invert L_s to find

$$L_s^{-1} \circ \equiv \frac{1}{\Sigma_t} \circ + \frac{1}{\Sigma_t} \sum_{l=0}^N \sum_{m=-l}^l \Sigma_l (\Sigma_t - \Sigma_l)^{-1} Y_{lm}(\hat{\Omega}) \int d\hat{\Omega}' Y_{lm}^*(\hat{\Omega}') \circ$$

We consider this scheme further in Section 8.3.2.

Discontinuous Trial Functions □ Although the true solutions to the transport equation are usually continuous in space and angle, we are frequently interested in obtaining a “discontinuous” approximation to these solutions. An example is the approximation of a continuous function by a sequence of step functions (see Figure 7.3) or localized polynomials, which are better suited for numerical analysis. Such discontinuous approximations are particularly useful for describing the angular dependence of the particle density near boundaries or interfaces.

But there is an obvious barrier to deriving such discontinuous approximations from a variational principle. If our original equation involves derivatives (as it does in transport problems), the variational functional is only defined for continuous trial functions. Hence we would actually like to extend the domain of the functional to include discontinuous trial functions.

The general scheme for accomplishing this is to employ Lagrange multipliers.^{36,37} That is, suppose we wish to solve

$$f(\phi, \mathbf{r}) = 0 \Rightarrow \delta F[\phi] = 0$$

subject to the constraint $H[\phi] = 0$. Then we would consider the functional

$$F[\varphi] \rightarrow F[\varphi] + \lambda H[\varphi]$$

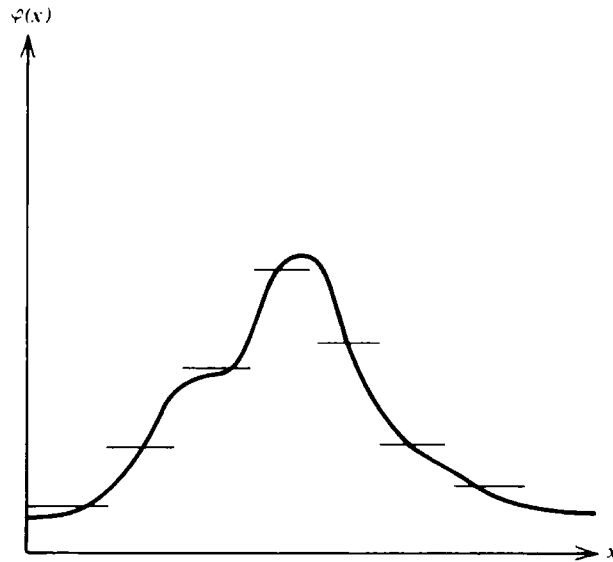


Fig. 7.3 □ Discontinuous representation of $\varphi(x)$ as a sequence of step functions.

where λ is regarded as an arbitrary parameter (the Lagrange multiplier). If we now take variations with respect to both φ and λ , we find both the original equation and the constraint.

Therefore the idea is to represent the continuity condition as a constraint, say relating two functions across a surface

$$\phi_+(\mathbf{R}_s) - \phi_-(\mathbf{R}_s) = 0, \quad \mathbf{R}_s \in S$$

Then the functional is augmented by a Lagrange multiplier characterizing this constraint

$$F[\varphi] \rightarrow F[\varphi] + \int dS \lambda(\mathbf{r}) [\varphi_+(\mathbf{r}) - \varphi_-(\mathbf{r})]$$

Chapter 8 develops in some detail the use of discontinuous trial functions in both space and angle for both the discrete ordinate and finite element methods for solving the transport equation.

Higher Order Methods □ It is possible to develop higher order perturbation and variational methods.³⁸ To illustrate, let us consider the generalized eigenvalue problem characterizing the criticality of a nuclear system

$$M\phi = \lambda F\phi \quad (7.34)$$

where the criticality eigenvalue is denoted by $\lambda = 1/k$. In traditional

perturbation theory, we decompose or partition the operators M and F into unperturbed parts and “small” perturbations

$$M = M_0 + \delta M \quad \text{and} \quad F = F_0 + \delta F$$

How do we choose this partitioning? Two constraints are used: (i) we must be able to solve the unperturbed eigenvalue problem

$$M_0 \phi_0 = \lambda_0 F_0 \phi_0$$

and (ii) in some sense, the perturbations must be small

$$\|\delta M\| \ll \|M_0\|, \quad \|\delta F\| \ll \|F_0\|$$

If we substitute this partitioning into the eigenvalue problem (7.34) and take the inner product with the adjoint unperturbed eigenfunction $\phi_0^\dagger$, we can find the perturbation in the eigenvalue as

$$\delta\lambda = \frac{(\phi_0^\dagger, (\delta M - \lambda_0 \delta F) \phi)}{(\phi_0^\dagger, F \phi)}$$

Our remaining task is to estimate the perturbed eigenfunction. In first order perturbation theory, we would simply replace ϕ by the unperturbed eigenfunction ϕ_0 . But we can do better than this by rewriting the eigenvalue problem as

$$M(\phi_0 + \delta\phi) - (\lambda_0 + \delta\lambda)F(\phi_0 + \delta\phi) = 0$$

or in a rearranged form

$$(M_0 - \lambda F_0) \delta\phi = -(\delta M - \lambda \delta F) \phi + \delta\lambda F_0 \phi_0$$

We can now use this as the basis of an iterative method

$$\delta\lambda^{(n)} = \frac{(\phi_0^\dagger, (\delta M - \lambda_0 \delta F) \phi^{(n-1)})}{(\phi_0^\dagger, F \phi^{(n-1)})}$$

$$\delta\phi^{(n)} = (M_0 - \lambda^{(n-1)} F_0)^{-1} [-(\delta M - \lambda^{(n-1)} \delta F) \phi^{(n-1)} + \delta\lambda^{(n)} F_0 \phi_0]$$

$$\phi^{(n)} = \phi_0 + \delta\phi^{(n)}$$

to generate higher order estimates of the eigenvalue. In particular one can show that $\delta\lambda^{(1)} = O(\delta M) = O(\delta F) \equiv O(\epsilon)$, $\delta\phi^{(1)} = O(\epsilon)$, $\delta\lambda^{(n)} = O(\epsilon^n)$, $\delta\phi^{(n)} = O(\epsilon^n)$.

So far, so good. This is the standard way to approach the development of a higher order perturbation theory. But we can accelerate this scheme dramatically by using variational methods based on the Ritz functional

$$F[\varphi^\dagger, \varphi] = \frac{(\varphi^\dagger, M\varphi)}{(\varphi^\dagger, F\varphi)}$$

The general idea is to use this functional to estimate the eigenvalue, but to calculate the trial functions by using perturbation theory

$$\delta\phi^{(n)} = (M_0 - \lambda^{(n-1)}F_0)^{-1} [-(\delta M - \lambda^{(n-1)}\delta F)\phi^{(n-1)} + \delta\lambda^{(n)}F_0\phi_0]$$

$$\delta\phi^{\dagger(n)} = (M_0^\dagger - \lambda^{(n-1)}F_0^\dagger)^{-1} [-(\delta M^\dagger - \lambda^{(n-1)}\delta F^\dagger)\phi^{\dagger(n-1)} + \delta\lambda^{(n)}F_0^\dagger\phi_0^\dagger]$$

This differs from the previous scheme because we now go up $O(\epsilon^2)$ at each step of the iteration

$$\lambda^{(n)} = F[\varphi^{\dagger(n-1)}, \varphi^{(n-1)}] = O(\|\phi^{(n-1)}\|^2) = O(\epsilon^{2(n+1)-2})$$

Of course there is much more work at each iteration level, since one must evaluate both $\delta\phi$ and its adjoint $\delta\phi^\dagger$. Nevertheless, this “supervariational” approach to calculating eigenvalues can yield very impressive results.¹⁰

Blending together variational and perturbation methods to develop a very rapidly converging iterative method is ideally suited to the acceleration of numerical solution methods. We consider such acceleration methods in more detail in Chapter 8.

7.2.4 □ Synthesis Techniques □ In “flux synthesis,” a very popular method of approximation in transport theory, one tries to synthesize the solution to a complicated transport problem out of solutions to several simpler problems.³⁹⁻⁴² In a way this approach might be viewed as kind of a poor man’s variational method.

Although this method has been used extensively for the solution of the transport equation, it can be most easily described by considering a comparable two-dimensional diffusion theory problem

$$-\nabla \cdot D(x,y)\nabla\phi + \Sigma(x,y)\phi(x,y) = S(x,y) \quad (7.35)$$

where $\phi(x,y)$ is assumed to be subject to suitable boundary conditions. The principal idea in the synthesis method is to decompose such problems into a set of simpler problems of lower dimension. In this case we would

decompose the two-dimensional diffusion equation into several one-dimensional problems, which are considerably easier to solve.

In its simplest form we might apply the synthesis method by expressing $\phi(x, y)$ in a separable form

$$\phi(x, y) = \phi_1(x)\phi_2(y) \quad (7.36)$$

In the original formulation of the synthesis method one assumed that one of these functions was known, say $\phi_2(y)$. The scheme was then to attempt to satisfy Eq. 7.35 with the form Eq. 7.36 in some weighted sense. That is, one demanded that a weighted integral of the equation vanish:

$$\int dy w(y) [-\nabla \cdot D \nabla \phi_1(x)\phi_2(y) + \Sigma(x, y)\phi_1(x)\phi_2(y) - S(x, y)] = 0$$

Since $\phi_2(y)$ was presumed known, this integral (referred to as a “weighted residual”) would then yield an effective one-dimensional problem for the unknown function $\phi_1(x)$

$$-\frac{d}{dx} D(x) \frac{d\phi_1}{dx} + [\Sigma(x) + D(x)B^2(x)] \phi_1(x) = S(x)$$

where

$$D(x) \equiv \int dy w(y) D(x, y)\phi_2(y)$$

$$\Sigma(x) \equiv \int dy w(y) \Sigma(x, y)\phi_2(y)$$

$$D(x)B^2(x) \equiv \int dy w(y) D(x, y) \left(\frac{d^2 \phi_2}{dy^2} \right)$$

The choice of a weighting function $w(y)$ was arbitrary. Frequently it was taken to be $\phi_2(y)$ itself.

A much less heuristic approach is to use a variational principle to accomplish the synthesis of the two-dimensional flux as a product of two one-dimensional fluxes as follows: The appropriate functional for Eq. 7.35 is

$$F[\varphi] = \int dx \int dy [D(x, y)(\nabla \varphi)^2 + \Sigma(x, y)\varphi^2(x, y) - 2S(x, y)\varphi(x, y)] \quad (7.37)$$

(We have noted that the diffusion equation is self-adjoint.) Suppose that we seek our trial function in the form Eq. 7.36 so that the functional (7.37) leads to the “reduced Lagrangian”

$$F_R[\varphi_1, \varphi_2] = \int dx \int dy \left\{ D(x, y) \left[\varphi_1^2 \left(\frac{d\varphi_2}{dy} \right)^2 + \varphi_2^2 \left(\frac{d\varphi_1}{dx} \right)^2 + \Sigma \varphi_1^2 \varphi_2^2 - 2S\varphi_1 \varphi_2 \right] \right\}$$

Now if we perform the variation δF_R with respect to the φ_2 , we find the approximate Euler equation

$$-\frac{d}{dx} D_1(x) \frac{d\phi_1}{dx} + [\Sigma_1(x) + D_1(x) B_1^2(x)] \phi_1(x) = S(x)$$

$$D_1(x) = \int dy \phi_2^2(y) D(x, y), \quad D_1(x) B_1^2(x) = \int dy D(x, y) \left(\frac{d\phi_2}{dy} \right)^2,$$

$$\Sigma_1(x) = \int dy \Sigma(x, y) \phi_2^2(y) \quad (7.38)$$

If we guess $\phi_2(y)$, we arrive at an approximate one-dimensional equation for $\phi_1(x)$. Thus we can use the variational principle to develop a synthesis approximation.

A more consistent procedure would be to take the variation δF_R also with respect to $\varphi_1(x)$ to find

$$-\frac{d}{dy} D_2(y) \frac{d\phi_2}{dy} + [\Sigma_2(y) + D_2(y) B_2^2(y)] \phi_2(y) = S(y) \quad (7.39)$$

$$D_2(y) = \int dx \phi_1^2(x) D(x, y), \quad D_2(y) B_2^2(y) = \int dx D(x, y) \left(\frac{d\phi_1}{dx} \right)^2,$$

$$\Sigma_2(y) = \int dx \Sigma(x, y) \phi_1^2(x)$$

We could then iterate between Eqs. 7.38 and 7.39 to obtain a solution of the form Eq. 7.36.

One can easily generalize this approach to synthesize three-dimensional solutions out of one- and two-dimensional solutions, and so on. For example, a common procedure is to attempt to represent the solution as a superposition of separable terms

$$\phi(x, y, z) = \sum_{n=1}^N \phi_n(z) \chi_n(x, y)$$

where the functions $\chi_n(x, y)$ are presumed known and the unknown $\phi_n(z)$ functions are then determined by using weighted residual or variational methods to arrive at a set of N effective one-dimensional equations.

More generally, we can summarize the synthesis approach⁴³ to solving a problem of the form

$$H(x_1, x_2, \dots, y)\phi(x_1, x_2, \dots, y) = f(x_1, x_2, \dots, y)$$

by first seeking the solution as an expansion in known functions in one (or more) of the variables, say $\chi_n(y)$:

$$\phi(x_1, \dots, y) \cong \sum_{n=1}^N \varphi_n(x_1, \dots) \chi_n(y) \equiv \varphi_{\text{approx}}$$

Then one can choose from several prescriptions to determine the unknown coefficient functions $\varphi_n(x_1, x_2, \dots)$:

i *Variational synthesis.* One utilizes the appropriate variational functional

$$F[\varphi^\dagger, \varphi] = (g, \varphi) + (\varphi^\dagger, f) - (\varphi^\dagger, H\varphi)$$

to find the appropriate Euler equations

$$\sum_m \left[\int dy \chi_m^\dagger(y) H \chi_m(y) \right] \varphi_m(x_1, \dots) = \int dy \chi_m^\dagger(y) f(x_1, \dots, y)$$

ii *Weighted residual method.* Since $\varphi_{\text{approx}} \neq \varphi$, we know that $H\varphi_{\text{approx}} \neq f$. Let us define the "residual error" as

$$\mathcal{E} \equiv H\varphi_{\text{approx}} - f$$

Then the weighted residual method would determine the coefficient functions $\varphi_n(x_1, x_2, \dots)$ by demanding that

$$\int dy w_i(y) [H\varphi_{\text{approx}} - f] = 0$$

where $w_i(y)$ are specified weighting functions. This leads to the set of equations:

$$\sum_m \left[\int dy w_i(y) H \chi_m(y) \right] \varphi_m(x_1, \dots) = \int dy w_i(y) f$$

If we choose the weighting functions as the expansion functions themselves, $w_i(y) = \chi_i(y)$, we arrive at the *Galerkin* weighting scheme. Note that if we choose the weighting functions to be the adjoint to these expansion functions, $w_i(y) = \chi_i^\dagger(y)$, we return to the variational synthesis method.

The general procedure of synthesizing a complicated solution out of simple (but not elementary) component parts has received considerable attention in a variety of transport problems. Synthesis methods have been applied in space, angle, and energy variables to simplify the form of the transport equation. Such methods are particularly valuable for the simplification of those problems in which significant details of the solution can be predicted in advance. Then the “trial modes” in the synthesis solution can be chosen in a manner consistent with these known properties, and a major part of the calculational effort can be eliminated.

7.3 □ APPROXIMATE TREATMENT OF PARTICLE ENERGY DEPENDENCE □

The cross sections characterizing the probabilities of collision events depend very sensitively on the particle kinetic energy or speed. This strong energy dependence has given rise to a variety of specialized approximation methods that can be used to treat this variable. In most cases these methods seek to replace the dependence of the particle phase space density on the continuous variables E or v by a discrete representation. This section reviews a variety of methods that are designed to discretize the particle energy or speed dependence. To simplify this discussion, we illustrate such methods by considering only the very simple infinite medium problem

$$\Sigma_t(E)\phi(E) = \int_0^\infty dE' \Sigma_s(E', E)\phi(E') + S(E) \quad (7.40)$$

The extensions to problems with space, angle, and time dependence will be obvious.

7.3.1 □ Discrete Ordinates Methods □ The most pedestrian approach is simply to replace the continuous variable $0 \leq E < \infty$ by a set of discrete mesh points $E_1, \dots, E_N$.⁴⁴ The transport equation is then written for each such energy E_i , and the energy integration is replaced by a numerical quadrature over this set (with quadrature weights w_j):

$$\Sigma_t(E_i)\phi(E_i) = \sum_{j=1}^N w_j \Sigma_s(E_j, E_i)\phi(E_j) + S(E_i), \quad i = 1, \dots, N$$

This set of algebraic equations can be rewritten in an obvious matrix notation

$$\Sigma_t \phi = S \phi + S \quad (7.41)$$

The discrete ordinate approach has received some attention in rarefied gas dynamics⁴⁵ (where discrete velocity models have also been studied), since the cross sections characterizing molecular collisions are rather smooth functions of particle energy. However a discrete ordinates approach in energy is rarely adequate to describe the more complicated interaction processes encountered in neutron or photon transport.

7.3.2 □ Multigroup Energy Methods □ The most common approach in neutron and photon transport problems involves breaking the energy range into intervals or "energy groups" $0 = E_G, E_{G-1}, \dots, E_1, E_0$, then averaging the energy-dependent cross sections over some assumed form of the flux $\phi(E)$ within each energy group.^{6,7} To illustrate, we integrate Eq. 7.40 over the energy group $E_g < E < E_{g-1}$

$$\int_{E_g}^{E_{g-1}} dE \Sigma_t(E) \phi(E) = \int_{E_g}^{E_{g-1}} dE \sum_{g'=1}^G \int_{E_g}^{E_{g'-1}} dE' \Sigma_s(E', E) \phi(E') + \int_{E_g}^{E_{g-1}} dE S(E)$$

and define the group fluxes

$$\phi_g \equiv \int_{E_g}^{E_{g-1}} dE \phi(E)$$

and the group averaged cross sections or group constants

$$\Sigma_{tg} \equiv \frac{1}{\phi_g} \int_{E_g}^{E_{g-1}} dE \Sigma_t(E), \quad \Sigma_{sg'g} \equiv \frac{1}{\phi_{g'}} \int_{E_g}^{E_{g-1}} dE \int_{E_g}^{E_{g'-1}} dE' \Sigma_s(E', E)$$

to arrive at the multigroup equations

$$\Sigma_{tg} \phi_g = \sum_{g'=1}^G \Sigma_{sg'g} \phi_{g'} + S_g, \quad g = 1, \dots, G$$

Once again we have replaced the original integral equation by a system of algebraic equations. These can be written in a matrix form similar to Eq. 7.41.

Of course the multigroup equations are of only formal interest until we prescribe a method for determining the group constants. The general approach involves guessing or calculating an approximate form for the intragroup flux $\phi(E)$ so that, for example,

$$\Sigma_{ig} = \frac{1}{\phi_g} \int_{E_g}^{E_{g-1}} dE \Sigma_i(E) \phi(E) \cong \frac{1}{\phi_{g \text{ approx}}} \int_{E_g}^{E_{g-1}} dE \Sigma_i(E) \phi_{\text{approx}}(E)$$

It should be apparent that the successful application of the multigroup method to transport problems with strongly energy-dependent cross sections requires a very careful choice of the energy spectrum $\phi_{\text{approx}}(E)$. Most commonly this is accomplished by way of a set of auxiliary calculations. For example, the group constants to be used in a “few group” multigroup transport calculation are typically determined by first solving a finely structured multigroup problem in an infinite medium for $\phi_{\text{approx}}(E)$. The subject of group constant generation has become a very highly developed art in nuclear reactor analysis, and the interested reader is referred to several of the standard texts on this subject for further details.^{6,7}

7.3.3 □ Series Expansions □ Yet another common approach involves the representation of the energy dependence as an expansion in a finite series of known functions $\chi_k(E)$

$$\phi(E) \cong \sum_{k=1}^N \phi_k \chi_k(E) \quad (7.42)$$

A variety of possible choices for $\chi_k(E)$ have been considered. For thermalization problems the $\chi_k(E)$ are usually taken as Laguerre polynomials multiplied by a Maxwell-Boltzmann distribution⁴⁶ (or Hermite polynomials if the speed variable is used⁴⁷). If we substitute an expansion in such polynomials into Eq. 7.40 and use the standard orthogonality properties, we arrive once again at a matrix problem similar to Eq. 7.41 where now the matrix elements are given as

$$[\Sigma_i]_{ij} = (\chi_i, \Sigma_i \chi_j), \quad [\mathcal{S}]_{ij} = (\chi_i, \mathcal{S} \chi_j), \quad [\phi]_i = (\chi_i, \phi) = \phi_i \quad (7.43)$$

Actually, the multigroup representation is nothing more than a special choice of orthogonal functions

$$\chi_k(E) = \phi_{\text{approx}}(E) u_k(E)$$

where $u_k(E)$ is the unit square wave function

$$u_k(E) \equiv \begin{cases} 1, & E_k \leq E \leq E_{k+1} \\ 0, & \text{otherwise} \end{cases}$$

One can also choose an arbitrary nonorthogonal set of functions^{48,49} in which to expand $\phi(E)$. However it then becomes necessary to provide some prescription for determining the matrix equation for the coefficients ϕ_k . Two of the most common schemes for accomplishing this are variational principles and weighted residual methods. In the first method one usually begins with the Roussopoulos functional for Eq. 7.40

$$F[\varphi^\dagger, \varphi] = (\varphi^\dagger, S) + (S^\dagger, \varphi) - (\varphi^\dagger, L\varphi)$$

then substitutes in trial functions of the form Eq. 7.42 for φ and $\varphi^\dagger$ and equates the first variation of the resulting reduced Lagrangian with respect to $\phi_k^\dagger$ and ϕ_k equal to zero to find, respectively,

$$(\Sigma_t - \mathcal{S})\varphi = S \quad \text{and} \quad (\Sigma_t^\dagger - \mathcal{S}^\dagger)\phi^\dagger = S^\dagger$$

where

$$[\Sigma_t]_{ij} = (\chi_i^\dagger, \Sigma_t \chi_j), \quad [\mathcal{S}]_{ij} = (\chi_i^\dagger, \mathcal{S} \chi_j)$$

Here we should notice that if we choose trial functions of the form $\chi_k(E) = \phi_{k \text{ guess}}(E) u_k(E)$, we would obtain an alternative derivation of the multigroup equations, but with adjoint or bilinear weighting. In neutron or gas thermalization problems, one can use detailed balance to symmetrize $\Sigma_s(E', E)$ and thereby obtain a self-adjoint collision operator (and variational principle):

$$F[\varphi] = 2(\varphi, S) - (\varphi, \tilde{L}\varphi) \quad (7.44)$$

Then by demanding $\delta F_R = 0$, we find that the matrix system (7.41) is defined by

$$[\Sigma_t]_{ij} = (\chi_i, \Sigma_t \chi_j), \quad [\mathcal{S}]_{ij} = (\chi_i, \mathcal{S} \chi_j)$$

A second approach is the weighted residual method in which the ϕ_k are determined by requiring

$$\int_0^\infty dE w_j(E) \left\{ (\Sigma_t - \mathcal{S}) \sum_{k=1}^N \phi_k \chi_k - S \right\} = 0, \quad j = 1, \dots, N$$

which yields

$$[\Sigma_t]_{ij} = (w_i, \Sigma_t \chi_j), \quad [\mathcal{S}]_{ij} = (w_i, \mathcal{S} \chi_j), \quad [S]_i = (w_i, S)$$

Here the $\{w_j(E)\}$ are some chosen set of weighting functions [sometimes chosen as the $\chi_j(E)$ themselves].

Such nonorthogonal function expansions or “overlapping” group techniques have been moderately successful in a variety of applications.

7.3.4 □ Synthetic Kernel Models □ Thus far we have discussed methods that approximate the energy dependence of the *solution* $\phi(E)$ to the transport equation. A quite different tactic is to approximate the *equation* itself by approximating or modeling the form of the scattering kernel. One such approach replaces $\Sigma_s(E', E)$ by the Green's function for a second order differential operator. There are two models commonly encountered in neutron thermalization studies in which this form occurs naturally.^{6,7}

i *Proton gas model.*

$$\Sigma_s(E', E) = \begin{cases} \left(\frac{\Sigma_s}{E'}\right) \exp\left(\frac{E' - E}{kT}\right) \operatorname{erf} \sqrt{E'/kT}, & E > E' \\ \left(\frac{\Sigma_s}{E'}\right) \operatorname{erf} \sqrt{E/kT}, & E < E' \end{cases}$$

ii *Heavy gas model.*

$$\begin{aligned} \Sigma_s(E', E) = & \Sigma_s \delta(E' - E) \\ & + \frac{\Sigma_s(E + E')}{kT} \left(\frac{E}{E'}\right)^{1/2} [-\delta'(E' - E) + kT\delta''(E' - E)] \end{aligned}$$

In each instance the integral equation (7.40) can be reduced to a second order differential equation.

A natural extension of these ideas is the generalized heavy gas or *primary model* of the scattering operator $S = \mathcal{S} - \Sigma_s$ proposed by Horowitz⁵⁰

$$S\phi = \xi \Sigma_s \frac{d}{dE} \left\{ f(E) \left[EkT \frac{d\phi}{dE} + (E - kT)\phi(E) \right] \right\} \quad (7.45)$$

where $f(E)$ is an arbitrary function that is determined either by fitting to

experimental measurements or by a fit to an integral of the scattering kernel itself, $\Sigma_s(E', E)$. This model satisfies detailed balance and includes some accounting of chemical binding effects. Moreover, the storage requirements and computer time required to solve the differential equation generated by Eq. 7.45 are quite small when compared to the labor involved in solving the integral equation (7.40) directly.

Unfortunately this model fails to yield satisfactory results when strong absorption is present (e.g., near a resonance in the absorption cross section). To circumvent this, Cadilhac⁵¹ has developed a slightly more general differential operator model of the scattering operator known as the *secondary model*, which contains two free functions. If one writes the scattering kernel as

$$M(E)\Sigma_s(E', E) = \begin{cases} u(E)v(E'), & E > E' \\ u(E')v(E), & E < E' \end{cases}$$

then, in fact,

$$S\phi = \frac{dq}{dE}$$

where $q(E)$ is the solution to the differential equation

$$\frac{d}{dE} \left[\frac{\phi(E)}{M(E)} \right] = \left[j(E) - \frac{d}{dE} k(E) \frac{d}{dE} \right] q(E)$$

Here the free functions $j(E)$ and $k(E)$ can be evaluated as

$$j(E) = \left[\int_0^E dE' u(E') \right]^{-1} \frac{d}{dE} [u(E)k(E)], \quad k(E) = [M(E)\Sigma_s(E)]^{-1}$$

For proper choices of $j(E)$ and $k(E)$, this model will yield the proton gas, heavy gas, Fermi age, or Goertzel-Greuling model under the appropriate limiting conditions.⁷ Hence the secondary model is capable of bracketing the thermalizing properties of the actual scattering kernel.

7.3.5 □ Degenerate Kernel Representations of Finite Rank □ Perhaps the most direct approach to approximating $\Sigma_s(E', E)$ involves its replacement by a finite sum of separable kernels

$$\Sigma_s(E', E) \cong \sum_{k=1}^N \alpha_k(E) \beta_k(E') \quad (7.46)$$

so that our integral equation (7.40) becomes

$$\Sigma_t(E)\phi(E) = \sum_{k=1}^N \alpha_k(E) \int_0^\infty dE' \beta_k(E') \phi(E') + S(E)$$

If we multiply by $\beta_j(E)/\Sigma_t(E)$ and integrate over energy, we arrive at a set of algebraic equations that can be written in matrix form as follows:

$$(I - A)\phi = S$$

where

$$[A]_{ij} = \int_0^\infty dE \frac{\beta_i(E) \alpha_j(E)}{\Sigma_t(E)}, \quad [\phi]_i \equiv \int_0^\infty dE \beta_i(E) \phi(E),$$

$$[S]_i \equiv \int_0^\infty dE \frac{\beta_i(E)}{\Sigma_t(E)} S(E)$$

The approximation of the square-integrable kernel of a Fredholm integral equation by a sum of separable terms such as Eq. 7.46 is a well-known technique in the theory of integral equations.⁵² [The degenerate kernel (7.46) is sometimes referred to as a Pincherle-Goursat kernel.] This approximation has been used for some time in linearized gas dynamics in the form of the BGK kernel⁵³ and its extensions.⁵⁴⁻⁵⁶ The kernel was first introduced in neutron transport theory in a one-term form

$$\Sigma_s(E', E) = \beta \Sigma_s(E) M(E) \Sigma_s(E'), \quad \beta^{-1} \equiv \int_0^\infty dE M(E) \Sigma_s(E)$$

for modeled studies of time-dependent thermalization by Corngold,⁵⁷ Nelkin,⁵⁸ and others. More general N -term expansions have been utilized in formal analytical studies by a number of authors, including Koppel⁵⁹ and Kuščer.⁶⁰

Several attempts have been made to develop this method into a calculational tool for detailed thermal spectrum calculations. A preliminary step in this direction was made by Shapiro and Corngold⁶¹ in a numerical study of time eigenvalues for the pulsed neutron experiment. Gritton and Leonard⁶² have applied this technique to a numerical study of the Kottwitz problem with very limited success, while Turinsky and Duderstadt⁶³ and Mockel⁶⁴ have combined the degenerate kernel representation with the invariant embedding approach to transport problems.

There are a number of schemes available for determining the components $\{\alpha_k(E)\}$ and $\{\beta_k(E')\}$ in the degenerate kernel expansion.

i *Orthogonal polynomials.* The most obvious approach is to choose $\alpha_k(E)$ and $\beta_k(E')$ as orthogonal polynomials. However it can be easily verified that this choice leads to the same matrix system that was obtained for a direct polynomial expansion of $\phi(E)$ itself.

ii *Moments methods.* Shapiro and Corngold⁶¹ constructed the kernel by requiring that it preserve the total scattering cross section $\Sigma_s(E)$, detailed balance, and the first N energy transfer moments of $\Sigma_s(E', E)$. This construction was found to yield reasonable results, provided the flux was not far from Maxwellian. However significant discrepancies arise when one applies this kernel to highly nonequilibrium phenomena. Versluis and Mockel⁶⁵ attempted to correct this poor convergence by using moment preservation to determine the behavior of the kernel only near $E_{th} = kT$. For higher energies $E \gg E_{th}$ they model the kernel using the higher order eigenfunctions of the scattering operator $\mathfrak{S}$:

$$\Sigma_s(E', E) = M(E) \sum_n \lambda_n \psi_n(E) \psi_n(E')$$

iii *Least square convergence criterion.* Turinsky⁶³ has taken a different approach to overcome the inadequacies of moments methods. He avoided an explicit requirement that detailed balance or energy transfer moments be preserved, and instead tried to obtain the best possible pointwise convergence to the true scattering kernel in a least squares sense. This particular choice of the degenerate kernel representations appears to yield the most satisfactory results for a wide range of transport problems.

7.3.6 □ Concluding Remarks □ Our description of techniques for replacing the integral equation (7.40) by an equivalent matrix representation suitable for computer calculation has passed from essentially “brute force” mathematical methods such as discrete ordinates or multigroup methods to more physically motivated approaches such as variational-synthesis and kernel approximations. If intuition is satisfactory, this “input” of physical information into constructing the matrix representation will result in algebraic systems of much smaller dimension, hence lower storage and computing speed requirements.

Several specific comments comparing these approaches are appropriate. Since the physical information involved in the discrete ordinates approach is nil, one would expect such methods to require a very fine mesh structure, that is, to involve large matrix systems. The size of the system can be reduced somewhat by going to an orthogonal polynomial representation, but applications of this method in the past have encountered very slow

convergence unless the spectrum was very close to a Maxwellian. Multi-group representations remain the most popular method for treating the energy variable. But again the size of the matrix system depends on how well we can guess the intragroup fluxes $\phi_{\text{guess}}(E)$, and many ambiguities arise when space, time, and angle dependence are included. The variational (overlapping group) methods are very powerful, provided one chooses suitable trial functions [which again involves guessing the form of $\phi(E)$]. They are usually applied only for very low order systems ($N=3,4$) and yield excellent results if the spectrum is not perturbed too much from the trial function shapes.

Each of these approaches attempts to approximate the unknown flux itself. Hence there is no a priori way to evaluate the accuracy of such approximations. In this sense, the alternative schemes that approximate the scattering kernel itself exhibit a slight advantage, since the adequacy of the particular approximation can be evaluated before one solves for $\phi(E)$.

A somewhat more technical drawback of the methods that approximate the solution $\phi(E)$ is that they fail to preserve the eigenvalue spectrum of the transport operator (either space or time eigenvalues), and in particular they destroy the continuous eigenvalue spectrum. This can be a rather serious shortcoming when one is studying relaxation problems (e.g., pulsed neutron or sound wave propagation experiments). Both the secondary model and the degenerate kernel models preserve the continuous eigenvalue spectrum, hence both methods have been quite successful in the analysis of asymptotic relaxation phenomena.

The secondary model of Cadilhac presents an extremely attractive scheme for treating energy dependence in neutron thermalization calculations. It requires very little storage and machine time, yet it is capable of describing the gross features of the scattering kernel that are important to neutron thermalization. It furthermore possesses the very desirable feature of yielding the proper epithermal behavior of the scattering kernel. Perhaps its only drawback is that it does involve only two free functions, $j(E)$ and $k(E)$. If these are insufficient to model the details of the scattering kernel, there is no obvious way to generalize the model to include more information. That is, it is impossible to achieve convergence (in the mathematical sense) of the secondary model to the true scattering kernel.

The degenerate kernel approximation does not suffer from this difficulty, since by taking more and more terms in the expansion Eq. 7.46 one can approximate the true scattering kernel to an arbitrary degree of accuracy. This mathematical feature may be quite important when one is concerned with very fine details of the scattering kernel. The degenerate kernel approximation possesses in addition all the attractive features of the secondary model (generates small matrix systems, preserves the continuous

eigenvalue spectrum, is capable of describing solutions quite far from equilibrium, and allows an a priori estimate of the accuracy of the approximation) as well as numerous others. The only relative drawbacks are a slight increase in storage requirements over the secondary model, and a somewhat poorer treatment of the kernel behavior in the epithermal range.

In summary then, we have reviewed and compared several of the more popular methods available for treating the energy dependence in particle transport processes. Although these methods can be implemented to simplify an analytical study of a transport problem, they are more appropriately applied to facilitate a direct numerical solution of the transport equation. Indeed, as we have noted, the mathematical complexity of the transport equations that realistically describe particle transport processes almost always forces one to a heavy reliance on numerical (i.e., computer) methods of analysis.

□ PROBLEMS □

7.1 Why is the adjoint system introduced in developing the perturbation equations? Illustrate your answer with an example showing that only the use of the adjoint system will yield the desired result.

7.2 Derive an expression for the second order correction to the perturbed eigenvalue in terms of the unperturbed eigenfunctions. (Use the usual Rayleigh-Schrödinger perturbation theory familiar from quantum mechanics.)

7.3 Derive the adjoint of the one-speed diffusion equation

$$-\frac{d}{dx} \left[D(x) \frac{d\phi}{dx} \right] + \Sigma_a(x) \phi(x) = S(x)$$

with boundary conditions such that the inward partial current at either end of a slab is zero, $j_+(0) = j_-(a) = 0$.

7.4 Derive the adjoint boundary conditions characterizing (i) reflecting boundaries, (ii) periodic boundaries, and (iii) diffuse reflection for the one-speed transport equation.

7.5 Determine the first order change in the reactivity $\Delta\rho = \delta k/k$ due to a perturbation in the scattering and absorption cross sections.

7.6 The accurate flux and adjoint flux in a subcritical system can be calculated readily. The configuration of another system is only slightly different. Find an expression for any desired reaction rate integrated over

the second system such that the expression has only second order errors and does not depend on variations from the flux or adjoint flux of the first system.

7.7 Demonstrate the validity of the result obtained in Problem 7.6 by considering the following example. An infinite medium extends from $x=0$ to $x=\infty$ and contains a plane source at $x=x_0$. The flux is to be described by one-group diffusion theory. The first system has an absorption cross section Σ_a and a diffusion constant D . The second system has the same source and diffusion constant, but an absorption cross section $\Sigma_a + \delta\Sigma_a$. Calculate the absorption rate throughout the second system exactly and according to the derived perturbation procedure. Then show that the results differ by second order terms in $\delta\Sigma_a$.

7.8 Develop the Euler equations for the following Lagrangians: (i) $L[q, q', q'', \dots, q^{(n)}, x]$, and (ii) $L[q_1, \dots, q_n; q'_1, \dots, q'_n, x]$.

7.9 Explicitly calculate each of the functional derivatives listed in Table 7.1.

7.10 Demonstrate that the total variation of the Roussopoulos functional is of second order in the variations [i.e., $\delta F = -(\delta\phi^\dagger, H\delta\phi)$].

7.11 By choosing trial functions $\varphi = c\phi$, $\varphi^\dagger = c^\dagger\phi^\dagger$, derive the Schwinger variational principle from the Roussopoulos principle.

7.12 Evaluate the numerical value of the first zero, ν_0 , of $J_0(x)$ by using the Ritz principle for the differential operator that generates $J_0(\nu_n x)$ as eigenfunctions. Use simple polynomial estimates as the trial functions.

7.13 Use the Roussopoulos functional to estimate the total absorption rate occurring in a bare slab in which the particle flux is maintained by a plane source at the origin. Use simple polynomials as trial functions and compare the variational estimate with the exact expression for the absorption as given by one-speed diffusion theory.

7.14 Prove that the Ritz functional for a self-adjoint eigenvalue problem is indeed an extremum principle. Give an explicit example of this feature by using this principle to estimate eigenvalues for a bare slab geometry and compare these to the actual eigenvalue.

7.15 Use the Ritz functional as a Lagrangian to derive the multigroup transport equations. Choose the trial functions as

$$\varphi(\mathbf{r}, E, \hat{\Omega}) = \sum_{g=1}^G \varphi_g(\mathbf{r}, \hat{\Omega}) \chi_g(E)$$

where the $\chi_g(E)$ are disjoint step functions over the interval $E_g < E < E_{g+1}$. In particular, develop expressions for the group constants appearing in these equations.

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Numerical Methods in Transport Theory

The complexity of the equations describing particle transport processes usually forces one to implement numerical (i.e., computer-based) methods of solution. Such methods seek to introduce approximations that convert the integrodifferential (or integral) form of the transport equation into a system of algebraic equations that is most amenable to solution by a digital computer.

The most direct procedure is the discrete ordinate approach in which the dependent variable in the transport equation $\varphi(\mathbf{r}, E, \hat{\Omega}, t)$ is replaced by a discrete set of values at a discrete set of points $(\mathbf{r}_i, E_j, \hat{\Omega}_k, t_n)$. The derivatives and integrals appearing in the transport equation must also be replaced by a corresponding discrete representation by using finite difference and numerical integration schemes. In this way one arrives at a set of algebraic equations for the discrete representation of the dependent variable.

An alternative approach involves expanding the dependent variables in the transport equation in a finite set of known basis functions, then using either orthogonality properties or more elaborate schemes such as weighted residual or variational methods to arrive at a set of algebraic equations for the expansion coefficients. We studied one example of this approach in Chapter 4 when we developed the P_N expansion of the angular dependence in spherical harmonics (or Legendre polynomials). A somewhat more general and powerful scheme involves expansions in localized basis functions (so-called finite elements) and is considered in some detail later in this chapter.

Such procedures eventually lead to a large system of algebraic equations for the discretized representation of the solution to the transport equation. These algebraic equations can then be solved using standard numerical algorithms on a digital computer.

Unfortunately, such a calculation becomes an immense undertaking if only a “brute force” discretization of the transport equation is employed. For example, a typical mesh size of $100 \times 100 \times 100$ space points, 10 energy points, and 10 angle points would yield a set of 10^8 simultaneous algebraic equations for each time step—a rather formidable task, even on modern digital computers.

Hence we cannot blindly depend on the computer to solve transport equations; rather, we must rely as well on physical insight to reduce the transport equation to more manageable form before applying discretization methods. For example, we can usually eliminate several of the independent variables in the transport equation in the analysis of most problems of interest. Or we can utilize an approximate form of the transport equation as the starting point for the development of a discrete representation.

To be more specific, it is customary in most transport calculations to begin with the multigroup form of the transport equation (cf. Sections 2.2.1 and 7.3.2) in which the scattering kernel has been expanded in a finite set of Legendre polynomials (cf. Section 4.2.2)

$$\begin{aligned} \frac{1}{v_g} \frac{\partial \varphi_g}{\partial t} + \hat{\Omega} \cdot \nabla \varphi_g + \Sigma_{tg} \varphi_g \\ = \sum_{g'=1}^G \sum_{l=0}^L \sum_{m=-l}^l Y_{lm}(\hat{\Omega}) \Sigma_{lg'g} \int d\hat{\Omega}' Y_{lm}^*(\hat{\Omega}') \varphi_{g'}(\mathbf{r}, \hat{\Omega}', t) + s_g \end{aligned}$$

In the vast majority of transport problems, one solves the multigroup equations *successively* as a sequence of effective one-group or one-speed problems in which the contribution from other energy groups g' is treated as an effective source term and combined with s_g

$$s_g^{\text{eff}} = \sum_{g' \neq g} \sum_{l=0}^L \sum_{m=-l}^l Y_{lm}(\hat{\Omega}) \Sigma_{lg'g} \int d\hat{\Omega}' Y_{lm}^*(\hat{\Omega}') \varphi_{g'}(\mathbf{r}, \hat{\Omega}', t) + s_g$$

Therefore we can confine our attention to the numerical solution of the “in group” transport equation that assumes the one-speed form

$$\hat{\Omega} \cdot \nabla \varphi + \Sigma_t \varphi = \sum_{l=0}^L \sum_{m=-l}^l Y_{lm}(\hat{\Omega}) \Sigma_{sl} \int d\hat{\Omega}' Y_{lm}^*(\hat{\Omega}') \varphi(\mathbf{r}, \hat{\Omega}', t) + s(\mathbf{r}, \hat{\Omega}) \quad (8.1)$$

In this equation we have suppressed the group index g and restricted our discussion (at least for the present) to time-independent problems. We now examine a variety of powerful numerical methods for solving this equation, including the discrete ordinate or S_N method, the P_N method, finite element methods, and collision probability or integral transport methods. (References 1 to 4 are excellent reviews of these methods.)

8.1 □ THE DISCRETE ORDINATES METHOD □ We begin our consideration of numerical schemes for solving transport equations by examining the method of *discrete ordinates*⁵ (sometimes known as the S_N method) in which the angular variable is discretized into a small number of directions or rays, then the particle transport equation is written for each ray, including various coupling terms describing ray-to-ray transfer. This method is certainly the most popular as well as one of the most direct and powerful approaches to numerical transport calculations.

We can summarize the major steps of the discrete ordinates approach to solving Eq. 8.1 as follows:

- i We begin by choosing a set of M discrete directions or rays $\hat{\Omega}_m$, $m=1, 2, \dots, M$ and corresponding quadrature weights $w_1, w_2, \dots, w_M$ (for numerical integrations over angle).
- ii The transport equation (8.1) is now evaluated at each of the discrete directions $\hat{\Omega}_m$:

$$\hat{\Omega}_m \cdot \nabla \varphi(\mathbf{r}, \hat{\Omega}_m) + \Sigma_t \varphi(\mathbf{r}, \hat{\Omega}_m) = \sum_{l=0}^L \sum_{n=-l}^l Y_{ln}(\hat{\Omega}_m) \Sigma_{sl} \int d\hat{\Omega}' Y_{ln}^*(\hat{\Omega}') \varphi(\mathbf{r}, \hat{\Omega}') + s(\mathbf{r}, \hat{\Omega}_m) \quad (8.2)$$

- iii The integral terms are evaluated as accurately as possible using the directions $\{\hat{\Omega}_m\}$ and quadrature weights $\{w_m\}$ chosen in step i. For example, the angular moments of the flux in Eq. 8.2 may be approximated as follows:

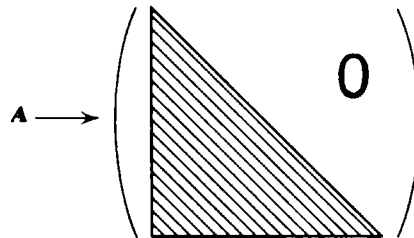
$$\varphi_{ln}(\mathbf{r}) \equiv \int d\hat{\Omega} Y_{ln}^*(\hat{\Omega}) \varphi(\mathbf{r}, \hat{\Omega}) \cong \sum_{m=1}^M w_m Y_{ln}^*(\hat{\Omega}_m) \varphi(\mathbf{r}, \hat{\Omega}_m)$$

- iv A discrete spatial mesh is chosen, and finite difference representations of derivative terms are introduced for this mesh at the discrete spatial and angular points $\mathbf{r}_i$, $i=1, 2, \dots, I$ and $\hat{\Omega}_m$, $m=1, 2, \dots, M$. This results in a system of algebraic equations for the angular fluxes at the discrete mesh points $\{r_i\}$ and $\{\hat{\Omega}_m\}$. If we define $\varphi_m^i = \varphi(\mathbf{r}_i, \hat{\Omega}_m)$ and $\boldsymbol{\varphi} = \text{col}(\varphi_1^1, \varphi_1^2, \dots, \varphi_m^i, \dots, \varphi_M^i)$, this system of equations may be expressed in matrix form as follows:

$$\mathbf{A}\boldsymbol{\varphi} = \mathbf{B}\boldsymbol{\varphi} + \mathbf{S}$$

where $\mathbf{A}$ represents the discretized streaming-collision operator, $\hat{\Omega}_m \cdot \nabla + \Sigma_t(\mathbf{r})$, $\mathbf{B}$ is the discretized form of the inscatter term, and $\mathbf{S}$ is the discretized source term.

v If we rearrange A so that it is a lower triangular matrix



(this is always possible and corresponds physically to solving in the direction of neutron motion), we can easily invert A to arrive at an iterative solution method

$$\varphi^{(n)} = A^{-1} B \varphi^{(n-1)} + A^{-1} S \quad (8.3)$$

Of course, the iterative scheme represented by Eq. 8.3 is similar to the collision (or Neumann) iteration we studied in Section 2.2.2. We continue this iteration process until some suitable convergence criterion is met.

The foregoing steps constitute an outline of the method of discrete ordinates. Although this approach is apparently quite straightforward in principle, several complications arise in practice.⁶ The choice of discrete directions $\{\hat{\Omega}_m\}$ and $\{w_m\}$ is not obvious in many cases—particularly in multidimensional geometries. Even for one-dimensional geometries, the choice of an optimum set is frequently problem dependent. Moreover, the discretization of the streaming operator in curvilinear geometries involves angular derivatives to account for ray-to-ray transfer or “angular redistribution.” If not treated carefully, the resulting finite difference scheme may be nonconservative insofar as it will fail to conserve particle number.

The discretization scheme may give rise to other deleterious numerical effects such as negative fluxes or flux oscillations. One particularly serious malady is the “ray effect” in which the finite number of rays used in a discrete ordinates representation may “miss” localized sources or absorbers. Measures must be taken to alleviate or eliminate this effect when it occurs.

Because the size of transport calculations implies large computing times, acceleration methods (e.g., coarse mesh rebalancing) are employed to speed up the convergence of the collision iteration represented by Eq. 8.3. This is especially true in weakly absorbing systems ($c \sim 1$).

The following sections, which discuss in more detail the steps in a discrete ordinates calculation, examine each of these complications.

8.1.1 □ Selection of Discrete Ordinates Quadrature Sets □ This section covers the criteria for choosing the discrete directions $\{\hat{\Omega}_m\}$ and corresponding weights $\{w_m\}$. Because the situations are somewhat different, the discussion of quadrature sets for one-angle (e.g., one-dimensional slab or spherical) geometries is separated from the discussion for two-angle (one-dimensional cylindrical or multidimensional) geometries.

One-Angle Quadrature Sets □ For one-dimensional plane or spherical geometries, the angular flux depends only on the direction cosine $\mu = \hat{\Omega} \cdot \hat{e}_x$ or $\mu = \hat{\Omega} \cdot \hat{e}_r$. For these cases, the angular integrals become simply

$$\varphi_{lm}(\mathbf{r}) = \int d\hat{\Omega} Y_{lm}^*(\hat{\Omega}) \varphi(\mathbf{r}, \hat{\Omega}) \rightarrow \left(\frac{2l+1}{4\pi} \right)^{1/2} 2\pi \int_{-1}^{+1} d\mu P_l(\mu) \varphi(x, \mu) \quad (8.4)$$

and the selection of discrete directions and weights over the unit sphere is reduced to the interval $-1 \leq \mu \leq 1$. Denoting the discrete directions and weights as $\{\mu_m\}$ and $\{w_m\}$, respectively, we can replace the integral Eq. 8.4 by the quadrature formula

$$\int_{-1}^{+1} d\mu P_l(\mu) \varphi(x, \mu) \cong \sum_{m=1}^M w_m P_l(\mu_m) \varphi(x, \mu_m)$$

Our goal is to determine suitable quadrature sets $\{\mu_m, w_m\}$.

The following criteria should be satisfied by the selected quadrature set $\{\mu_m, w_m\}$.⁷⁻⁹

i *Projection invariance.* The quadrature set should be invariant with respect to allowable orientations of the physical domain. For one-dimensional slab geometry with azimuthal (rotation about the x -axis) symmetry, the only change in geometric orientation allowable is reflection ($x \rightarrow -x$). Any other orientation would change the symmetry and necessitate a different coordinate system. But reflection about $x=0$ implies that if $\mu_i = \cos \theta_i$ is chosen, the $\mu_j = \cos(\pi - \theta_i) = -\mu_i$ must also be included. Therefore the discrete directions $\{\mu_m\}$ should be symmetric about $\mu=0$. Physically, this corresponds to treating particles traveling from left to right ($\mu > 0$) the same as particles traveling from right to left ($\mu < 0$).

Projection invariance is desirable if one has no a priori knowledge concerning the solution. For radiation shielding calculations, however, one

may know that the angular flux is forward peaked (concentrated near $\mu = 1$) for large distances into the shield. In this case one may wish to tailor a nonsymmetric quadrature set with several points clustered near $\mu = +1$.¹⁰

ii *Positivity of the scalar flux.* The zeroth moment of the angular flux, the scalar flux

$$\phi(x) = 2\pi \int_{-1}^{+1} d\mu \varphi(x, \mu) \cong 2\pi \sum_{m=1}^M w_m \varphi(x, \mu_m)$$

is always positive. Choosing the $w_m > 0$ will ensure this property as long as the angular flux is positive.

iii *Accurate evaluation of angular integrals.* The various moments of the flux (e.g., Eq. 8.4) and source should be evaluated accurately with a minimum of directions and weights.

In early discrete ordinates schemes it was common to use trapezoidal quadrature in which it was assumed that the angular flux varied linearly between any two quadrature points μ_i :⁵

$$\varphi(x, \mu) = \left(\frac{\mu - \mu_{j-1}}{\mu_j - \mu_{j-1}} \right) \varphi(x, \mu_j) + \left(\frac{\mu_j - \mu}{\mu_j - \mu_{j-1}} \right) \varphi(x, \mu_{j-1}), \quad \mu_{j-1} \leq \mu \leq \mu_j$$

This particular scheme in which the angular flux was represented by N straight-line segments was referred to as the S_N method. Such a nomenclature has persisted to the present day, and discrete ordinates schemes are still occasionally referred to as S_N methods—even though the quadrature scheme may bear no resemblance to the earlier straight-line interpolation.

Perhaps the most popular quadrature set for one-dimensional geometries is the *Gaussian quadrature* set. It is well known that Gaussian quadrature will integrate exactly a polynomial of a given degree with the least number of quadrature points (and weights). In particular, M point Gaussian quadrature will exactly integrate a polynomial of degree $2M - 1$. Since the various angular integrals are moments of Legendre polynomials (see Eq. 8.1), the use of Gaussian quadrature points and weights would seem to be the optimum choice. Interestingly enough, Gaussian quadrature sets also satisfy criteria i and ii above; that is, the $\{\mu_m\}$ are symmetric about $\mu = 0$, and the $\{w_m\}$ are all positive.

Table 8.1 contains standard Gaussian quadrature sets for several choices of the number of directions (weights) M . This table gives only quadrature sets for even M (i.e., S_2, S_4 , etc.), since the Gaussian sets for odd M all have a quadrature point at $\mu = 0$. In slab geometry the angular flux may be discontinuous at $\mu = 0$; therefore we might expect evaluating the flux at

Table 8.1 □ **Gaussian Quadrature Sets^a**

μ_i			w_i		
$n = 2$					
0.57735	02691	89626	1.00000	00000	00000
$n = 4$					
0.33998	10435	84856	0.65214	51548	62546
0.86113	63115	94053	0.34785	48451	37454
$n = 6$					
0.23861	91860	83197	0.46791	39345	72691
0.66120	93864	66265	0.36076	15730	48139
0.93246	95142	03152	0.17132	44923	79170
$n = 8$					
0.18343	46424	95650	0.36268	37833	78362
0.52553	24099	16329	0.31370	66458	77887
0.79666	64774	13627	0.22238	10344	53374
0.96028	98564	97536	0.10122	85362	90376
$n = 10$					
0.14887	43389	81631	0.29552	42247	14753
0.43339	53941	29247	0.26926	67193	09996
0.67940	95682	99024	0.21908	63625	15982
0.86506	33666	88985	0.14945	13491	50581
0.97390	65285	17172	0.06667	13443	08688
$n = 12$					
0.12523	34085	11469	0.24914	70458	13403
0.36783	14989	98180	0.23349	25365	38355
0.58731	79542	86617	0.20316	74267	23066
0.76990	26741	94305	0.16007	83285	43346
0.90411	72563	70475	0.10693	93259	95318
0.98156	06342	46719	0.04717	53363	86512
$n = 16$					
0.09501	25098	37637	0.18945	06104	55068
0.28160	35507	79258	0.18260	34150	44923
0.45801	67776	57227	0.16915	65193	95002
0.61787	62444	02643	0.14959	59888	16576
0.75540	44083	55003	0.12462	89712	55533
0.86563	12023	87831	0.09515	85116	82492
0.94457	50230	73232	0.06225	35239	38647
0.98940	09349	91649	0.02715	24594	11754

^aWeights are normalized to $\int_{-1}^1 d\mu = \sum_{i=1}^n w_i = 2$.

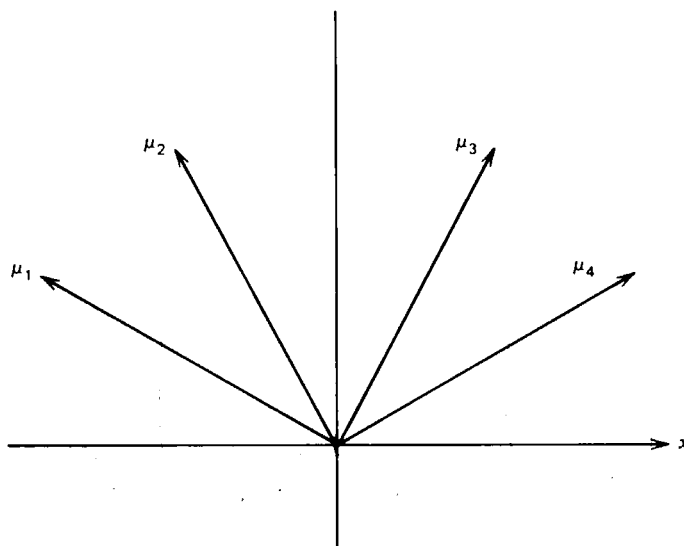


Fig. 8.1 □ S_4 (or P_4) quadrature set: $\mu_3 = -\mu_2 = .33998$, $\mu_4 = -\mu_1 = .86114$, $w_1 = w_4 = .34785$, $w_2 = w_3 = .65215$.

$\mu=0$ to lead to numerical difficulties. In addition, since the angular flux at $\mu=0$ is neither incoming nor outgoing, there would be some questions about the correct application of boundary conditions.

The possibility of a discontinuity in the angular flux at $\mu=0$ points out an apparent inconsistency, since Gaussian quadrature implicitly assumes that the integrand is continuous over the entire interval. But if the flux is discontinuous at $\mu=0$, the result of an integration by way of Gaussian quadrature could be significantly in error. In this case the analytical procedures for performing an integral with a discontinuous integrand (i.e., splitting up the integral into two or more separate integrals) suggests a better approach. One can split up the angular range into two parts, $-1 \leq \mu < 0$ and $0 < \mu \leq 1$, and perform Gaussian quadrature separately over each half-range. This approach, known as the double P_N method¹¹ in discrete ordinates (after a similar method in the spherical harmonics or P_N method—see Section 4.2.2) is used frequently for one dimensional slab problems. An example of the S_4 quadrature set is given in Figure 8.1. (See also Problem 8.8.)

Two Angle Quadrature Sets □ The choice of discrete directions $\{\hat{\Omega}_m\}$ and weights $\{w_m\}$ is complicated somewhat when two angles are necessary to specify a given direction $\hat{\Omega}_m$. In the most general situation, we must consider the entire unit sphere of directions (Figure 8.2). It is convenient to associate the weights w_m with an area on the unit sphere associated with the direction $\hat{\Omega}_m$. Such an “area” method derives sets of discrete directions

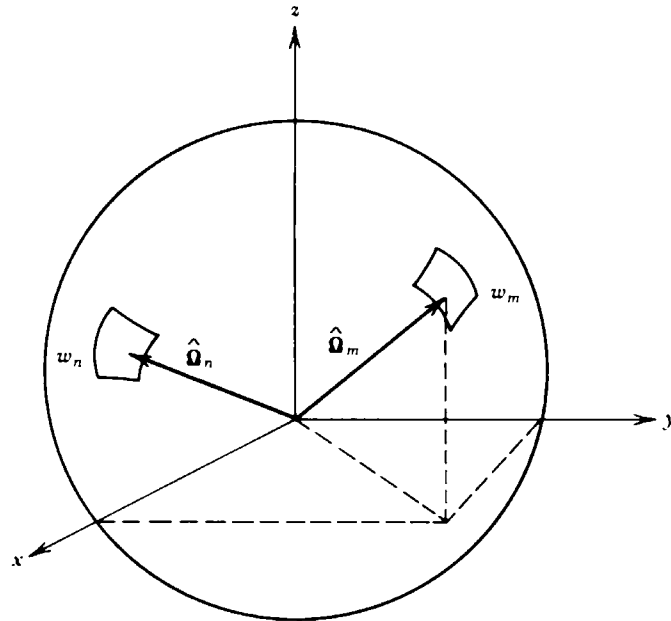


Fig. 8.2 □ Directions defined on the unit sphere.

$\{\hat{\Omega}_m\}$ and weights $\{w_m\}$ by representing the weights as explicit areas on the unit sphere and using projection invariance.¹² We consider briefly the restrictions placed on the set of directions and weights because of projection invariance, but further discussion of direction sets for two-angle applications must be sought in the references.

Let us consider a three-dimensional Cartesian geometry (see Figure 8.3), assuming no advance knowledge of the angular flux solution within the block. In this case our choice of the discrete directions $\{\hat{\Omega}_m\}$ should be independent of the labeling of the three axes. That is, we have no a priori reason to treat particles traveling in the $+z$ -direction any differently from particles traveling in the $-z$ - or $\pm x$ - or $\pm y$ -directions. Therefore the

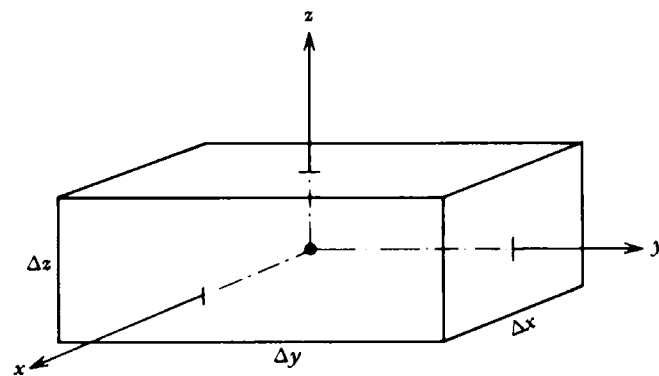


Fig. 8.3 □ Spatial mesh cell in Cartesian geometry.

angular direction set should be invariant under arbitrary 90° rotations (x to y , y to $-z$, etc.) about the coordinate axes, and 180° reflections about the xy , xz , or yz planes. This implies that each octant of the unit sphere is similar, therefore we need consider only one octant.⁸

Let us now denote the direction cosines with respect to the x , y , and z axes as μ , η , and ξ , respectively, and assume that we have chosen a direction set $\{\hat{\Omega}_m\}$ that satisfies the projection invariance restrictions discussed above. If we denote the direction $\hat{\Omega}_m$ with the direction cosine triplet (μ_m, η_m, ξ_m) , then since $\hat{\Omega}_m$ is a unit vector, we must have $\mu_m^2 + \eta_m^2 + \xi_m^2 = 1$. If we collect the set of μ 's for all the $\hat{\Omega}_m$'s (some μ 's may be repeated several times) and order them in some manner (e.g., $-1 < \mu_1 < \mu_2 < \dots < \mu_M < 1$), call this set $\{\mu_m\}$, and do the same for the η 's and the ξ 's, we must arrive at identical sets $\{\mu_m\} = \{\eta_m\} = \{\xi_m\}$ because the x , y , and z axes must not be distinguishable among one another with respect to the direction set $\{\hat{\Omega}_m\}$. Let us denote the unique set of direction cosines as $\{\alpha_m\}$. The reflection property implies that the direction cosine set $\{\alpha_m\}$ is symmetric about $\alpha = 0$. Apparently, then, we need only choose $\alpha_1, \alpha_2, \dots, \alpha_{M/2}$ to specify the direction cosines along all the coordinate axes, where we have denoted the positive direction cosines by $\alpha_1, \alpha_2, \dots, \alpha_{M/2}$. However, we learn shortly that there is actually only one degree of freedom, namely the choice of α_1 . Choosing α_1 is sufficient to specify $\alpha_2, \alpha_3, \dots, \alpha_{M/2}$ regardless of the number of direction cosines being used. These, in turn, will determine all the direction cosines.

The symmetric distribution of direction cosines forces the discrete directions $\hat{\Omega}_m$ to lie on latitudes (i.e., loci of constant μ , η , or ξ) on the unit sphere. This may be seen schematically in Figure 8.4, where one octant of the unit sphere is shown. The arrangement of points on the octant must be invariant under 120° rotations of the octant, and this corresponds to a rotation of one axis into the other. If the points were not arranged on latitudes, this condition would not be satisfied.

Let us now demonstrate that the specification of one direction cosine α_1 uniquely determines all direction cosines if projection invariance is satisfied.¹² Assume that we are at a discrete direction $\hat{\Omega}_a = (\mu_i, \eta_j, \xi_k)$, and we traverse along the μ_i latitude in the direction of increasing η latitude to the next discrete direction $\hat{\Omega}_b$. By hypothesis, we are at μ_i and η_{j+1} , and clearly the ξ value must be ξ_{k-1} because both latitudes cannot increase (or decrease) while the other latitude is constant. Consideration of Figure 8.4 may aid in visualizing this argument. Therefore $\hat{\Omega}_b = (\mu_i, \eta_{j+1}, \xi_{k-1})$. But we have noted the equivalence of the sets $\{\mu_m\} = \{\eta_m\} = \{\xi_m\} = \{\alpha_m\}$. Therefore $\hat{\Omega}_a = (\alpha_i, \alpha_j, \alpha_k)$ and $\hat{\Omega}_b = (\alpha_i, \alpha_{j+1}, \alpha_{k-1})$. Furthermore, the restriction that $\mu^2 + \eta^2 + \xi^2 = 1$ implies that

$$\alpha_i^2 + \alpha_j^2 + \alpha_k^2 = 1, \quad \alpha_i^2 + \alpha_{j+1}^2 + \alpha_{k-1}^2 = 1$$

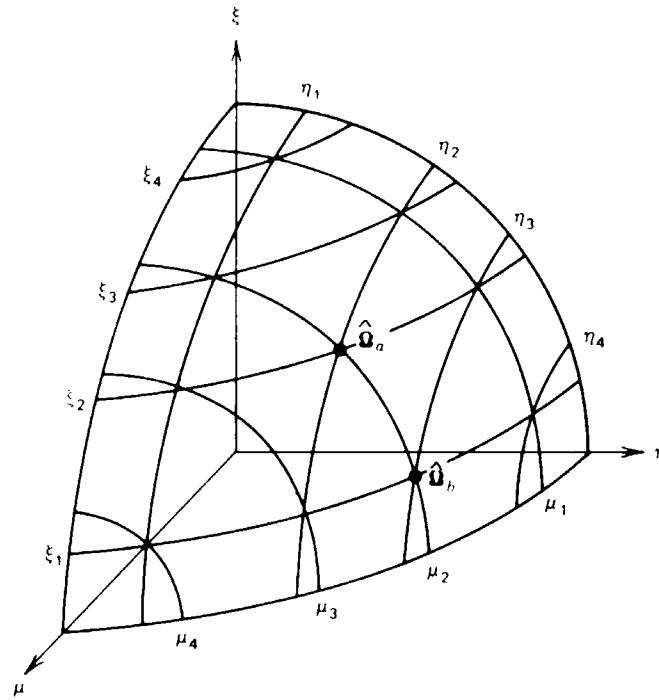


Fig. 8.4 □ Symmetric point arrangement on one octant of unit sphere.

Subtracting these two equations, we find

$$\alpha_{j+1}^2 - \alpha_j^2 = \alpha_k^2 - \alpha_{k-1}^2 \quad (8.5)$$

Since i, j , and k were arbitrary, Eq. 8.5 implies that

$$\alpha_i^2 = \alpha_{i-1}^2 + C$$

for all i , or

$$\alpha_i^2 = \alpha_1^2 + C(i-1) \quad (8.6)$$

But if we have M direction cosines along each axis, there is a direction $\hat{\Omega}_m$ corresponding to $(\alpha_1, \alpha_1, \alpha_{M/2})$ because there are $M/2$ points for $\alpha > 0$. This implies

$$\alpha_1^2 + \alpha_1^2 + \alpha_{M/2}^2 = 1 \quad (8.7)$$

Then if we combine Eq. 8.6 with Eq. 8.7, we can evaluate the constant C as follows:

$$C = \frac{2(1 - 3\alpha_1^2)}{M - 2}$$

Thus the specification of α_1 determines the remaining α_j , $j=2, \dots, M/2$. We can tailor the points to be clustered close to $\alpha=0$ by choosing α_1 large ($\leq 1/\sqrt{3}$) or clustered near the poles $\alpha = \pm 1$ by choosing α_1 to be small.

Projection invariance also forces the weights to be symmetric with respect to rotations and reflections. Instead of discussing this issue further, however, we direct the interested reader to more detailed references on this subject.^{12,13} From a more practical point of view, it should be noted that a variety of quadrature sets are usually supplied with the more popular discrete ordinates transport computer codes.

8.1.2 □ Derivation and Solution of the Discretized Equations □ The previous sections have discussed the derivation of the discrete ordinates equations from the transport equation and have considered the choice of quadrature sets $\{\hat{\Omega}_m, w_m\}$ for one- and multidimensional geometries. We are now in a position to solve the resultant system of discrete ordinates equations, assuming that we have chosen a suitable set of discrete directions and weights. We must discretize the remaining variables in this system of coupled partial differential equations (i.e., the discrete ordinates equations) to arrive at an equivalent set of algebraic equations, which can then be solved on a digital computer.

To simplify this discussion, we assume isotropic scattering (for the present) so that the discrete ordinates equations can be written as

$$\hat{\Omega}_m \cdot \nabla \varphi(\mathbf{r}, \hat{\Omega}_m) + \Sigma_t(\mathbf{r}) \varphi(\mathbf{r}, \hat{\Omega}_m) = (4\pi)^{-1} \Sigma_s(\mathbf{r}) \sum_{n=1}^M w_n \varphi(\mathbf{r}, \hat{\Omega}_n) + s(\mathbf{r}, \hat{\Omega}_m) \quad \text{for } m = 1, 2, \dots, M \quad (8.8)$$

We first consider the simple case of one-dimensional plane geometries, since many of the principles illustrated in connection with this application hold for more general geometries.

One-Dimensional Plane Geometry □ For the case of one-dimensional slab geometry with azimuthal symmetry (see Figure 8.5) the transport equation becomes

$$\mu \frac{\partial \varphi}{\partial x} + \Sigma_t(x) \varphi(x, \mu) = \frac{1}{2} \Sigma_s(x) \int_{-1}^{+1} d\mu' \varphi(x, \mu') + s(x, \mu)$$

and the corresponding discrete ordinates equations are

$$\mu_m \frac{d}{dx} \varphi(x, \mu_m) + \Sigma_t(x) \varphi(x, \mu_m) = \frac{1}{2} \Sigma_s(x) \sum_{n=1}^M w_n \varphi(x, \mu_n) + s(x, \mu_m), \quad m = 1, 2, \dots, M \quad (8.9)$$

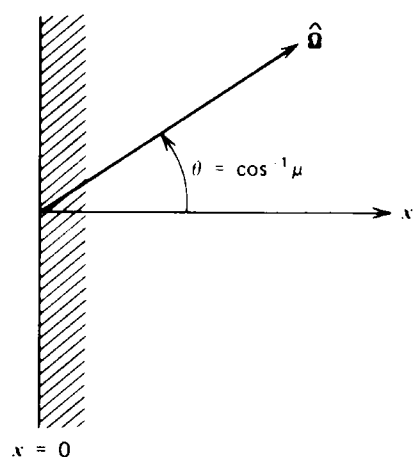


Fig. 8.5 □ One-dimensional slab geometry.

A variety of boundary conditions may be applied to the left and right sides of the slab. For purposes of illustration, we assume a reflecting boundary at $x=0$ and a vacuum boundary at $x=a$. Table 8.2 contains the one-dimensional versions of the other standard boundary conditions, which may be used with only minor modifications to the following discussion.

The discretized equations are derived by applying finite difference techniques directly to Eq. 8.9. The next section reveals that such a direct application of finite difference methods to the transport equation in curvilinear geometries may lead to a nonconservative difference scheme in that the resultant finite difference equations may not conserve the total number of particles in a computational cell. In such cases it is advisable to derive the discretized equations using a particle balance argument for each mesh cell (similar in spirit to the original derivation of the transport equation in Chapter 1). This approach is illustrated later for both one-dimensional spherical geometry and general two-dimensional geometries.

To proceed with the direct discretization of Eq. 8.9, we introduce a spatial mesh $x_1, x_2, \dots, x_I$, where x_i is the midpoint of the i th mesh cell (see Figure 8.6). The boundaries of the i th cell, which also coincide with any material boundaries, are labeled $x_{i \pm 1/2}$. Equation 8.9 is then approximated for each mesh cell with a cell-centered finite difference expression for the derivative term $\mu_m d\varphi/dx$ and cell-averaged expressions for the remaining terms

$$\begin{aligned} \mu_m \left(\frac{\varphi(x_{i+1/2}, \mu_m) - \varphi(x_{i-1/2}, \mu_m)}{x_{i+1/2} - x_{i-1/2}} \right) + \Sigma_i(x_i) \varphi(x_i, \mu_m) \\ = \frac{1}{2} \Sigma_s(x_i) \sum_{n=1}^M w_n \varphi(x_i, \mu_n) + s(x_i, \mu_m), \quad \begin{matrix} m = 1, 2, \dots, M \\ i = 1, 2, \dots, I \end{matrix} \end{aligned}$$

Table 8.2 □ Discrete Ordinate Boundary Conditions for One-Dimensional Plane Geometry

Vacuum

$$\varphi_m^{1/2} = 0, \quad m > \frac{M}{2}; \quad \varphi_m^{I+1/2} = 0, \quad m \leq \frac{M}{2}$$

Inhomogeneous

$$\varphi_m^{1/2} = f_m, \quad m > \frac{M}{2}; \quad \varphi_m^{I+1/2} = f_m, \quad m \leq \frac{M}{2}$$

Reflecting ($\alpha = 1$) or albedo

$$\varphi_m^{1/2} = \alpha \varphi_{M-m+1}^{1/2}, \quad m > \frac{M}{2}; \quad \varphi_m^{I+1/2} = \alpha \varphi_{M-m+1}^{I+1/2}, \quad m \leq \frac{M}{2}$$

Periodic

$$\varphi_m^{1/2} = \varphi_m^{I+1/2}, \quad m > \frac{M}{2}; \quad \varphi_m^{I+1/2} = \varphi_m^{1/2}, \quad m \leq \frac{M}{2}$$

White

$$\varphi_m^{1/2} = \frac{\sum_{n=1}^{M/2} w_n \varphi_n^{1/2} \mu_n}{\sum_{n=1}^{M/2} w_n \mu_n}, \quad m > \frac{M}{2}; \quad \varphi_m^{I+1/2} = \frac{\sum_{n=M/2+1}^M w_n \varphi_n^{I+1/2} \mu_n}{\sum_{n=M/2+1}^M w_n \mu_n}, \quad m \leq \frac{M}{2}$$

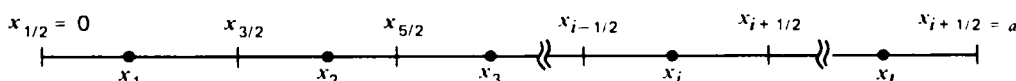
or in an obvious notation

$$\mu_m \left(\frac{\varphi_m^{i+1/2} - \varphi_m^{i-1/2}}{\Delta x_i} \right) + \sum_i^i \varphi_m^i = \frac{1}{2} \sum_{n=1}^M w_n \varphi_n^i + s_m^i \equiv q_m^i \quad (8.10)$$

Notice that Eq. 8.10 represents IM equations in $(2I+1)M$ unknowns. To reduce the number of unknowns, we relate the cell-centered fluxes φ_m^i to the cell-edged fluxes $\varphi_m^{i\pm 1/2}$ by a simple arithmetic mean expression

$$\varphi_m^i = \frac{\varphi_m^{i+1/2} + \varphi_m^{i-1/2}}{2} \quad (8.11)$$

This relation is the one-dimensional version of the well known “diamond

**Fig. 8.6 □ Spatial mesh for discretization of discrete ordinates equations in plane geometry.**

difference" scheme.⁶ If we now substitute Eq. 8.11 into Eq. 8.10, we arrive at

$$\mu_m \left(\frac{\varphi_m^{i+1/2} - \varphi_m^{i-1/2}}{\Delta x_i} \right) + \Sigma_i \left(\frac{\varphi_m^{i+1/2} + \varphi_m^{i-1/2}}{2} \right) = q_m^i \quad (8.12)$$

We have chosen not to express q_m^i in terms of the cell-edged fluxes because the iterative solution method Eq. 8.3 proceeds by assuming that q_m^i is known, then updating this quantity with each iteration.

The set of equations (8.12) now contains $(I+1)M$ unknowns, since we have utilized Eq. 8.11 to eliminate IM unknowns. The boundary conditions on the $M/2$ incoming fluxes at each boundary provide the additional M equations to complete the set and allow a solution. Equation 8.12 can be solved for either $\varphi_m^{i+1/2}$ or $\varphi_m^{i-1/2}$

$$\varphi_m^{i+1/2} = \left(\frac{1 - \Sigma_i \Delta x_i / 2\mu_m}{1 + \Sigma_i \Delta x_i / 2\mu_m} \right) \varphi_m^{i-1/2} + \frac{q_m^i}{\mu_m / \Delta x_i + \Sigma_i / 2} \quad (8.13)$$

$$\varphi_m^{i-1/2} = \left(\frac{1 + \Sigma_i \Delta x_i / 2\mu_m}{1 - \Sigma_i \Delta x_i / 2\mu_m} \right) \varphi_m^{i+1/2} + \frac{q_m^i}{-\mu_m / \Delta x_i + \Sigma_i / 2} \quad (8.14)$$

It is crucial to choose the proper equation (8.13) or (8.14) as the basis for the iterative solution. This choice will be determined by the particular direction μ_m being considered. If we note that boundary conditions are imposed on the incoming boundaries, it is apparent that we should advance the solution away from the incoming boundaries and in the direction of neutron motion. That is, if we know the incoming flux at $x=a$, $\varphi_m^{I+1/2}$ for $\mu_m < 0$, we are forced to use Eq. 8.14 because otherwise Eq. 8.13 would yield $\varphi_m^{I+3/2}$, which is not a valid flux. Similarly, if we know the incoming fluxes at $x=0$, $\varphi_m^{1/2}$, $\mu_m > 0$, we must use Eq. 8.13. In summary, then, we would choose Eq. 8.13 for $\mu_m > 0$ and Eq. 8.14 for $\mu_m < 0$.

These arguments remain valid for the case of implicit boundary conditions (e.g., reflecting or periodic boundary conditions). For example, if we had specified a reflecting boundary condition at $x=0$ and an inhomogeneous boundary condition at $x=a$, we would begin with the known fluxes at $x=a$, $\varphi_m^{I+1/2}$, $\mu_m < 0$, and progress through the slab to $x=0$. At this point we would have computed the outgoing flux at $x=0$, $\varphi_m^{1/2}$, $\mu_m < 0$. We could then impose the reflecting boundary condition $\varphi_{M-m+1}^{1/2} = \varphi_m^{1/2}$ and use Eq. 8.14 to proceed back across the slab toward $x=a$. This scheme is represented schematically in Figure 8.7.

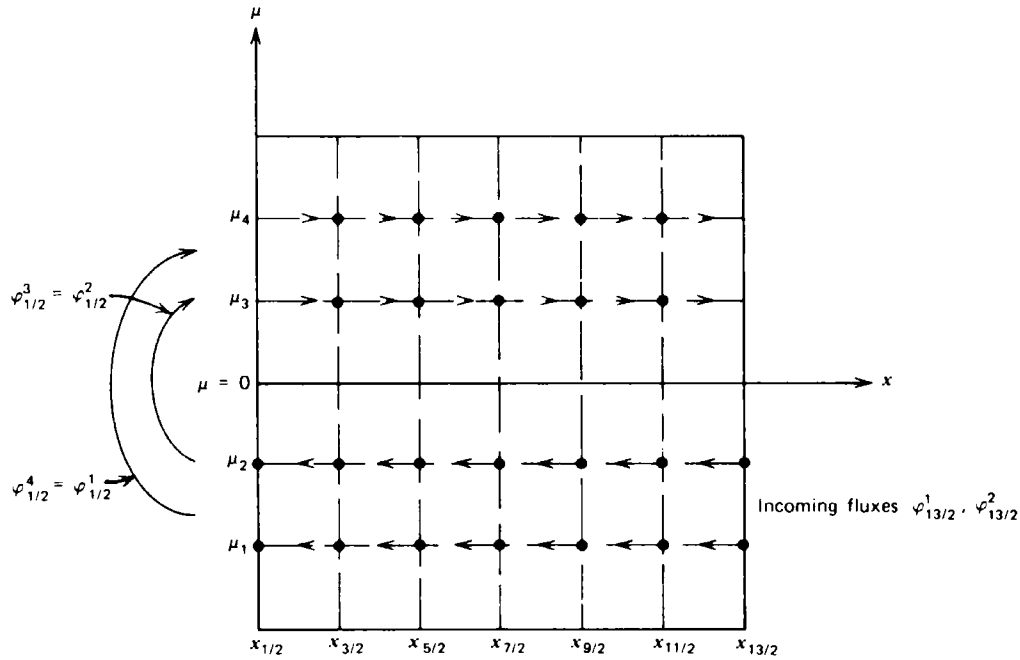


Fig. 8.7 □ Solution strategy for plane geometry.

If there are implicit boundary conditions on both sides, a less direct approach must be taken. One can iterate on a guessed boundary flux, which is then used to calculate the interior fluxes. Other procedures may also be used for this case.⁹ However the significant point is that we still use Eq. 8.13 for $\mu_m > 0$ and Eq. 8.14 for $\mu_m < 0$, regardless of the choice of boundary conditions.

This particular choice is also required to ensure the numerical stability of the solution algorithm. This may be illustrated for the simple case of a homogeneous slab with constant mesh spacing, zero source, and a known incoming flux at $x=0$. In this case $\varphi_m^{i+1/2}$ can be expressed in terms of the boundary flux $\varphi_m^{1/2}$ using Eq. 8.13:

$$\varphi_m^{i+1/2} = \left(\frac{1 - \sum_l \Delta x / 2\mu_m}{1 + \sum_l \Delta x / 2\mu_m} \right)^i \varphi_m^{1/2}$$

Now if there is some error ε in the initial flux, say $\tilde{\varphi}_m^{1/2} = \varphi_m^{1/2} + \varepsilon$, then clearly the error in the solution $\varphi_m^{i+1/2}$ is damped because for $\mu_m > 0$,

$$\varepsilon_i = \left(\frac{1 - \sum_l \Delta x / 2\mu_m}{1 + \sum_l \Delta x / 2\mu_m} \right)^i \varepsilon$$

However if we had chosen Eq. 8.14 to compute $\varphi_m^{i+1/2}$, the resultant error would have been

$$\varepsilon_i = \left(\frac{1 + \sum_i \Delta x / 2\mu_m}{1 - \sum_i \Delta x / 2\mu_m} \right)^i \varepsilon$$

In this case the initial error in the solution would have been amplified by the choice of the wrong difference scheme; that is, the difference scheme would be unstable. Note that even if the initial solution were known exactly, a computer would generate some roundoff error for its representation of the initial solution; therefore there would be an initial disturbance in the solution that could easily be magnified by an unstable scheme, destroying the calculation.

Another desirable property of such difference schemes is positivity, an attribute of a difference scheme that results in a positive solution for any positive source. Since the analytical angular flux is always positive, it is desirable to ensure (if possible) that the numerical approximation is also positive. To be more explicit, let us consider the positivity of the diamond difference scheme represented by Eqs. 8.13 and 8.14. Examination of Eq. 8.13 indicates that for $q_m^i > 0$ and $\varphi_m^{i-1/2} > 0$, the condition

$$\frac{\sum_i \Delta x_i}{2\mu_m} \leq 1 \quad (8.15)$$

will guarantee that $\varphi_m^{i+1/2} > 0$. (Note that we have $\mu_m > 0$ when using Eq. 8.13.) In other words, the diamond difference scheme in one-dimensional plane geometry is positive if Eq. 8.15 is satisfied. In practice, however, it is difficult to meet this constraint because the quadrature point μ_m with smallest magnitude may be quite close to zero. By way of example, for S_{16} quadrature the smallest direction cosine is $\mu_m = 0.095$ which, when substituted into Eq. 8.15, implies a mesh spacing $\Delta x_i \leq 0.2 / \sum_i$ —that is, a mesh spacing less than one-fifth of a mean free path. This rather severe restriction for the spatial mesh clearly could result in significant increases in computing effort. Furthermore, in two-dimensional geometries it can be shown that the diamond difference scheme cannot be guaranteed to be positive.⁶ As a consequence of this feature, most discrete ordinates codes have some form of “negative flux fixup” prescription to treat negative fluxes if they appear during a calculation. These “fixup” schemes all involve local modifications of the difference schemes whenever a negative flux is encountered.

The simplest such fixup scheme merely sets the offending flux equal to zero. This may seem to be somewhat artificial, but actually it should be

kept in mind that a zero flux is probably the best approximation to the actual solution, since the computed negative flux is based on the accurate diamond difference scheme.

An alternative fixup procedure involves switching to a positive difference scheme whenever negative fluxes are encountered. To be more explicit, let us generalize the diamond difference relations (8.11) that express the cell-centered flux in terms of the cell-edged fluxes by including a weighting factor α :¹⁴

$$\begin{aligned}\varphi_m^i &= \alpha \varphi_m^{i+1/2} + (1 - \alpha) \varphi_m^{i-1/2}, & \mu_m > 0 \\ \varphi_m^i &= \alpha \varphi_m^{i-1/2} + (1 - \alpha) \varphi_m^{i+1/2}, & \mu_m < 0\end{aligned}\quad (8.16)$$

Notice here that choosing $\alpha = \frac{1}{2}$ results in the diamond difference relations, Eq. 8.11.

Now let us assume that $q_m^i = 0$ and that we are considering the case $\mu_m > 0$. If we substitute Eq. 8.16 into Eq. 8.10 and solve for $\varphi_m^{i+1/2}$, we find

$$\varphi_m^{i+1/2} = \left(\frac{1 - (1 - \alpha) \Sigma_i^j \Delta x_i / \mu_m}{1 + \alpha \Sigma_i^j \Delta x_i / \mu_m} \right) \varphi_m^{i-1/2}$$

Clearly, $\varphi_m^{i+1/2} > 0$ if $\alpha = 1$ and $\varphi_m^{i-1/2} > 0$. Therefore the weighted diamond difference relations are strictly positive for $\alpha = 1$. This “step function” scheme may be substituted for the diamond difference scheme whenever $\varphi_m^{i+1/2}$ is negative. Once a positive $\varphi_m^{i+1/2}$ is obtained, one can switch back to the usual diamond difference scheme ($\alpha = \frac{1}{2}$). This prescription to avoid negative fluxes is included as an option in discrete ordinates computer codes such as ANISN.¹⁵ There is a disadvantage, however, in that the resulting difference scheme is no longer of second order accuracy in the mesh spacing. Therefore we must sacrifice accuracy for positivity—which is a frequent tradeoff in the application of discrete ordinates methods.

We have explicitly solved the resulting finite difference relations Eqs. 8.13 and 8.14 in the direction of neutron motion. The net effect of this prescription is that the matrix of coefficients **A** has been rearranged into a lower triangular form and simply inverted by progressing through the space angle mesh. But we have not yet addressed the fact that the source term q_m^i contains the unknown flux φ_m^i in the inscatter term as indicated by Eq. 8.10. As we noted earlier, however, an iterative strategy is used to update the inscatter and source terms as follows:

- i Estimate the initial source $q_m^{i(0)}$.
- ii Use Eqs. 8.13 and 8.14 as appropriate to solve for the first flux iterate $\varphi_m^{i(1)}$ for all i and m .

iii Reconstruct the source terms for all i, m as

$$q_m^{i(1)} = \frac{1}{2} \sum_s^i \sum_{n=1}^M w_n \varphi_n^{i(1)} + s_m^i$$

iv Repeat step ii and compute $\varphi_m^{i(2)}$ for all i, m .

(This procedure can readily be generalized to include anisotropic scattering or implicit source terms such as those due to fission.)

In practice one accumulates the inscattering and source terms as the computation advances through the mesh. In this way the angular flux need not be stored except for the components necessary for the calculation in an adjacent mesh cell.

In summary, we have described in some detail the derivation and solution of the discretized discrete ordinates equations in one-dimensional slab geometry. But several of the principles discussed in this section are also applicable to more general geometries: the solution of the discretized equations in the direction of particle motion is a general requirement for numerical stability and is equivalent to arranging the equations in such a way that the coefficient matrix becomes lower triangular. Furthermore, the assurance of positivity of a difference scheme may place undue restrictions on the mesh spacing or may force one to sacrifice accuracy to obtain positivity. Finally, the method of source iterations is necessary to obtain a lower triangular coefficient matrix, which, in turn, is necessary for an efficient solution algorithm.

One-Dimensional Spherical Geometry □ Let us now consider a spherically symmetric problem in which we can describe the angular dependence of the flux by one variable, the direction cosine with respect to the r -axis (see Figure 8.8). We have noted that a direct application of finite difference approximations can lead to nonconservative difference equations. Therefore we rederive the finite difference equations for one-dimensional spherical geometry by implementing particle balance conditions for each mesh cell. It can be shown that in the limit of infinitesimal mesh cells, the resulting finite difference equations become identical with a particular form of the transport equation in one-dimensional spherical geometries. This equation, known as the “conservative form” of the transport equation, has the following attractive feature: it leads to conservative finite difference equations when subjected to the standard difference approximations. We conclude this section by discussing how such difference equations can be solved.

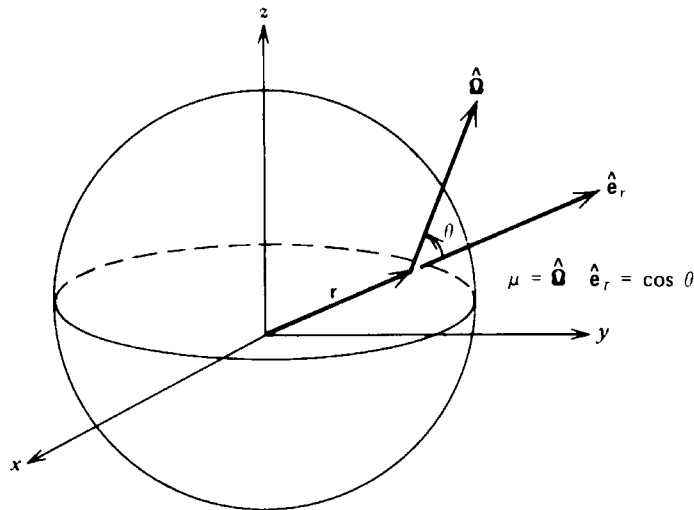


Fig. 8.8 □ Spherical geometry.

Let us begin by considering a spherical mesh cell of thickness Δr_i , volume ΔV_i , and centered at radius r_i . The inner and outer radii of the cell are $r_{i+1/2}$ and $r_{i-1/2}$, respectively. We also need an angular mesh cell centered at μ_m with “volume” $\Delta\mu_m$, which can be identified as simply the quadrature weight $w_m = \Delta\mu_m$. The angular volume is necessary because we must account for the phenomenon of ray-to-ray transfer of particles (so-called angular redistribution). This phenomenon occurs because the angular coordinate system is defined relative to the radius vector $\mathbf{r}$; therefore it is not fixed in space. That is, a particle that is streaming along a straight-line trajectory will have different direction vectors $\hat{\Omega}$ in the angular coordinate system defined with respect to $\mathbf{r}$. This tendency of a particle to experience a change in its direction cosine during streaming is illustrated in Figure 8.9. This will give rise to a transfer of particles between “adjacent” angular mesh cells.

We now equate particle gain to losses in the phase space volume $\Delta V_i \Delta\mu_m$. More explicitly, the net gain of neutrons in $\Delta V_i \Delta\mu_m$ due to streaming across the spatial edges at $r_{i \pm 1/2}$ is easily computed as

$$\begin{aligned} \text{gain} = & -\hat{\Omega}_m \cdot \hat{\mathbf{e}}_r \left[\varphi\left(r_i + \frac{\Delta r_i}{2}, \mu_m\right) 4\pi \left(r_i + \frac{\Delta r_i}{2}\right)^2 \right. \\ & \left. - \varphi\left(r_i - \frac{\Delta r_i}{2}, \mu_m\right) 4\pi \left(r_i - \frac{\Delta r_i}{2}\right)^2 \right] \Delta\mu_m \end{aligned}$$

(note that this term may be negative, thereby representing a loss). The gain

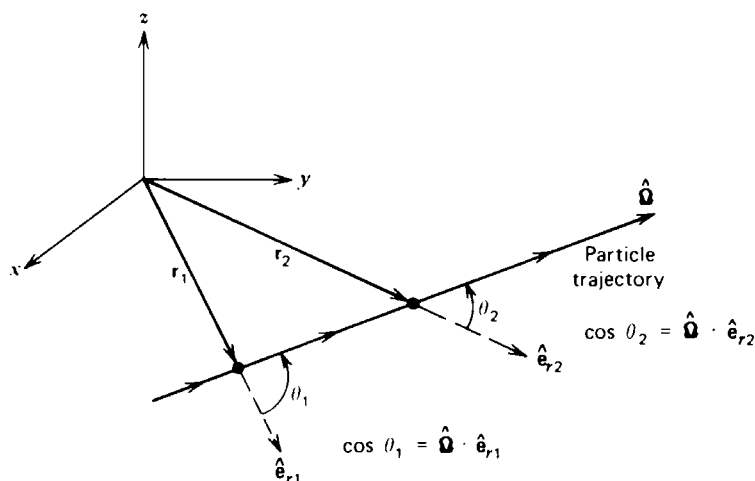


Fig. 8.9 □ Change in direction cosine during particle streaming in curvilinear coordinate system.

due to neutrons that suffer a scattering collision in ΔV_i and end up in $\Delta\mu_m$ can be obtained by adding up all the scattering collisions (including self-scatter):

$$\text{gain} = \sum_{n=1}^M [\varphi(r_i, \mu_n) \Delta\mu_n] [\Sigma_s(r_i) P(\mu_n \rightarrow \mu_m) \Delta\mu_m]$$

where $P(\mu_n \rightarrow \mu_m) / \Delta\mu_m$ is the probability that the scattering collision will transfer a particle from direction μ_n to $\Delta\mu_m$. The loss due to neutrons in $\Delta\mu_m$ that suffer any collision in ΔV_i is just

$$\text{loss} = \varphi(r_i, \mu_m) \Delta\mu_m \Sigma_t(r_i) 4\pi r_i^2 \Delta r_i$$

and the gain due to external sources is

$$\text{gain} = s(r_i, \mu_m) 4\pi r_i^2 \Delta r_i \Delta\mu_m$$

Finally we turn to the net gain of particles in ΔV_i due to angular redistribution of particles from $\Delta\mu_{m-1}$ to $\Delta\mu_m$ across $\mu_{m-1/2}$ and from $\Delta\mu_m$ to $\Delta\mu_{m+1}$ across $\mu_{m+1/2}$. (Here the directions are ordered so that redistribution takes place only in the direction of increasing m .) To compute this term, we define effective areas $\alpha_{m\pm 1/2}$ at $\mu_{m\pm 1/2}$, which, when multiplied by $\varphi(r_i, \mu_{m\pm 1/2})$, result in the net number of particles leaving (–) or entering (+) $\Delta V_i \Delta\mu_m$.^{7,8} (These “areas” are evaluated below.) The net gain

term due to angular redistribution can then be written as

$$\varphi\left(r_i, \mu_m - \frac{\Delta\mu_m}{2}\right)\alpha_{m-1/2} - \varphi\left(r_i, \mu_m + \frac{\Delta\mu_m}{2}\right)\alpha_{m+1/2}$$

If we now equate the loss and gain terms, we find

$$\begin{aligned} & 4\pi\mu_m\Delta\mu_m\left[\varphi\left(r_i + \frac{\Delta r_i}{2}, \mu_m\right)\left(r_i + \frac{\Delta r_i}{2}\right)^2 - \varphi\left(r_i - \frac{\Delta r_i}{2}, \mu_m\right)\left(r_i - \frac{\Delta r_i}{2}\right)^2\right] \\ & + \varphi\left(r_i, \mu_m + \frac{\Delta\mu_m}{2}\right)\alpha_{m+1/2} - \varphi\left(r_i, \mu_m - \frac{\Delta\mu_m}{2}\right)\alpha_{m-1/2} \\ & + \Sigma_t(r_i)4\pi r_i^2\Delta r_i\Delta\mu_m\varphi(r_i, \mu_m) \\ & = \sum_{n=1}^M \varphi(r_i, \mu_n)\Delta\mu_n\Sigma_s(r_i)P(\mu_n \rightarrow \mu_m)\Delta\mu_m4\pi r_i^2\Delta r_i + s(r_i, \mu_m)4\pi r_i^2\Delta r_i\Delta\mu_m \end{aligned} \quad (8.17)$$

For convenience, we assume isotropic scattering $P(\mu_n \rightarrow \mu_m) = \frac{1}{2}$, then divide Eq. 8.17 by $4\pi r_i^2\Delta r_i\Delta\mu_m$ to obtain

$$\begin{aligned} & \frac{\mu_m}{r_i^2} \left[\frac{\varphi\left(r_i + \frac{\Delta r_i}{2}, \mu_m\right)\left(r_i + \frac{\Delta r_i}{2}\right)^2 - \varphi\left(r_i - \frac{\Delta r_i}{2}, \mu_m\right)\left(r_i - \frac{\Delta r_i}{2}\right)^2}{\Delta r_i} \right] \\ & + \frac{1}{4\pi r_i^2\Delta r_i} \left[\frac{\varphi\left(r_i, \mu_m + \frac{\Delta\mu_m}{2}\right)\alpha_{m+1/2} - \varphi\left(r_i, \mu_m - \frac{\Delta\mu_m}{2}\right)\alpha_{m-1/2}}{\Delta\mu_m} \right] \\ & + \Sigma_t(r_i)\varphi(r_i, \mu_m) = \frac{1}{2}\Sigma_s(r_i) \sum_{n=1}^M \varphi(r_i, \mu_n)\Delta\mu_n + s(r_i, \mu_m) \end{aligned} \quad (8.18)$$

Equation 8.18 is the required finite difference equation, but we have still to determine the $\alpha_{m\pm 1/2}$ terms. These angular area terms are evaluated by considering the case of divergenceless flow in an infinite absorbing medium with a constant source, that is,

$$\Sigma_a\varphi(\mathbf{r}, \hat{\Omega}) = s(\mathbf{r}, \hat{\Omega}) = \frac{S_0}{4\pi}$$

This yields a constant angular flux

$$\varphi(\mathbf{r}, \hat{\Omega}) = \frac{S_0}{4\pi \Sigma_a} = \text{constant}$$

The numerical approximation to this case should also result in a constant flux, and the finite difference expressions for the streaming operator should vanish. If we apply Eq. 8.18 to this problem, we find

$$\left(\frac{\mu_m}{r_i^2}\right) \frac{\left(r_i + \frac{\Delta r_i}{2}\right)^2 - \left(r_i - \frac{\Delta r_i}{2}\right)^2}{\Delta r_i} + \left(\frac{1}{4\pi r_i^2 \Delta r_i}\right) \left(\frac{\alpha_{m+1/2} - \alpha_{m-1/2}}{\Delta \mu_m}\right) = 0$$

This can be rearranged as

$$\alpha_{m+1/2} - \alpha_{m-1/2} = -\mu_m \Delta \mu_m 8\pi r_i \Delta r_i \quad (8.19)$$

We now redefine the α terms as follows:

$$\alpha_{m \pm 1/2} \rightarrow \alpha_{m \pm 1/2} (8\pi r_i \Delta r_i)^{-1}$$

so that Eq. 8.19 can be rewritten as follows:

$$\alpha_{m+1/2} - \alpha_{m-1/2} = -\mu_m \Delta \mu_m$$

This redefinition of α is clearly allowed when we remember that α was originally defined in terms of an equivalent “area,” and we are simply normalizing this original definition for convenience.

With this definition of the α term, Eq. 8.18 becomes

$$\begin{aligned} & \left(\frac{\mu_m}{r_i^2}\right) \left[\frac{\varphi\left(r_i + \frac{\Delta r_i}{2}, \mu_m\right) \left(r_i + \frac{\Delta r_i}{2}\right)^2 - \varphi\left(r_i - \frac{\Delta r_i}{2}, \mu_m\right) \left(r_i - \frac{\Delta r_i}{2}\right)^2}{\Delta r_i} \right] \\ & + \left(\frac{2}{r_i}\right) \left[\frac{\varphi\left(r_i, \mu_m + \frac{\Delta \mu_m}{2}\right) \alpha_{m+1/2} - \varphi\left(r_i, \mu_m - \frac{\Delta \mu_m}{2}\right) \alpha_{m-1/2}}{\Delta \mu_m} \right] \\ & + \Sigma_s(r_i) \varphi(r_i, \mu_m) = \frac{1}{2} \Sigma_s(r_i) \sum_{n=1}^M \varphi(r_i, \mu_n) \Delta \mu_n + s(r_i, \mu_m) \end{aligned} \quad (8.20)$$

Notice that the angular redistribution can only take place in the direction

of increasing μ . That is, if a particle is streaming outward ($\mu > 0$), then as r increases, μ increases. Conversely, if the particle is streaming inward ($\mu < 0$), then as r decreases, μ increases (becomes less negative). It should be noted that there is no angular redistribution out of $\mu = +1$ or into $\mu = -1$. Therefore we should have zero areas for these limiting cases, $\alpha_{1/2} = \alpha_{M+1/2} = 0$. The first condition, $\alpha_{1/2} = 0$ initiates the recursion formula ($\alpha_{m+1/2} - \alpha_{m-1/2} = -\mu_m \Delta\mu_m$) and allows the calculation of the remaining α terms. If the $\{\mu_m\}$ direction set is symmetric about $\mu = 0$, the recursion formula will also result in $\alpha_{M+1/2} = 0$ if $\alpha_{1/2} = 0$.

If we define $\varphi_{m\pm 1/2}^i \equiv \varphi(r_i, \mu_m \pm \Delta\mu_m/2)$, the angular redistribution portion of the discretized streaming operator in Eq. 8.18 can be written (using the redefined α terms) as

$$A_m^i = \frac{2}{r_i} \left(\frac{\varphi_{m+1/2}^i \alpha_{m+1/2} - \varphi_{m-1/2}^i \alpha_{m-1/2}}{\Delta\mu_m} \right) \quad (8.21)$$

If we multiply A_m^i by $\Delta\mu_m$ and sum over all m , we obtain

$$\begin{aligned} \sum_{m=1}^M A_m^i \Delta\mu_m &= \frac{2}{r_i} \sum_{m=1}^M (\varphi_{m+1/2}^i \alpha_{m+1/2} - \varphi_{m-1/2}^i \alpha_{m-1/2}) \\ &= \frac{2}{r_i} (\varphi_{M+1/2}^i \alpha_{M+1/2} - \varphi_{1/2}^i \alpha_{1/2}) = 0 \quad \text{if } \alpha_{M+1/2} = \alpha_{1/2} = 0 \end{aligned}$$

But this is essentially a statement that there is no net gain or loss of particles due to angular redistribution. Therefore the foregoing difference scheme for the angular redistribution term Eq. 8.21 is conservative.

We now demonstrate that in the limit of infinitesimal mesh cells (i.e., $\Delta r_i \rightarrow 0$ and $\Delta\mu_m \rightarrow 0$), the discretized equation (8.20) is indeed equivalent to the analytical one-dimensional spherical transport equation.⁸ To show this, we take the limit of each of the terms in Eq. 8.20 as $\Delta r_i, \Delta\mu_m \rightarrow 0$:

$$\begin{aligned} \lim_{\Delta r \rightarrow 0} \left(\frac{\mu_m}{r_i^2 \Delta r_i} \right) r^2 \varphi(r, \mu_m) \bigg|_{r_i - \Delta r_i/2}^{r_i + \Delta r_i/2} &= \frac{\mu}{r^2} \frac{\partial}{\partial r} (r^2 \varphi) \\ \lim_{\Delta\mu_m \rightarrow 0} \frac{1}{2} \Sigma_s(r_i) \sum_{n=1}^M \varphi(r_i, \mu_n) \Delta\mu_n &= \frac{1}{2} \Sigma_s(r) \int_{-1}^{+1} d\mu \varphi(r, \mu) \end{aligned}$$

If we note that α is a function of μ [i.e., $\alpha_{m+1/2} = \alpha(\mu_m + \Delta\mu_m/2)$], the

angular redistribution term becomes

$$\lim_{\Delta\mu_m \rightarrow 0} \left(\frac{2}{r_i \Delta\mu_m} \right) \alpha(\mu) \varphi(r_i, \mu) \bigg|_{\mu_m - \Delta\mu_m/2}^{\mu_m + \Delta\mu_m/2} = \frac{2}{r} \frac{\partial}{\partial \mu} (\alpha \varphi)$$

To determine the continuous form of the α function, we take the limit of $(\alpha_{m+1/2} - \alpha_{m-1/2} = -\mu_m \Delta\mu_m)$ as $\Delta\mu_m \rightarrow 0$ to find

$$\frac{\partial \alpha}{\partial \mu} = -\mu$$

If we integrate this equation, we obtain

$$\alpha = -\frac{\mu^2}{2} + c$$

But we have noted that there is no angular redistribution into $\mu = -1$ or out of $\mu = +1$. Hence $\alpha = 0$ for $\mu = \pm 1$, and we can evaluate $c = \frac{1}{2}$. Therefore $\alpha = (1 - \mu^2)/2$.

If we combine these results, we arrive at the desired limit of the difference equations (8.20):

$$\begin{aligned} \frac{\mu}{r^2} \frac{\partial}{\partial r} (r^2 \varphi) + \frac{1}{r} \frac{\partial}{\partial \mu} [(1 - \mu^2) \varphi] + \Sigma_s(r) \varphi(r, \mu) \\ = \frac{1}{2} \Sigma_s(r) \int_{-1}^{+1} d\mu' \varphi(r, \mu') + s(r, \mu) \end{aligned} \quad (8.22)$$

which is referred to as the *conservative form* of the transport equation in one-dimensional spherical geometry.⁹ As with the discretized case, we use the term “conservative” to indicate that the angular redistribution term vanishes when integrated over all angle:

$$\int_{-1}^{+1} d\mu \frac{1}{r} \frac{\partial}{\partial \mu} [(1 - \mu^2) \varphi(r, \mu)] = \frac{1}{r} (1 - \mu^2) \varphi(r, \mu) \bigg|_{-1}^{+1} = 0$$

The equivalence of the conservative form of the transport equation with a finite difference equation based on particle conservation for each mesh cell implies that the conservative form of the transport equation should be used

if finite difference methods are to be applied directly. Application of difference approximations to other forms of the transport equation in curvilinear coordinate systems will lead to nonconservative difference schemes.

Although we have already obtained a discretized form of the discrete ordinates equations, it is instructive to rederive this form directly from the conservative form of the transport equation (8.22) to illustrate this alternative approach. We assume that a quadrature set $\{\mu_m, w_m\}$ has been chosen according to the criteria listed in Section 8.1.1. The corresponding discrete ordinates equations become

$$\begin{aligned} \frac{\mu_m}{r^2} \frac{\partial}{\partial r} [r^2 \varphi(r, \mu_m)] + \frac{1}{r} \frac{\partial}{\partial \mu} [(1 - \mu^2) \varphi(r, \mu)] + \Sigma_t(r) \varphi(r, \mu_m) \\ = \frac{1}{2} \Sigma_s(r) \sum_{n=1}^M w_n \varphi(r, \mu_n) + s(r, \mu_m) \end{aligned} \quad (8.23)$$

The boundary at $r=0$ is a symmetry boundary, and we therefore use a reflecting boundary condition. This is not strictly correct because by definition a particle exactly at $r=0$ will change discontinuously from $\mu = -1$ to $\mu = +1$.

To discretize Eq. 8.23, we introduce a spatial mesh similar to that used for one-dimensional slab geometry (see Figure 8.10). Here the cell-edged mesh points are labeled as $r_{i \pm 1/2}$ and are chosen to coincide with any material boundaries that might be present. Since we must consider the angular derivatives explicitly, we incorporate the quadrature set $\{\mu_m\}$ into an angular mesh structure, where the integral points μ_m are the discrete directions (see Figure 8.11). We use a centered difference expression for

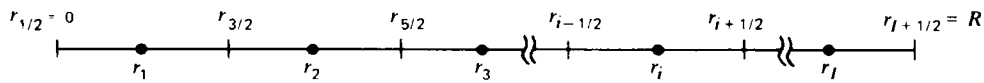


Fig. 8.10 □ Spatial mesh structure.

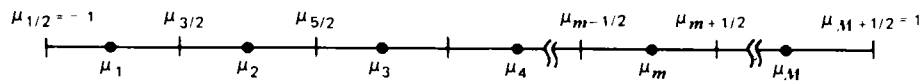


Fig. 8.11 □ Angular mesh structure.

the angular derivative

$$\left. \frac{\partial}{\partial \mu} (1 - \mu^2) \varphi \right|_{\mu_m} = \frac{(1 - \mu_{m+1/2}^2) \varphi_{m+1/2} - (1 - \mu_{m-1/2}^2) \varphi_{m-1/2}}{\Delta \mu_m}$$

where we define $\Delta \mu_m = \mu_{m+1/2} - \mu_{m-1/2}$. Hence the finite-differenced form of the discrete ordinates equations (8.23) is

$$\begin{aligned} \frac{\mu_m}{r_i^2} \left(\frac{r_{i+1/2}^2 \varphi_m^{i+1/2} - r_{i-1/2}^2 \varphi_m^{i-1/2}}{\Delta r_i} \right) \\ + \left(\frac{(1 - \mu_{m+1/2}^2) \varphi_{m+1/2}^i - (1 - \mu_{m-1/2}^2) \varphi_{m-1/2}^i}{r_i \Delta \mu_m} \right) + \Sigma_i^i \varphi_m^i = q_m^i \end{aligned} \quad (8.24)$$

where

$$q_m^i = \frac{1}{2} \Sigma_s^i \sum_{n=1}^M \varphi_n^i w_n + s_m^i$$

If we compare Eq. 8.24 with our earlier discretized equation (8.20), evidently we must identify

$$\alpha_{m+1/2} = \frac{1 - \mu_{m+1/2}^2}{2} \quad \text{and} \quad \alpha_{m-1/2} = \frac{1 - \mu_{m-1/2}^2}{2}$$

Subtracting these terms, we find

$$\begin{aligned} \alpha_{m+1/2} - \alpha_{m-1/2} &= - \frac{\mu_{m+1/2}^2 - \mu_{m-1/2}^2}{2} \\ &= - \frac{(\mu_{m+1/2} - \mu_{m-1/2})(\mu_{m+1/2} + \mu_{m-1/2})}{2} \end{aligned}$$

which is identical to the earlier recursion formula [if we assume $\mu_m = (\mu_{m+1/2} + \mu_{m-1/2})/2$]. Therefore the direct discretization of the conservative form of the transport equation in one-dimensional spherical geometry yields the discretized equations based on conservation of particles for each mesh cell.

To generalize these results, we introduce the following notation:

$$\begin{aligned} V_i &= \text{volume of spatial mesh cell at } r_i = 4\pi r_i^2 \Delta r_i \\ A_{i\pm 1/2} &= \text{area of cell edge at } r_{i\pm 1/2} = 4\pi r_{i\pm 1/2}^2 \\ \alpha_{m\pm 1/2} &= \frac{1 - \mu_{m\pm 1/2}^2}{2} \end{aligned}$$

and express Eq. 8.24 in terms of these definitions as follows:

$$\begin{aligned} & \frac{\mu_m (A_{i+1/2} \varphi_m^{i+1/2} - A_{i-1/2} \varphi_m^{i-1/2})}{V_i} \\ & + \frac{(A_{i+1/2} - A_{i-1/2})(\alpha_{m+1/2} \varphi_{m+1/2}^i - \alpha_{m-1/2} \varphi_{m-1/2}^i)}{V_i \Delta \mu_m} + \sum_i \varphi_m^i = q_m^i \end{aligned} \quad (8.25)$$

This result applies to one-dimensional plane and cylindrical as well as spherical geometries with the appropriate definitions for the V_i , $A_{i\pm 1/2}$, and $\alpha_{m\pm 1/2}$ terms. Table 8.3 gives the specific values for these three one-dimensional geometries.

Table 8.3 □ Area and Volume Elements for Standard One-Dimensional Geometries

Parameter	Slab	Spherical	Cylindrical
$A_{i\pm 1/2}$	1	$4\pi r_{i\pm 1/2}^2$	$2\pi r_{i\pm 1/2}$
V_i	Δx_i	$4\pi r_i^2 \Delta r_i$	$2\pi r_i \Delta r_i$

We now turn to the solution of Eq. 8.24 for the space angle mesh illustrated in Figure 8.12. As in the one-dimensional slab geometry problem, Eq. 8.24 contains too many unknowns for the number of equations ($3IM + I + M$ unknowns, IM equations). Therefore we relate the cell-centered fluxes to the cell-edged fluxes with the symmetric arithmetic mean or diamond difference relations

$$\varphi_m^i = \frac{1}{2} (\varphi_m^{i+1/2} + \varphi_m^{i-1/2}), \quad \varphi_m^i = \frac{1}{2} (\varphi_{m+1/2}^i + \varphi_{m-1/2}^i) \quad (8.26)$$

Equation 8.26 represents $2IM$ equations that when added to the IM equations and the M incoming boundary conditions above, is still insufficient to determine the $3IM + I + M$ unknowns. The additional I equations necessary to balance the number of unknowns may be obtained by considering the “starting” direction $\mu = -1$ or $\mu_{1/2}$. For this special direction, which corresponds to streaming inward along a radius vector, there is no angular redistribution. In this case, the transport equation

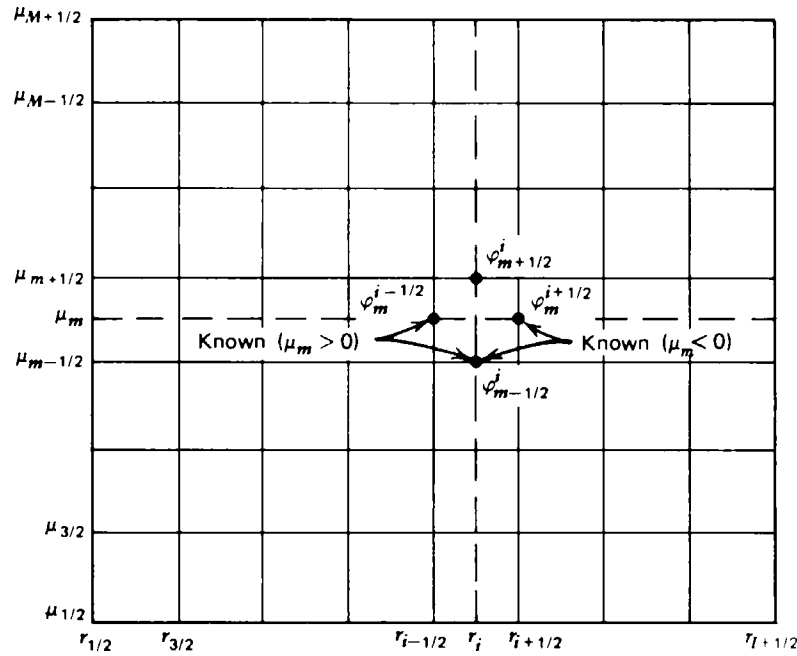


Fig. 8.12 □ Space angle mesh structure.

becomes

$$\mu \frac{\partial \varphi}{\partial r} + \Sigma_r(r) \varphi(r, \mu) = \frac{1}{2} \Sigma_s(r) \int_{-1}^{+1} d\mu' \varphi(r, \mu') + s(r, \mu)$$

which is identical to the one-dimensional slab equation. Thus if we know $\varphi(R, -1)$, the inward radially directed flux at the surface of the sphere (i.e., $\varphi_{1/2}^{I+1/2}$), we can solve for $\varphi_{1/2}^{I-1/2}$, $\varphi_{1/2}^{I-3/2}$, and so on, by using Eq. 8.14 with $\mu_m = -1$. Therefore we can calculate the I fluxes along the special direction $\mu_{1/2} = -1$ just by specifying the incoming flux for this direction, thereby finding the additional I equations necessary to reduce the number of unknowns. At this point in the calculation we know $\varphi_{1/2}^i$ for $i = \frac{1}{2}, \frac{3}{2}, \dots, I + \frac{1}{2}$.

To proceed with the calculation, we note that for any angular “sweep” m , the *incoming* angular redistribution flux is $\varphi_{m-1/2}^i$, and this term is known from the previous sweep. Therefore we can solve for $\varphi_{m+1/2}^i$ using Eq. 8.26

$$\varphi_{m+1/2}^i = 2\varphi_m^i - \varphi_{m-1/2}^i$$

Now we must determine the flux on the incoming spatial boundary. As in the plane geometry case, for $\mu_m > 0$, $\varphi_m^{i-1/2}$ is the incoming flux, and $\varphi_m^{i+1/2}$

is the outgoing flux. Therefore for $\mu_m > 0$, we solve for $\varphi_m^{i+1/2}$ using Eq. 8.26

$$\varphi_m^{i+1/2} = 2\varphi_m^i - \varphi_m^{i-1/2}$$

These expressions can be used to eliminate $\varphi_{m+1/2}^i$ and $\varphi_m^{i+1/2}$ to solve Eq. 8.25 for φ_m^i :

$$\varphi_m^i = a_m^i \varphi_m^{i-1/2} + b_m^i \varphi_{m-1/2}^i + c_m^i q_m^i \quad (8.27)$$

where $\mu_m > 0$, and the coefficients a_m^i , b_m^i , and c_m^i are constants. For $\mu_m < 0$, we eliminate $\varphi_m^{i-1/2}$ instead of $\varphi_m^{i+1/2}$, and the resulting expression is

$$\varphi_m^i = a_m^i \varphi_m^{i+1/2} + b_m^i \varphi_{m-1/2}^i + c_m^i q_m^i \quad (8.28)$$

where the a_m^i , b_m^i , and c_m^i are the same as in Eq. 8.27 if the angular quadrature satisfies $\mu_m = (\mu_{m+1/2} + \mu_{m-1/2})/2$. (Note that this would not be true for standard Gauss-Legendre quadrature sets.) Therefore we can calculate the cell-centered flux φ_m^i from either Eq. 8.27 or Eq. 8.28, and the outgoing flux ($\varphi_m^{i+1/2}$ or $\varphi_m^{i-1/2}$) can be determined from Eq. 8.27. This quantity is then used as the incoming flux for the next mesh cell.

The order of the progression through the space angle mesh in Figure 8.12 should now be evident. Remembering that all fluxes φ_m^i along $m = \frac{1}{2}$ have been computed, we start with the known incoming boundary flux $\varphi_1^{i+1/2} = \varphi(R, \mu_1)$ and progress to the left computing φ_1^i and then the edge fluxes $\varphi_m^{i-1/2}$ and $\varphi_{m+1/2}^i$. After $r=0$ has been reached, the next angular sweep ($m=2$) is begun. Once all φ_m^i for $\mu_m < 0$ have been determined, we can use the reflecting boundary condition at $r=0$ to determine $\varphi_m^{1/2} = \varphi_{M-m+1}^{1/2}$ for $\mu_m > 0$, and sweep back to the right for each μ_m . Figure 8.13 illustrates this procedure schematically.

8.1.3 □ Multidimensional Geometries □ In the previous sections we have discussed in some detail the application of the discrete ordinates method to one-dimensional slab and spherical geometry problems. In the slab application we found that the solution could be obtained easily by solving along each discrete direction in the direction of particle motion. This progression through the space angle mesh was particularly simple for one-dimensional slab geometry because there was no coupling between angular directions (no angular redistribution). The situation was a bit more complicated for one-dimensional spherical geometry because the discrete directions $\{\mu_m\}$ were coupled by the angular redistribution term characteristic of curvilinear geometries. But again the progression through the space

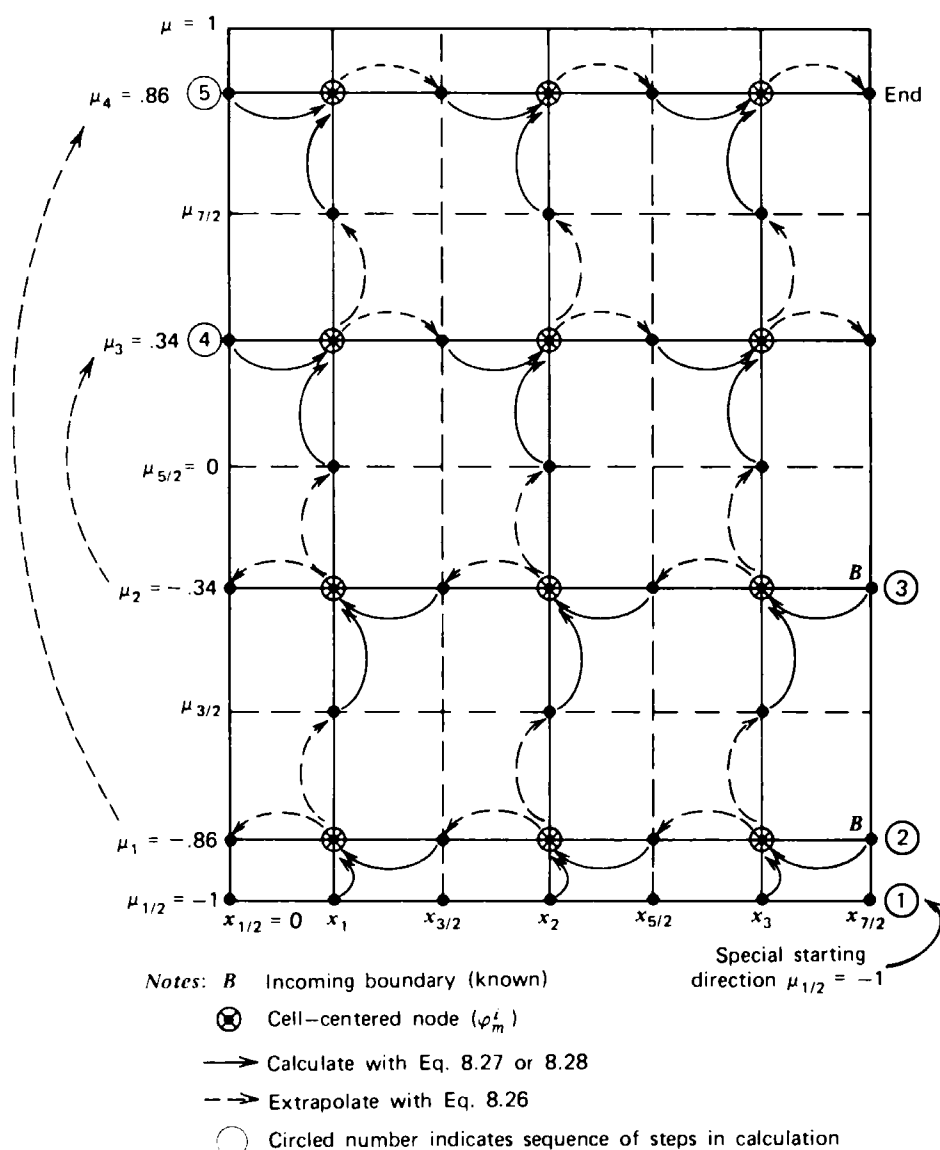


Fig. 8.13 □ Progression through typical spherical space angle mesh ($I=3$, $M=4$).

angle mesh was relatively simple once the calculation was suitably initiated.

As we might expect, the solution of the discrete ordinates equations becomes considerably more complex in cylindrical or multidimensional geometries. In these cases two angles are needed to specify $\hat{\Omega}_m$ because there is no longer azimuthal symmetry (in angular space). This complicates both the discretization of the discrete ordinates equations and the algorithm to solve the resultant system of algebraic equations.

For multidimensional geometries it is advisable to derive the finite difference relations directly from a statement of particle conservation for each mesh cell, rather than introducing finite difference approximations directly into the transport equation.⁸ Therefore this section first derives the finite difference equations applicable to an arbitrary two-dimensional geometry. Although the coordinate system is labeled x - y , the discussion also is applicable to r - θ and r - z geometries. The extension to three-dimensional geometries, though computationally challenging, is based on such principles of the two-dimensional application as the concept of conservative difference relations for curvilinear geometries or progression through the mesh in the direction of particle motion. Just as in the numerical solution of the diffusion equation, one finds that the extension from one- to two-dimensional problems is the significant conceptual step; subsequent extensions from two to three dimensions generally result in severe computational problems because of the sheer size of the system of equations rather than any basic complications in finite difference methods or numerical solution algorithms from the added dimension. Therefore we do not consider the solution of three-dimensional transport problems beyond mentioning that there does exist a discrete ordinates code, **THRETRAN**,¹⁶ which is capable of treating three-dimensional geometry.

The difference equations for a general two-dimensional geometry are derived⁸ by considering the overall particle balance in the computational mesh cell $V_{ij}\Delta\Omega_m$. We assume that a suitable set of discrete directions $\{\hat{\Omega}_m\}$ and weights $\{w_m\}$ has been selected. The spatial mesh is characterized by the notation indicated in Figure 8.14 where, as always, we denote cell-centered quantities by integer indices and cell-edged quantities with half-integer indices. Here the center of the spatial cell V_{ij} is (x_i, y_j) , and the center of the angular cell is $\hat{\Omega}_m$. We define the "edges" of the angular cell to be at $\hat{\Omega}_{m \pm 1/2}$ and as in the one-dimensional spherical case,

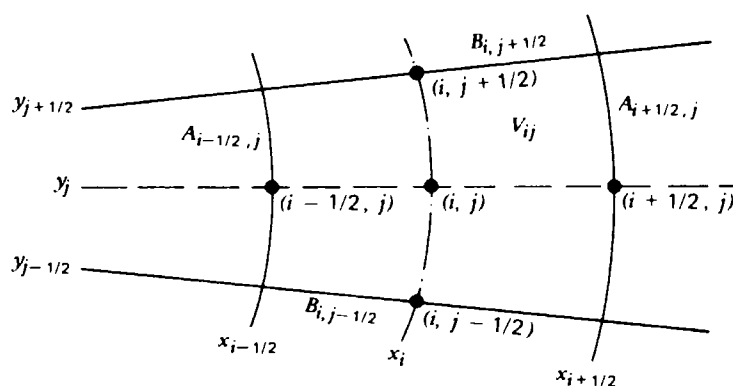


Fig. 8.14 □ Spatial mesh structure for two-dimensional geometry.

the “areas” of these edges are denoted by $\alpha_{m\pm 1/2}$. If there are two coordinates with curvature, we define additional areas $\beta_{m\pm 1/2}$. We introduce (μ_m, η_m) as the direction cosine pair with respect to the x - y axes (or r - θ or r - z), $\mu_m \equiv \hat{\Omega}_m \cdot \hat{e}_x$ and $\eta_m \equiv \hat{\Omega}_m \cdot \hat{e}_y$. Using the conventional index notation [e.g., $\varphi_m^{ij} \equiv \varphi(x_i, y_j, \hat{\Omega}_m)$], we can now write down the particle balance equation for the mesh cell $V_{ij} w_m$. First note that the total number of particles in $\Delta\Omega$ about $\hat{\Omega}$ crossing an area A at position $\mathbf{r}$ per second is $\varphi(\mathbf{r}, \hat{\Omega}) \hat{\Omega} \cdot \hat{\mathbf{n}} \Delta\Omega A$, where $\hat{\mathbf{n}}$ is the normal to the area A at $\mathbf{r}$, and a positive sign indicates a net number crossing in the same direction as $\hat{\mathbf{n}}$. Therefore the net number of particles leaving V_{ij} across the area $A_{i+1/2,j}$ is just $\varphi_m^{i+1/2,j} \mu_m w_m A_{i+1/2,j}$ (where we have noted $w_m = \Delta\Omega_m$), whereas the net number leaving V_{ij} across $A_{i-1/2,j}$ is $-\varphi_m^{i-1/2,j} \mu_m w_m A_{i-1/2,j}$. Similar terms can be written for the net number of particles leaving V_{ij} at the areas $B_{i,j\pm 1/2}$. Therefore the combined result of loss from V_{ij} across the spatial boundaries is

$$\begin{aligned} & \mu_m w_m (A_{i+1/2,j} \varphi_m^{i+1/2,j} - A_{i-1/2,j} \varphi_m^{i-1/2,j}) \\ & + \eta_m w_m (B_{i,j+1/2} \varphi_m^{i,j+1/2} - B_{i,j-1/2} \varphi_m^{i,j-1/2}) \end{aligned}$$

The loss due to particle collisions is

$$\Sigma_i^{ij} \varphi_m^{ij} V_{ij} w_m$$

and the gain due to inscatter (under the assumption of isotropic scattering) and sources is

$$q_m^{ij} = \left[(4\pi)^{-1} \Sigma_s^{ij} \sum_{n=1}^M w_n \varphi_n^{ij} \right] V_{ij} w_m + s_m^{ij} V_{ij} w_m$$

We can use the methods employed for one-dimensional spherical geometry to compute the angular redistribution terms. In that case we assumed that the effective areas for angular flow across $\hat{\Omega}_{m\pm 1/2}$ were $\alpha_{m\pm 1/2}$. However, rather than repeating the step in which the terms were renormalized, we note here that the net effect was to multiply the angular redistribution term by the quantity (for spherical geometry)

$$8\pi r_i \Delta r_i = 4\pi \left(r_i + \frac{\Delta r_i}{2} \right)^2 - 4\pi \left(r_i - \frac{\Delta r_i}{2} \right)^2 = A_{i+1/2} - A_{i-1/2}$$

Therefore we express the net loss from $V_{ij} w_m$ due to angular redistribution

across $\alpha_{m\pm 1/2}$ as

$$(A_{i+1/2,j} - A_{i-1/2,j})(\alpha_{m+1/2}\varphi_{m+1/2}^{ij} - \alpha_{m-1/2}\varphi_{m-1/2}^{ij})$$

where we must still determine $\alpha_{m\pm 1/2}$. Note that we could also allow for angular redistribution in a second direction by defining a similar term

$$(B_{i,j+1/2} - B_{i,j-1/2})(\beta_{m+1/2}\varphi_{m+1/2}^{ij} - \beta_{m-1/2}\varphi_{m-1/2}^{ij})$$

However in the standard two-dimensional geometries, there is curvature in at most one direction, and we continue to treat this case only.

Combining these gain and loss terms and dividing through by w_m , we obtain the basic particle balance equation for the phase space cell $V_{ij}w_m$:

$$\begin{aligned} \mu_m(A_{i+1/2,j}\varphi_m^{i+1/2,j} - A_{i-1/2,j}\varphi_m^{i-1/2,j}) \\ + \eta_m(B_{i,j+1/2}\varphi_m^{i,j+1/2} - B_{i,j-1/2}\varphi_m^{i,j-1/2}) \\ + (A_{i+1/2,j} - A_{i-1/2,j})\left(\frac{\alpha_{m+1/2}}{w_m}\varphi_{m+1/2}^{ij} - \frac{\alpha_{m-1/2}}{w_m}\varphi_{m-1/2}^{ij}\right) \\ + \Sigma_i^j \varphi_m^{ij} V_{ij} = q_m^{ij} V_{ij} \end{aligned} \quad (8.29)$$

Table 8.4 contains the explicit expressions for the A , B , and V coefficients for the standard two-dimensional geometries. Moreover, Eq. 8.29 is applicable to Cartesian geometries because in this case $A_{i+1/2,j} = A_{i-1/2,j}$ and $B_{i,j+1/2} = B_{i,j-1/2}$ (no area divergence) so that the angular redistribution terms will vanish.

We can evaluate the α and β terms in a manner similar to that used for one-dimensional spherical geometries (Section 8.1.2). Again we want to consider a situation in which divergenceless flow exists in a region with a constant absorption cross section and a constant source. In this case the

Table 8.4 □ **Area and Volume Elements^a**

Geometry	dV	dA	dB	$A_{i+1/2,j}$	$B_{i,j+1/2}$	V_{ij}
(x,y)	$dx dy$	dy	dx	Δy_j	Δx_i	$\Delta x_i \Delta y_j$
(r,θ)	$r d\theta dr$	$r d\theta$	dr	$2\pi r_{i+1/2} \Delta\theta_j$	Δr_i	$2\pi r \Delta r_i \Delta\theta_j$
(r,z)	$2\pi r dr dz$	$2\pi r dz$	$2\pi r dr$	$2\pi r_{i+1/2} \Delta z_j$	$2\pi \bar{r} \Delta r_i$	$2\pi \bar{r} \Delta r_i \Delta z_j$

^aIn this table $\bar{r} \equiv (r_{i+1/2} + r_{i-1/2})/2$.

flux is a constant ϕ_0 and Eq. 8.29 becomes

$$\begin{aligned} \mu_m(A_{i+1/2,j} - A_{i-1/2,j})\phi_0 + \eta_m(B_{i,j+1/2} - B_{i,j-1/2})\phi_0 \\ + (A_{i+1/2,j} - A_{i-1/2,j})\left(\frac{\alpha_{m+1/2} - \alpha_{m-1/2}}{w_m}\right)\phi_0 + \Sigma_i \phi_0 V_{ij} = \left(\frac{S_0}{4\pi}\right)V_{ij} \end{aligned}$$

But since this solution satisfies

$$\Sigma_i \phi_0 V_{ij} = \left(\frac{S_0}{4\pi}\right)V_{ij}$$

and $B_{i,j+1/2} = B_{i,j-1/2}$ by assumption, we conclude

$$\mu_m(A_{i+1/2,j} - A_{i-1/2,j}) + \frac{(A_{i+1/2,j} - A_{i-1/2,j})(\alpha_{m+1/2} - \alpha_{m-1/2})}{w_m} = 0$$

This yields a relation to calculate the α terms

$$\alpha_{m+1/2} - \alpha_{m-1/2} = -\mu_m w_m \quad (8.30)$$

For such multidimensional problems the evaluation of the α terms is more complicated because $\hat{\Omega}_m$ depends on both μ_m and η_m . For a given value η_k , we may have several μ_i . (In this regard, keep in mind the latitudinal point arrangement schemes outlined in Section 8.1.1.) In particular, there will be a most negative μ_i into which there is no angular redistribution, and also a most positive μ_i , out of which there is no angular redistribution. These directions approximately represent streaming inward along a radius vector or streaming outward. In general one sets the $\alpha_{1/2} = 0$ for the smallest μ_i for each η_k . If symmetric sets in μ are used, this ensures that the last α is also zero and results in a conservative difference relation when multiplied by w_m and summed over all angles. However details of the actual calculation of the various α terms are somewhat problem (and code) dependent, and perhaps it is best to refer the interested reader to the various code manuals (e.g., for TWOTRAN¹⁷ or DOT¹⁸).

The basic idea behind the method of solving the discrete ordinates equations in multidimensional geometry is the same as that for one-dimensional geometries. We attempt to rearrange the system of equations into a "lower triangular" form by proceeding to solve the discrete ordinates equations in the direction of particle motion.

Once again we must introduce relations between the cell-centered and cell-edged fluxes to reduce the number of unknowns. The symmetric diamond difference relations are chosen

$$\begin{aligned}\varphi_m^{ij} &= \frac{1}{2} (\varphi_m^{i+1/2,j} + \varphi_m^{i-1/2,j}) \\ \varphi_m^{ij} &= \frac{1}{2} (\varphi_m^{i,j+1/2} + \varphi_m^{i,j-1/2}) \\ \varphi_m^{ij} &= \frac{1}{2} (\varphi_{m+1/2}^{ij} + \varphi_{m-1/2}^{ij})\end{aligned}\tag{8.31}$$

The difference equations (8.29) are to be solved in the direction of particle motion; therefore the cell-edged fluxes $\varphi_m^{i\pm 1/2,j}, \varphi_m^{i,j\pm 1/2}$ represent either incoming or outgoing fluxes for a given spatial mesh cell and direction $\hat{\Omega}_m$. Since the incoming fluxes generally are known either from the boundary conditions or as a result of a calculation in an adjacent cell, our goal now is to express the cell-centered flux in terms of the incoming fluxes only. In addition, for curvilinear geometries the fluxes $\varphi_{m\pm 1/2}^{ij}$ also represent outgoing or incoming fluxes, respectively, across the angular edges at $\alpha_{m\pm 1/2}$. We now adopt the convention that the angular sweeps (iterations over index m) proceed in the direction of increasing m . This is consistent with the physical process of ray-to-ray transfer if the directions $\hat{\Omega}_m$ are indexed so that for a given n , the index m increases for increasing μ . The argument is the same as in the one-dimensional spherical geometry case; there can only be angular redistribution in the positive μ direction.

The effect of this convention is that $\varphi_{m-1/2}^{ij}$ is an incoming flux for the phase space mesh cell. Therefore we only need to identify the incoming fluxes on the spatial edges at $x_{i\pm 1/2}$ and $y_{j\pm 1/2}$. (Note that this discussion is applicable to r - θ and r - z geometries by simply replacing x and y with r and θ or r and z , respectively.) The identification of the incoming fluxes may be made by inspection if we remember that in all cases the (μ, η) coordinate system lines up with the (x, y) coordinate system (i.e., $\mu_m = \hat{\Omega}_m \cdot \hat{e}_x$ and $\eta_m = \hat{\Omega}_m \cdot \hat{e}_y$). First we group the directions $\{\hat{\Omega}_m\}$ into four categories depending on the quadrant in (μ, η) space. These are defined in Figure 8.15. Next we consider a typical mesh cell, as illustrated in Figure 8.16. Clearly the cell edges A and B are incoming boundaries for a direction $\hat{\Omega}_m$ in quadrant III. The incoming boundaries for other directions are similarly defined and are noted in the legend of Figure 8.16.

Therefore for a given mesh cell we know $\varphi_{m-1/2}^{ij}$ and one of each of the pairs $\varphi_m^{i\pm 1/2,j}$ and $\varphi_m^{i,j\pm 1/2}$. We then use Eqs. 8.29, 8.30, and 8.31 to

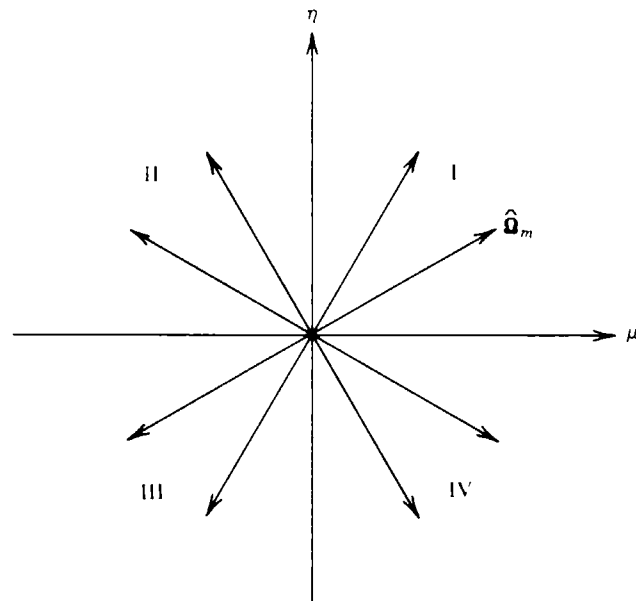


Fig. 8.15 □ Quadrant definition for two-dimension angular geometry.

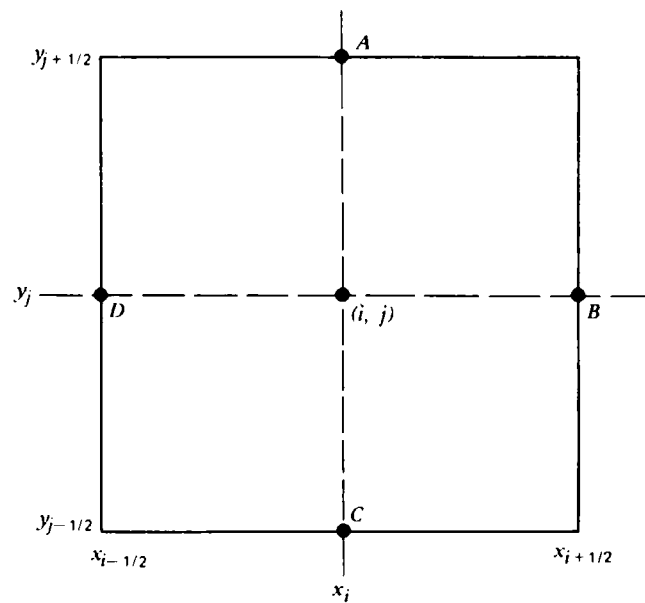


Fig. 8.16 □ Spatial mesh cell. The quadrants have the following incoming boundaries: I, C, D; II, B, C; III, A, B; IV, A, D.

eliminate the outgoing fluxes and arrive at an expression for the cell-centered flux φ_m^{ij} in terms of the incoming fluxes:

$$\begin{aligned} \varphi_m^{ij} = & \frac{|\mu_m|(A_{i+1/2,j} + A_{i-1/2,j})}{D} \varphi_m^{i\pm 1/2,j} + \frac{2|\eta_m|B_{ij}}{D} \varphi_m^{i,j\pm 1/2} \\ & + \frac{(A_{i+1/2,j} - A_{i-1/2,j})(\alpha_{m+1/2} + \alpha_{m-1/2})w_m^{-1}}{D} \varphi_{m-1/2}^{ij} + \frac{V_{ij}q_m^{ij}}{D} \end{aligned}$$

where

$$\begin{aligned} D \equiv & |\mu_m|(A_{i+1/2,j} + A_{i-1/2,j}) + 2|\eta_m|B_{ij} \\ & + (A_{i+1/2,j} - A_{i-1/2,j})(\alpha_{m+1/2} + \alpha_{m-1/2})w_m^{-1} + \Sigma_i^{ij}V_{ij} \end{aligned} \quad (8.32)$$

For example, if $\hat{\Omega}_m$ is in quadrant I, then $\varphi_m^{i-1/2,j}$ and $\varphi_m^{i,j-1/2}$ are incoming fluxes and therefore are used in Eq. 8.32 to determine φ_m^{ij} . Then the diamond difference relations can be used to extrapolate the outgoing fluxes $\varphi_m^{i+1/2,j}$, $\varphi_m^{i,j+1/2}$, and $\varphi_{m+1/2}^{ij}$ for the mesh cell. These may then be used as incoming fluxes for an adjacent cell.

For Cartesian geometries, there is no angular redistribution, hence no $\varphi_{m\pm 1/2}^{ij}$ terms. In this case the angular sweeps are decoupled, and one can proceed from the known incoming fluxes for each m through the spatial mesh. Thus the known boundary conditions are sufficient to begin the solution procedure. However with curvilinear geometries one must also have an initial condition for the incoming angular boundary. As noted previously, we initialize the angular redistribution recursion relation (8.30) for the smallest μ for each η level. Assuming this initial direction is $\hat{\Omega}_m = (\mu_m, \eta_m)$, we then use a step function relationship to relate the cell-edged and cell-centered fluxes for this direction:

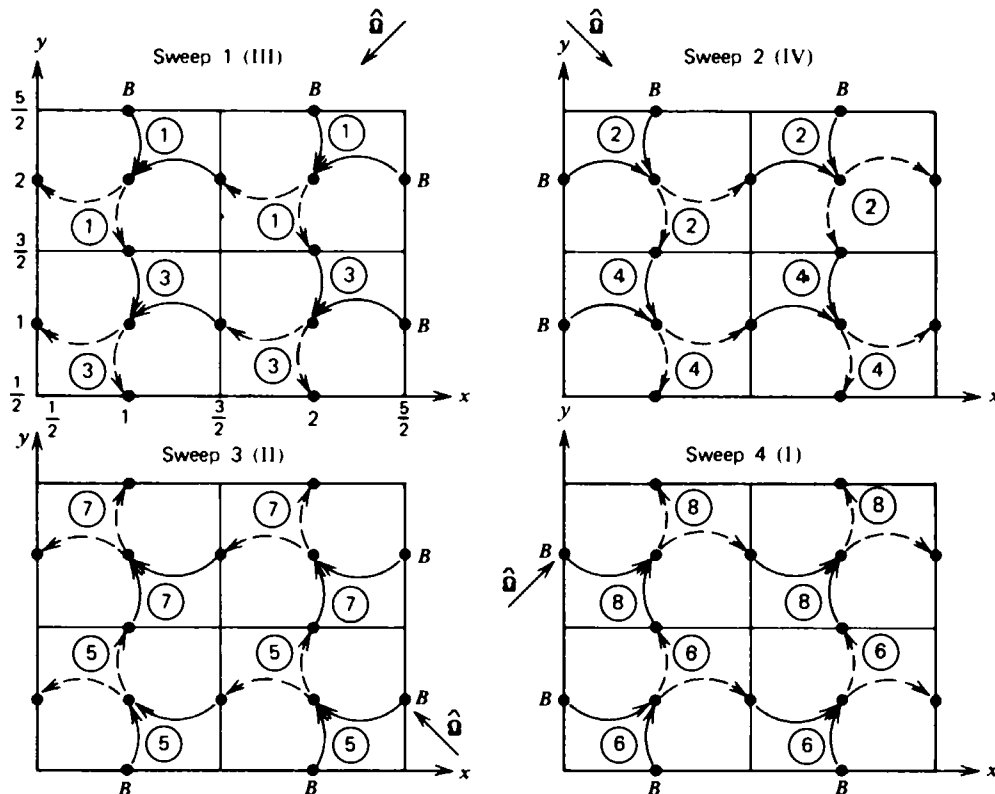
$$\varphi_m^{ij} = \varphi_{m+1/2}^{ij}$$

This can then be used in place of Eq. 8.31 to find the same equation for φ_m^{ij} as Eq. 8.32 except that the terms with $(\alpha_{m+1/2} + \alpha_{m-1/2})$ disappear.

In summary then, the steps for sweeping through the space angle mesh are as follows:¹⁷

- i Choose a quadrant of directions (μ, η) and begin at the mesh cell at the intersection of the two corresponding incoming boundaries.

- ii Use the known incoming boundary fluxes to compute the cell-centered flux from Eq. 8.32.
- iii Use Eq. 8.31 to compute the cell-edged fluxes on the outgoing boundaries of the cell.
- iv Proceed to the next cell and compute the cell-centered flux with Eq. 8.32 along with previously calculated cell-edged fluxes and known boundary fluxes.



Notes: —→ Calculation with Eq. 8.32

---→ Extrapolation with Eq. 8.31

Circled numbers indicate order of steps (e.g., step ① begins at the right-top boundary and proceeds left across the top row for all directions $\hat{\Omega}_m \in \text{quadrant III}$)

"B" Indicates that node is an incoming boundary for that particular direction

Fig. 8.17 □ Typical progression through space angle mesh.

Figure 8.17 illustrates the procedure for a typical mesh. It is assumed that initialization of the fluxes in the special starting directions is performed where needed.

8.1.4 □ Finite Element Treatment of the Spatial Variable in the Discrete Ordinates Equations □ The preceding discussion of the discrete ordinates method has been devoted to the “classical” approach, which combines a discrete ordinates treatment of the angle variable with standard finite difference techniques in the spatial variables. However a recently developed alternative formulation combines the discrete ordinates method in angle with the finite element method in space.¹⁹ This scheme, which is the basis for the TRIPLET/TRIDENT²⁰ and ONETRAN²¹ computer codes, has yielded impressive results for a variety of applications.

The particular application of the finite element method to the solution of the discrete ordinates equations is based on a unique implementation of the familiar Galerkin integral law formulation of the transport equation (cf. Section 8.3). By applying the finite element method locally on an individual mesh cell basis rather than on a global basis, the highly successful solution algorithm of discrete ordinates codes can be retained, and one can solve for the fluxes in the direction of particle motion. Thus the solution procedure is nearly the same as in the conventional finite difference–discrete ordinates computer codes in which one progresses from mesh cell to mesh cell, solving a system of equations relating the mesh cell fluxes in the direction of particle flight.

Although the basic approach is the same for both one- and two-dimensional discrete ordinates applications, the implementation for the latter case is somewhat more cumbersome because of the geometrical complexity of tracking particles through a triangular mesh. Therefore we consider the one- and two-dimensional applications separately.

One-Dimensional Geometries □ We begin with the finite element–discrete ordinates method as applied to one-dimensional geometries and as implemented in the ONETRAN²¹ discrete ordinates computer code. For simplicity, since the treatment of the angular edge fluxes (i.e., $\varphi_{m \pm 1/2}$) for curvilinear geometries is identical to the conventional discrete ordinates treatment, we consider only the slab geometry.

Before launching into details, let us demonstrate the similarity of the finite element and conventional formulations of the discrete ordinates method for the one-dimensional case. The mesh cell in Figure 8.18 is

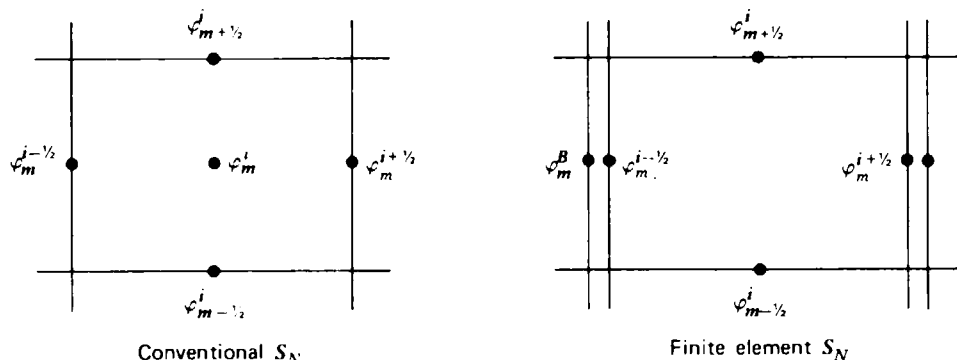


Fig. 8.18 □ Typical mesh cells for finite difference and finite element–discrete ordinates methods.

typical for such applications. If we now consider a direction $\mu_m > 0$, then clearly $\varphi_m^{i-1/2}$ is the incoming flux for the spatial boundary, and $\varphi_{m-1/2}^i$ is (always) the incoming flux on the angular boundary. In the conventional finite difference–discrete ordinates approach we solved for $\varphi_{m+1/2}^i$ and $\varphi_m^{i+1/2}$ by first computing the cell-centered flux φ_m^i , then using the diamond difference relations. However the solution for $\varphi_m^{i+1/2}$ could have been obtained directly by eliminating φ_m^i and $\varphi_{m+1/2}^i$ from the basic difference equation (8.29), using the diamond difference relations

$$\begin{aligned}\varphi_m^i &= \frac{1}{2}(\varphi_m^{i+1/2} + \varphi_m^{i-1/2}) \\ \varphi_{m+1/2}^i &= \varphi_m^{i+1/2} + \varphi_m^{i-1/2} - \varphi_{m-1/2}^i\end{aligned}\quad (8.33)$$

This would result in an equation for the outgoing flux $\varphi_m^{i+1/2}$ in terms of the incoming flux $\varphi_m^{i-1/2}$.

The finite element method is not significantly different. The diamond difference assumption for the angular edge fluxes, Eq. 8.33, is used, but the spatial edge fluxes are computed by solving two equations. There is no “cell-centered” flux in the finite element mesh cell; but then, we noted that it really is not necessary for the conventional application either. The main difference is that the outgoing flux from the adjacent cell, which is labeled φ_m^B , is *not* the flux on the incoming edge of the mesh cell as it is in the conventional finite difference–discrete ordinates method. Rather, the outgoing flux from the adjacent cell is treated as an incoming source of particles, and one solves for the incoming and outgoing cell-edged fluxes simultaneously. Thus the spatial flux can be discontinuous at the cell

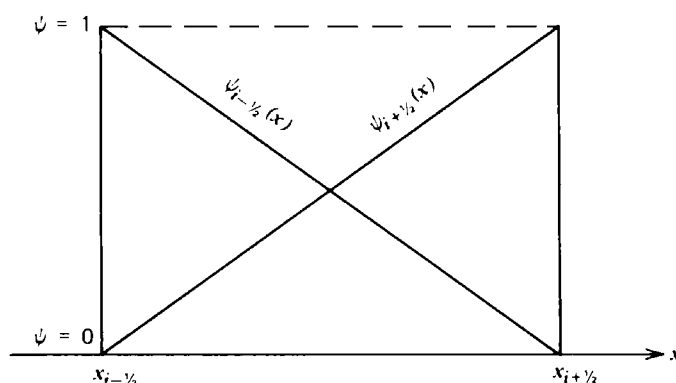


Fig. 8.19 □ Discontinuous finite element basis functions.

edges. This can lead to a marked improvement in accuracy for some problems.

The discussion above is intended to motivate our decision to consider only the derivation of the equations that relate the cell-edged fluxes (including treatment of the discontinuities), since this is the essential difference between the conventional finite difference and finite element formulations of the discrete ordinates equations. Only slab geometry is considered here because of the similarity to the spherical geometry case.

We now derive the equations relating the spatial cell-edged fluxes using the finite element method.²¹ (The reader may wish to refer ahead to Section 8.3 for a more general discussion of the finite element method.) If we consider a typical spatial mesh, the flux $\varphi_m(x)$ is expanded in terms of finite element basis functions over the mesh cell. These basis functions $\psi_{i\pm 1/2}(x)$ are unity at $x_{i\pm 1/2}$ and zero at $x_{i\mp 1/2}$, respectively, and are similar to the standard Lagrange basis functions (see Figure 8.19). These basis functions differ from the usual linear Lagrange basis functions, however, since they are discontinuous. This makes them particularly useful for the treatment of problems with material discontinuities.

More specifically, we define the finite element basis functions as

$$\psi_{i-1/2}(x) = \begin{cases} \frac{x_{i+1/2} - x}{x_{i+1/2} - x_{i-1/2}}, & x_{i-1/2} \leq x \leq x_{i+1/2} \\ 0, & \text{otherwise} \end{cases}$$

$$\psi_{i+1/2}(x) = \begin{cases} \frac{x - x_{i-1/2}}{x_{i+1/2} - x_{i-1/2}}, & x_{i-1/2} \leq x \leq x_{i+1/2} \\ 0, & \text{otherwise} \end{cases}$$

We now expand $\varphi_m(x)$ in terms of the $\psi_{i\pm 1/2}(x)$

$$\varphi_m(x) = \varphi_m^{i-1/2} \psi_{i-1/2}(x) + \varphi_m^{i+1/2} \psi_{i+1/2}(x)$$

where $\varphi_m^{i\pm 1/2}$ are the cell-edged fluxes. Using the explicit forms of $\psi_{i\pm 1/2}(x)$, we have

$$\varphi_m(x) = \frac{1}{\Delta x_i} \left[(x_{i+1/2} - x) \varphi_m^{i-1/2} + (x - x_{i-1/2}) \varphi_m^{i+1/2} \right]$$

where $\Delta x_i = x_{i+1/2} - x_{i-1/2}$. The source term $q_m(x)$ is similarly expanded in terms of its cell-edge values,

$$q_m(x) = \frac{1}{\Delta x_i} \left[(x_{i+1/2} - x) q_m^{i-1/2} + (x - x_{i-1/2}) q_m^{i+1/2} \right]$$

Introducing these expansions into the discrete ordinates equations, we find

$$\begin{aligned} \mu_m \frac{d\varphi_m}{dx} + \frac{\Sigma_i}{\Delta x_i} \left[(x_{i+1/2} - x) \varphi_m^{i-1/2} + (x - x_{i-1/2}) \varphi_m^{i+1/2} \right] \\ = \frac{1}{\Delta x_i} \left[(x_{i+1/2} - x) q_m^{i-1/2} + (x - x_{i-1/2}) q_m^{i+1/2} \right] \end{aligned} \quad (8.34)$$

The derivative term will be evaluated momentarily.

The Galerkin (or integral law) formulation of the finite element method typically proceeds by multiplying Eq. 8.34 by the finite element basis functions and integrating over the mesh cell. That is, the weighting functions for the finite element method are chosen as the basis functions $\psi_{i\pm 1/2}(x)$. However it is more convenient to choose the following alternative weighting functions:²¹

$$\varphi_1(x) = 1, \quad \varphi_2(x) = x - x_{i-1/2} \quad \text{for } \mu_m > 0$$

and

$$\varphi_1(x) = 1, \quad \varphi_2(x) = x_{i+1/2} - x \quad \text{for } \mu_m < 0$$

It can be shown that the use of the weighting functions above is equivalent to Galerkin weighting, although the exact form of the resulting equations is altered. This particular choice of weighting function simplifies the spatial integrations rather considerably.

Let us assume that $\mu_m > 0$ and perform the weighting explicitly:

$$\begin{aligned} \mu_m \int_{x_{i-1/2}}^{x_{i+1/2}} dx \, 1 \frac{d\varphi_m}{dx} \\ + \frac{\Sigma_i}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} dx \, 1 \left[(x_{i+1/2} - x) \varphi_m^{i-1/2} + (x - x_{i-1/2}) \varphi_m^{i+1/2} \right] \\ = \frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} dx \, 1 \left[(x_{i+1/2} - x) q_m^{i-1/2} + (x - x_{i-1/2}) q_m^{i+1/2} \right] \end{aligned}$$

The streaming term can be integrated and evaluated by imposing the boundary condition that the flux on a boundary be the limiting value of the angular flux as the boundary is approached in the direction of particle motion. In other words,

$$\lim_{x \rightarrow x_{i-1/2}} \varphi_m(x) = \varphi_m^B, \quad \lim_{x \rightarrow x_{i+1/2}} \varphi_m(x) = \varphi_m^{i+1/2}, \quad \mu_m > 0$$

and

$$\lim_{x \rightarrow x_{i-1/2}} \varphi_m(x) = \varphi_m^{i-1/2}, \quad \lim_{x \rightarrow x_{i+1/2}} \varphi_m(x) = \varphi_m^B, \quad \mu_m < 0$$

(The notation φ_m^B refers to the incoming flux on the boundary due to the adjacent cell.) Thus the streaming term becomes (noting $\mu_m > 0$)

$$\mu_m \varphi_m(x) \Big|_{x_{i-1/2}}^{x_{i+1/2}} = \mu_m (\varphi_m^{i+1/2} - \varphi_m^B)$$

The significance of this boundary condition is that an outgoing flux from a mesh cell is treated as an incoming source of particles for the adjacent mesh cell. However the flux just inside this adjacent mesh cell (e.g., $\varphi_m^{i-1/2}$ for $\mu_m > 0$) is not constrained to equal the incoming flux φ_m^B . If the actual angular flux exhibits a “near discontinuity” at the boundary, perhaps because of a material or source discontinuity, this behavior may be better approximated with the discontinuous basis functions. The use of discontinuous finite elements is discussed in greater detail in Section 8.3.

The remaining terms are readily integrated to yield the first equation:

$$\mu_m (\varphi_m^{i+1/2} - \varphi_m^B) + \Sigma_i \left(\frac{\Delta x_i}{2} \right) (\varphi_m^{i-1/2} + \varphi_m^{i+1/2}) = \frac{1}{2} \Delta x_i (q_m^{i-1/2} + q_m^{i+1/2})$$

or collecting terms,

$$\left(\Sigma_i \frac{\Delta x_i}{2} \right) \varphi_m^{i-1/2} + \left(\mu_m + \Sigma_i \frac{\Delta x_i}{2} \right) \varphi_m^{i+1/2} = \left(\frac{\Delta x_i}{2} \right) (q_m^{i-1/2} + q_m^{i+1/2}) + \mu_m \varphi_m^B \quad (8.35)$$

The second equation is obtained by weighting Eq. 8.34 with $\varphi_2(x) = x - x_{i-1/2}$:

$$\begin{aligned} \mu_m \int_{x_{i-1/2}}^{x_{i+1/2}} dx (x - x_{i-1/2}) \frac{d\varphi_m}{dx} \\ + \frac{\Sigma_i^i}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} dx (x - x_{i-1/2}) \left[(x_{i+1/2} - x) \varphi_m^{i-1/2} + (x - x_{i-1/2}) \varphi_m^{i+1/2} \right] \\ = \frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} dx (x - x_{i-1/2}) \left[(x_{i+1/2} - x) q_m^{i-1/2} + (x - x_{i-1/2}) q_m^{i+1/2} \right] \end{aligned}$$

The streaming term can be integrated by parts to find

$$\mu_m \int_{x_{i-1/2}}^{x_{i+1/2}} dx (x - x_{i-1/2}) \frac{d\varphi_m}{dx} = \mu_m \Delta x_i \varphi_m^{i+1/2} - \mu_m \left(\frac{1}{2} \right) (\varphi_m^{i+1/2} + \varphi_m^{i-1/2}) \Delta x_i$$

The remaining integrals can be easily evaluated so that our second equation becomes

$$\begin{aligned} (-3\mu_m + \Sigma_i^i \Delta x_i) \varphi_m^{i-1/2} + (3\mu_m + 2\Sigma_i^i \Delta x_i) \varphi_m^{i+1/2} \\ = \Delta x_i q_m^{i-1/2} + 2\Delta x_i q_m^{i+1/2} \end{aligned} \quad (8.36)$$

We can follow a very similar procedure for $\mu_m < 0$ to find

$$\left(-\mu_m + \frac{\Sigma_i^i \Delta x_i}{2} \right) \varphi_m^{i-1/2} + \left(\frac{\Sigma_i^i \Delta x_i}{2} \right) \varphi_m^{i+1/2} = \frac{\Delta x_i}{2} (q_m^{i-1/2} + q_m^{i+1/2}) - \mu_m \varphi_m^B \quad (8.37)$$

and

$$(-3\mu_m + 2\Sigma_i^i \Delta x_i) \varphi_m^{i-1/2} + (3\mu_m + \Sigma_i^i \Delta x_i) \varphi_m^{i+1/2} = 2\Delta x_i q_m^{i-1/2} + \Delta x_i q_m^{i+1/2} \quad (8.38)$$

Clearly Eqs. 8.35 and 8.36 are equivalent to Eq. 8.13 for $\mu_m > 0$ from the conventional finite difference-discrete ordinates method, and similarly Eqs. 8.37 and 8.38 replace Eq. 8.14 for $\mu_m < 0$. The difference, of course, is that both cell-edged fluxes are unknowns because the incoming flux is not continuous at the boundary. (Reference 21 should be consulted for the detailed equations for one-dimensional spherical and cylindrical geometries.)

Therefore the essential differences between the finite difference–discrete ordinates and finite element–discrete ordinates method can be summarized as follows: (i) the angular flux is not continuous in the spatial variable in the finite element method; (ii) the spatial diamond difference relations are not utilized to relate the cell-edged fluxes—rather, a weighted residual formulation of the finite element method is used to derive an alternative set of equations relating the spatial cell-edged fluxes. The systematic progression through the space angle mesh will be identical to the conventional discrete ordinates method except for the solution of the equations above.

The finite element scheme has two inherent disadvantages when compared with the conventional discrete ordinates method. First, computational times per mesh cell are increased substantially because two relatively complicated equations are solved at each mesh cell rather than the simple diamond difference equations. Second, computer storage requirements are increased considerably because the cell-edged fluxes and sources are needed instead of the cell-centered values. In addition, there are several more coefficients (e.g., the $\phi_m^{i\pm 1/2}$ terms) to be stored for each cell with the finite element scheme.

However these disadvantages are compensated by the ability of the finite element scheme to yield comparable accuracy with a significantly coarser spatial mesh. In addition, the finite element scheme reduces the propensity for negative fluxes and thereby avoids the need for costly negative flux fixup algorithms.

Two-Dimensional Geometries □ The finite element–discrete ordinates scheme has also been applied to two-dimensional x – y and r – z geometries.^{19,20} The mesh is partitioned into triangles (with certain restrictions), and the unknown angular flux is expanded in terms of a set of linear basis functions over each triangular mesh cell. As in the one-dimensional case, the angular flux in the direction of particle flight is assumed to be continuous within a mesh cell, and the flux on an incoming boundary is allowed to be discontinuous. The equations for the cell-edged fluxes are obtained by inserting the expansion for the flux in the discrete ordinates equations, then weighting and integrating. The general procedure is to sweep through the space angle mesh in the direction of particle flight, but now the triangular mesh complicates the situation somewhat. In contrast to orthogonal meshes, the incoming boundaries of a triangular mesh cell are determined by both the direction $\hat{\Omega}_m$ and the orientation of the triangle. Thus the progression through the mesh is not a well-defined operation. For this reason the triangles are restricted to lie on horizontal bands (see Figure 8.20). This allows for a relatively easy determination of the appropriate incoming boundaries.

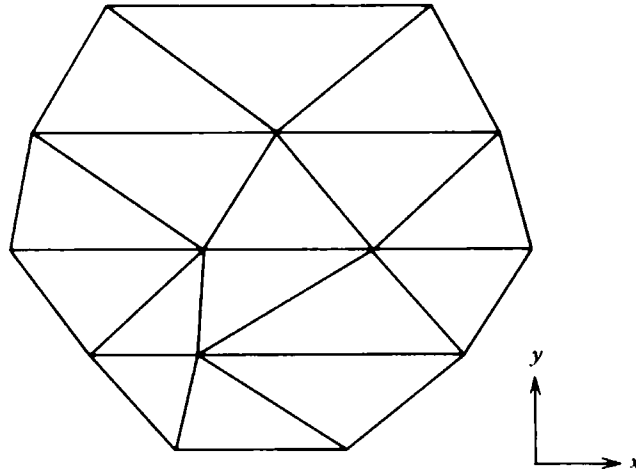


Fig. 8.20 □ TRIDENT mesh structure.

To be more specific, consider the representative triangular mesh cell sketched in Figure 8.21, where there may be triangles adjacent to the triangle of interest. The direction $\hat{\Omega}_m$ determines whether the sides a , b , or c correspond to incoming or outgoing fluxes. If we choose $\hat{\Omega}_m$ as indicated, clearly b is an incoming boundary and a and c are outgoing boundaries. Note that each vertex represents six angular fluxes, one for each triangle, since we are not assuming the flux to be continuous across the triangle boundaries.

The discrete ordinates equations

$$\mu_m \frac{\partial \varphi_m}{\partial x} + \eta_m \frac{\partial \varphi_m}{\partial y} + \Sigma_t(x, y) \varphi_m(x, y) = q_m(x, y) \quad (8.39)$$

are then approximated by the finite element method as follows.²⁰ First the flux $\varphi_m(x, y)$ is expanded in a linear polynomial (in x and y) over the

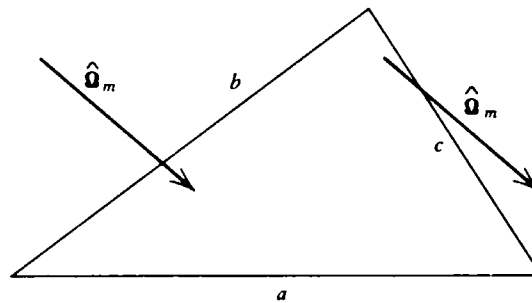


Fig. 8.21 □ Triangular mesh cell.

triangle. Since a linear polynomial in two variables contains three degrees of freedom, three pieces of data will be necessary. These are conveniently chosen to be the vertex fluxes. Therefore, with the appropriate basis functions ψ_i , we have

$$\varphi_m(x, y) = \sum_{j=1}^3 \varphi_m^j \psi_j(x, y) \quad (8.40)$$

Next we substitute Eq. 8.40 into the discrete ordinates equations (8.39), multiply by weighting functions φ_1 , φ_2 , and φ_3 , and integrate over the triangle. Here we use the boundary conditions that the angular flux on a boundary is the limit of the angular flux as the boundary is approached in the direction of particle motion.

The first step implies that the basis functions are unity at the vertex i (corresponding to φ_m^i) and zero at the other vertices. The explicit forms for these basis functions are

$$\begin{aligned} \psi_i^{(1)}(x, y) &= \frac{(x - x_2)(y_3 - y_2) - (x_3 - x_2)(y - y_2)}{(x_3 - x_2)(y_2 - y_1) - (x_2 - x_1)(y_3 - y_2)} \\ \psi_i^{(2)}(x, y) &= \frac{(x - x_3)(y_1 - y_3) - (x_1 - x_3)(y - y_3)}{(x_1 - x_3)(y_3 - y_2) - (x_3 - x_2)(y_1 - y_3)} \\ \psi_i^{(3)}(x, y) &= \frac{(x - x_1)(y_2 - y_1) - (x_2 - x_1)(y - y_1)}{(x_2 - x_1)(y_1 - y_3) - (x_1 - x_3)(y_2 - y_1)} \end{aligned}$$

The weighting functions $\varphi_i(x, y)$, $i = 1, 2, 3$ are chosen to be 1, $x - \bar{x}$, and $y - \bar{y}$, respectively, where $(\bar{x}, \bar{y})$ is the centroid of the triangle. These weighting functions are complete in the space of linear polynomials defined on the triangular domain, therefore could be used to expand the basis functions. That is, this weighting scheme is equivalent to Galerkin weighting.

As mentioned earlier, the progression through the space angle mesh is no longer straightforward. Since a triangle boundary can be incoming or outgoing, depending on its orientation with respect to the specific direction $\hat{\Omega}_m$, a test must be made at each boundary for each direction. The progression through the mesh is begun at the top band. For this band, the incoming directions are in quadrants II or III (see Figure 8.15). First, all directions in quadrant III are swept by progressing through the top band from right to left. If all its incoming fluxes are not known, a triangle is "skipped" temporarily when it is encountered. Figure 8.22 indicates the order in which the triangular mesh cells are analyzed for a typical row.

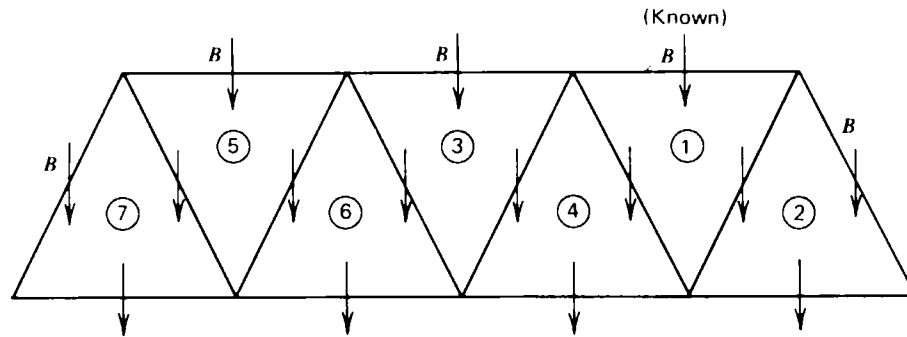


Fig. 8.22 □ Typical progression through triangular mesh (B denotes boundary or known flux from row above and number indicates order of calculation).

Then we can proceed from left to right for all angles in quadrants II. This procedure is repeated for the next band until the bottom band is reached, at which time quadrants I and IV are swept, and the bands are traversed from bottom to top.

Comparison with Conventional Discrete Ordinates Methods □ The finite element treatment in space may seem relatively cumbersome for two-dimensional geometry compared with the conventional diamond difference scheme. It furthermore exhibits a twofold to threefold increase in computation time requirements. Nevertheless the finite element–discrete ordinates method does offer some substantial advantages:

- i Negative fluxes and flux oscillations are strongly suppressed. Thus there is no need for the costly negative flux fixup schemes.
- ii Hexagonal and curvilinear geometries are conveniently treated with a triangular mesh.
- iii The discontinuous finite element scheme couples quite readily with the coarse mesh rebalance acceleration methods (cf. Section 8.1.5).

These advantages may far outweigh the greater complexity of the mesh cell calculations for finite element methods. However every problem is different, and the choice between conventional and finite element discrete ordinates methods should be made on a case-by-case basis.

8.1.5 □ Additional Numerical Considerations □ The efficient implementation of the discrete ordinates method requires several modifications in the basic numerical algorithm such as schemes to accelerate the scattering source iterations or prescriptions to mitigate a variety of deleteri-

ous numerical phenomena including negative fluxes, flux oscillations, and the ray effect. This section briefly considers these problems and examines their treatment in current discrete ordinates codes.

Acceleration Schemes □ The basic algorithm for solving the discrete ordinates equations can be represented by the following matrix iteration equation

$$\boldsymbol{\varphi}^{(n)} = \mathbf{A}^{-1}(\mathbf{B}\boldsymbol{\varphi}^{(n-1)} + \mathbf{S})$$

where $\mathbf{A}$ is the lower diagonal matrix representation of the streaming collision operator, $\hat{\Omega} \cdot \nabla + \Sigma_t$, and $\mathbf{B}$ is the matrix representation of the inscattering operator, $\int d\hat{\Omega}' \Sigma_s(\mathbf{r}, \hat{\Omega}' \rightarrow \hat{\Omega}) \phi(\mathbf{r}, \hat{\Omega}')$. The rate of convergence of the iterations is determined by the relative “sizes” of $\mathbf{A}$ and $\mathbf{B}$. In the extreme case of no scattering, $\mathbf{B} = 0$, and the method converges in one iteration. As the amount of scattering (or equivalently, the scattering ratio $c = \Sigma_s/\Sigma_t$) increases, so in general will the number of iterations required for convergence to an acceptable solution. For problems with large spatial domains that have scattering ratios near unity (e.g., a moderator channel in a nuclear reactor pin cell calculation), the rate of convergence can be unacceptably slow.

Several methods have been proposed and applied to accelerate the convergence of the scattering iteration including coarse mesh rebalance,²²⁻²⁴ Chebyshev acceleration,²⁵ and synthetic methods.²⁶ We discuss only the most popular of these methods, coarse mesh rebalance, and leave the details of the remaining methods to the references.

The essential idea behind the *coarse mesh rebalance* method is to force conservation of neutrons over “coarse” regions of the spatial domain (as compared to the “fine” mesh structure used in the discrete ordinates calculation). The approximate solution is forced to obey particle conservation over these larger regions in the following manner:⁴ Assume that we have partitioned the spatial domain V into coarse mesh regions V_I , $I = 1, 2, \dots, N$. Let us now integrate the neutron continuity equation (see Section 4.2.1) over an arbitrary cell V_I

$$\int_{V_I} d^3r \nabla \cdot \mathbf{J}(\mathbf{r}) + \int_{V_I} d^3r \Sigma_a(\mathbf{r}) \phi(\mathbf{r}) = \int_{V_I} d^3r S(\mathbf{r})$$

and use the divergence theorem to express the streaming term as

$$\int_{V_I} d^3r \nabla \cdot \mathbf{J} = \int_{S_I} dS \hat{\mathbf{e}}_s \cdot \mathbf{J}$$

Using the standard notation for the incoming (−) and outgoing (+) partial currents, we can write

$$\int_{S_I} dS \hat{\mathbf{e}}_s \cdot \mathbf{J} = \int_{S_I} dS J_+ - \int_{S_I} dS J_-$$

therefore the continuity equation yields a particle balance condition:

$$\int_{S_I} dS J_+ - \sum_J \int_{S_{IJ}} dS J_- + \int_{V_I} d^3r \Sigma_a \phi = \int_{V_I} d^3r S$$

Here S_{IJ} is the boundary between coarse mesh regions V_I and V_J , and the summation is taken over all coarse mesh regions V_J that are adjacent to V_I .

Now in general if we were to compute $J_+^{(n)}$, $J_-^{(n)}$, and $\phi^{(n)}$ directly from the results of the n th iteration, the balance condition would not be satisfied. Therefore we attempt to force agreement by determining the set of *rebalance factors* f_I , $I = 1, 2, \dots, N$, which result in the balance condition being satisfied when used as multiplicative factors for both the scalar flux $\phi^{(n)}(\mathbf{r})$ and the outgoing partial current $J_+^{(n)}(\mathbf{r})$ for the corresponding coarse mesh volumes

$$\int_{S_I} dS f_I J_+^{(n)} - \sum_J \int_{S_{IJ}} dS f_J J_-^{(n)} + \int_{V_I} d^3r \Sigma_a f_I \phi^{(n)} = \int_{V_I} d^3r S$$

Since this holds for all I , this is simply a system of equations for the rebalance factors f_I :

$$\mathbf{Rf} = \mathbf{S}$$

We then solve this relatively simple system of equations for the f_I and multiply each of the angular fluxes from the latest iterate $\boldsymbol{\varphi}^{(n)}$ by its corresponding rebalance factor. We then arrive at a rebalanced angular flux estimate, denoted $\tilde{\boldsymbol{\varphi}}^{(n)}$, which may then be used to find $\boldsymbol{\varphi}^{(n+1)}$.

In practice one obtains substantial reductions in computation time with the coarse mesh rebalance method. However the method can result in little or no acceleration²⁷ if one is simultaneously employing the discrete ordinates to spherical harmonics fictitious source scheme to alleviate the ray effect (see next section). In this case it has been found that the use of discontinuous spatial differencing schemes mitigates this difficulty to some extent.²⁸ Thus the use of coarse mesh rebalance has been found to be quite successful when used with the discrete ordinate–finite element methods (TRIPLET/TRIDENT). The general theory of the coarse mesh rebalance method may be found in References 29 and 30.

Negative Fluxes and Flux Oscillations □ Section 8.1.2 discussed the stability and positivity of the diamond difference scheme. We do not expand on this subject any further except to note that the presence of flux oscillations in the discrete ordinates solution is related to the problem of negative fluxes. That is, the diamond difference relations generally result in a prediction of the cell-edged fluxes that oscillate about the actual values. Of course, since the cell-centered flux is the arithmetic mean of the cell-edged fluxes, this would imply that the cell-centered fluxes will be predicted quite well in general. Since the cell-centered fluxes are used in the integral terms [i.e., $\int d^3r \Sigma_s(\mathbf{r})\phi(\mathbf{r})$], the net result of this is that reaction rates are predicted quite well at the expense of the annoying oscillatory behavior of the cell-edged fluxes.⁶ Thus the diamond difference scheme can result in oscillatory fluxes, but as long as they are damped, the net effect is not serious from a computational standpoint. As with negative fluxes, one can shift to a different scheme (e.g., a step function scheme), but then the inherent accuracy of the diamond difference scheme must be sacrificed to mitigate this oscillatory behavior.

The Ray Effect □ The most serious (and well-known) affliction of the discrete ordinates method is the *ray effect*.^{31,32} This phenomenon is not due to the numerical discretization schemes, but rather to the basic discrete ordinates approximation itself which, in essence, consists of solving the transport equation along a few discrete characteristics (i.e., rays). Alternatively, one can describe the discrete ordinates method as a transformation of the rotationally invariant transport equation to a finite set of coupled (via scattering) transport equations that are at most invariant under discrete rotations.

To illustrate why the loss of rotational invariance and the solution of the transport equation along discrete characteristics can lead to defective results, let us consider an isotropic line source in a purely absorbing medium.³ Then clearly the resultant analytical angular flux away from the source will possess azimuthal symmetry about the source. But if we apply the discrete ordinates method to this situation, the resultant angular flux will consist of δ -functions in the azimuthal angle (and polar angle) because only the specific directions emanating from the line source will contain source particles (see Figure 8.23). Although the solutions along the discrete directions $\hat{\Omega}_j$ will be satisfactory, we note that many of the mesh cells are not intersected by an allowable direction from the line source. Since the medium is a pure absorber and the only source of particles is the line source, the angular flux will be identically zero in these mesh cells. Thus the discrete ordinates method approximates the azimuthally uniform angular flux by a discrete set of δ -functions at discrete azimuthal angles. Hence

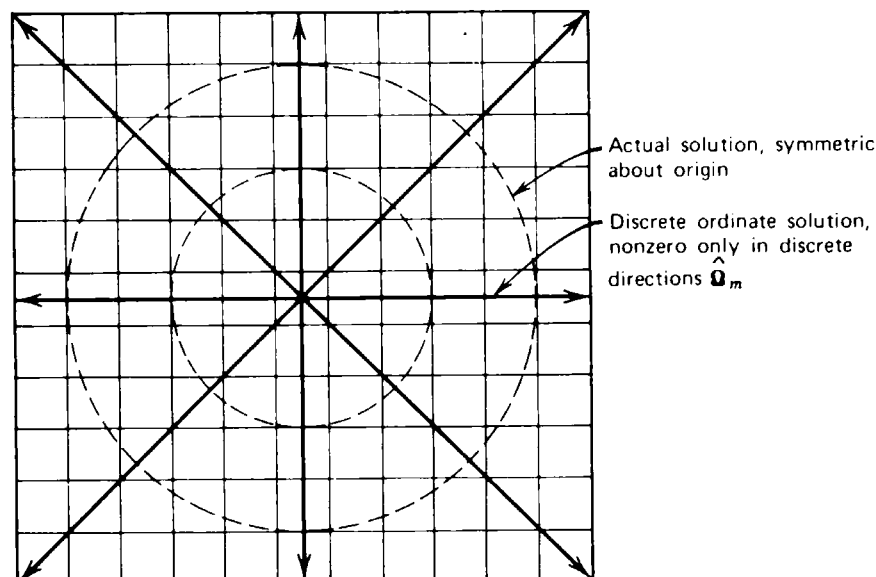


Fig. 8.23 □ Ray effect from an isotropic line source.

for this situation the discrete ordinates approximation is quite poor. This example is admittedly severe, yet there are frequent physical situations that contain elements of the example, such as an isolated source in a strongly absorbing medium.

One potential remedy would be to introduce additional discrete directions. However, in addition to increasing the computational effort significantly, it has been found that some realistic configurations result in ray effects for quadrature sets employing as many as 144 discrete directions.³² Therefore one cannot be assured that this remedy will help.

Another approach that has been quite successful is to transform the discrete ordinates equations to spherical-harmonicslike form. The motivation for this is that the spherical harmonics equations are invariant under arbitrary rotations, as is the transport equation. Therefore the spherical harmonics equations do not exhibit the ray effect under any circumstances. A variety of methods^{27,28,31-34} have been proposed to achieve this conversion by addition of a fictitious source to the discrete ordinates equations. These sources are not unique, and they consist of linear combinations of various derivatives of the angular flux. Numerical results indicate that the $S_N \rightarrow P_{N-1}$ conversion method works quite well in eliminating the ray effect. However it does introduce computer run time penalties because the fictitious source slows down the convergence significantly.²⁷ For example, the use of the $S_N \rightarrow P_{N-1}$ method in the two-dimensional discrete ordinates code TWOTRAN results in an increase in computer time by at least a factor of two.¹⁷

8.1.6 □ Discrete Ordinates Computer Codes □ We conclude this section with a brief review of the standard production-level discrete ordinates computer codes, without attempting to identify the latest versions of the codes. The interested reader should refer to either the Argonne Code Center (ACC) or the Radiation Shielding Information Center (RSIC) at Oak Ridge National Laboratory for current information on these codes and their various versions. Furthermore, we make no attempt to sort through the history of the various codes. (Reference 6 contains an excellent review of the history of various discrete ordinates codes along with a detailed summary of the options available in the codes.) Finally, since most of these codes have versions that are intended for specific computer systems, the user should consult either the ACC or RSIC catalogs for further information regarding which version is compatible for a particular system.

ANISN (ORNL). The ANISN code is an efficient, versatile multigroup discrete ordinates code that may be used directly for neutron or gamma transport in one-dimensional slab, spherical, or cylindrical geometries. ANISN allows general order anisotropic scattering. Cross section data can be prepared either by compatible cross section codes (e.g., TAPEMAKER) or directly as macroscopic data. ANISN offers a wide variety of boundary condition options, source options, and criticality search options. ANISN also allows the option of performing a diffusion theory solution to initiate the S_N algorithm.

DTF-IV (LASL). Similar to ANISN in its capabilities, DTF-IV is a general purpose multigroup discrete ordinates code for neutron or gamma transport in one-dimensional slab, spherical, or cylindrical geometries.

ONETRAN (LASL). ONETRAN employs discrete ordinates in angle with a local, discontinuous finite element method in space and is applicable for neutron or gamma transport in one-dimensional slab, spherical, or cylindrical geometries. It also allows a general angular treatment for one-dimensional slab geometries that do not exhibit any symmetries in the angular domain. ONETRAN offers roughly the same options as the ANISN/DTF-IV codes, but the computational time in general is greater because of the discontinuous finite element approach. However, as noted in Section 8.1.3, for problems with severe heterogeneities, ONETRAN should offer significant advantages over the standard discrete ordinates codes.

DOT (ORNL). The DOT code is a multigroup discrete ordinates code for two-dimensional geometries. DOT can treat general order anisotropic scattering and has a wide variety of options for sources, boundary conditions, criticality searches, and so on.

TWOTRAN (LASL). The capabilities of TWOTRAN are similar to those of DOT in that TWOTRAN is a multigroup discrete ordinates code for two-dimensional geometries with many of the same options as the ORNL code.

TRIDENT (LASL). TRIDENT, originally known as TRIPLET, was the first production level transport code to employ finite element methods. The code combines discrete ordinates methods in angle with a discontinuous finite element scheme in space. Although there are restrictions on the triangular mesh, TRIDENT may be applied to irregular domains such as a hexagonal mesh. The computer run times are greater by a factor of 2 or 3 than those for a conventional discrete ordinates code such as TWOTRAN, but the increased capability for treating strong heterogeneities and the flexibility allowed by using a triangular mesh may overcome this disadvantage for many applications.

8.2 □ SPHERICAL HARMONICS (P_N) METHOD □ In Chapter 4 we developed a consistent procedure for representing the angular dependence of the flux $\varphi(\mathbf{r}, \hat{\Omega})$ as an expansion in spherical harmonics $Y_{lm}(\hat{\Omega})$. This led to a set of equations for the expansion coefficients, which when appropriately truncated were known as the P_N equations or the P_N approximation. Although these equations have been used primarily for theoretical (i.e., analytical) investigations of solutions of the transport equation, under certain circumstances they can be used as the basis for numerical methods for solving the transport equation.

This section demonstrates the formal equivalence³⁵⁻³⁷ between the P_N equations in plane geometry and the discrete ordinates equations with Gaussian quadrature, then discusses the numerical solution of these equations.

8.2.1 □ Equivalence of the P_N and Discrete Ordinates Equations □ To demonstrate that the S_N equations using Gaussian quadrature are formally equivalent to the P_{N-1} equations with Mark boundary conditions, we first prove that the moments of the angular flux determined with the discrete ordinates equations satisfy the same equations as the spherical harmonics moments. To this end, we define the discrete ordinates moments for the angular flux and source as

$$\begin{aligned}\bar{\varphi}_l(x) &= 2\pi \sum_{m=1}^N w_m P_l(\mu_m) \varphi(x, \mu_m) \\ \bar{s}_l(x) &= 2\pi \sum_{m=1}^N w_m P_l(\mu_m) s(x, \mu_m)\end{aligned}$$

and the spherical harmonics moments as

$$\varphi_l(x) = 2\pi \int_{-1}^{+1} d\mu P_l(\mu) \varphi(x, \mu)$$

Next, multiply the discrete ordinates equations

$$\mu_m \frac{d\varphi_m}{dx} + \Sigma_l \varphi_m(x) = \sum_{l'=0}^L \left(\frac{2l'+1}{4\pi} \right) \Sigma_{sl'} \tilde{\varphi}_{l'}(x) P_{l'}(\mu_m) + s_m$$

by $2\pi w_m P_l(\mu_m)$ and sum over all m to find

$$\begin{aligned} 2\pi \sum_{m=1}^N w_m P_l(\mu_m) \mu_m \frac{d\varphi_m}{dx} + 2\pi \Sigma_l \sum_{m=1}^N w_m P_l(\mu_m) \varphi(x, \mu_m) \\ = 2\pi \sum_{l'=0}^L \left(\frac{2l'+1}{4\pi} \right) \Sigma_{sl'} \tilde{\varphi}_{l'}(x) \sum_{m=1}^N w_m P_l(\mu_m) P_{l'}(\mu_m) \\ + 2\pi \sum_{m=1}^N w_m P_l(\mu_m) s(x, \mu_m) \end{aligned} \quad (8.41)$$

If we use the definition for $\tilde{\varphi}_{l'}(x)$ and the identity

$$\mu P_l(\mu) = \frac{l+1}{2l+1} P_{l+1}(\mu) + \frac{l}{2l+1} P_{l-1}(\mu)$$

then Eq. 8.41 becomes

$$\begin{aligned} \frac{l+1}{2l+1} \frac{d\tilde{\varphi}_{l+1}}{dx} + \frac{l}{2l+1} \frac{d\tilde{\varphi}_{l-1}}{dx} + \Sigma_l \tilde{\varphi}_l(x) \\ = 2\pi \sum_{l'=0}^L \left(\frac{2l'+1}{4\pi} \right) \Sigma_{sl'} \tilde{\varphi}_{l'}(x) \sum_{m=1}^N w_m P_l(\mu_m) P_{l'}(\mu_m) + \tilde{s}_l \end{aligned} \quad (8.42)$$

This equation holds for $l=0, 1, 2, \dots, N-1$. But we recall from Section 8.1.1 that N point Gaussian quadrature will integrate a $2N-1$ degree polynomial exactly. Therefore if $l+l' \leq 2N-1$ in Eq. 8.42, then

$$\sum_{m=1}^N w_m P_l(\mu_m) P_{l'}(\mu_m) = \int_{-1}^{+1} d\mu P_l(\mu) P_{l'}(\mu) = \frac{2}{2l+1} \delta_{ll'} \quad (8.43)$$

But by assumption, $l \leq N-1$ and $l' \leq L$. Therefore if $L \leq N$, Eq. 8.43 is valid. This restriction on L that the order of anisotropy be less than or

equal to the order of the discrete ordinates approximation is very reasonable in practice. If we now substitute Eq. 8.43 into Eq. 8.42, we find that the $\tilde{\varphi}_l(x)$ satisfy the same equations as the true Legendre moments $\varphi_l(x)$.

Let us recall that in the P_N method, we truncate the set Eq. 8.42 by assuming

$$\frac{d\varphi_l}{dx} = 0 \quad \text{for } l \geq N$$

To achieve this with our S_N representation, we require

$$\tilde{\varphi}_N(x) = 2\pi \sum_{m=1}^N w_m P_N(\mu_m) \varphi(x, \mu_m) = 0$$

—that is, we would require the set of $\{\mu_m\}$ we have chosen to have the property that $P_N(\mu_m) = 0$ for all m . But the zeros of $P_N(\mu)$ are just the Gauss quadrature points $\{\mu_m\}$ of order N .

Finally we need only recognize that the discrete ordinate representation of the true vacuum boundary conditions for Eq. 8.41 correspond to Mark's prescription for obtaining boundary conditions for the P_N method. Therefore we have formally demonstrated that

$$\left[\begin{array}{l} S_N \text{ discrete ordinates} \\ \text{equations with} \\ \text{Gaussian quadrature} \end{array} \right] = \left[\begin{array}{l} P_{N-1} \text{ equations with} \\ \text{Mark boundary} \\ \text{conditions} \end{array} \right]$$

Furthermore, if we agree to define $\varphi(x, \mu)$ for $\mu \neq \mu_m$ as

$$\varphi(x, \mu) = \sum_{l=0}^N \left(\frac{2l+1}{4\pi} \right) \tilde{\varphi}_l(x) P_l(\mu)$$

we can generate the Legendre expansion coefficients $\tilde{\varphi}_l(x)$, hence the P_N solution using a discrete ordinates calculation. (The same argument can be used to relate DP_N to DS_N methods.)

8.2.2 □ Solution of the P_N Equations □ The most common methods used for a direct solution of the P_N equations involve the elimination of odd-order angular moments to yield a set of coupled-diffusionlike equations. To illustrate one such approach³⁸ we consider the P_3 equations in

plane geometry (adopting the notation $\varphi'_n = d\varphi_n/dx$ and $\Sigma_{ii} = \Sigma_i - \Sigma_{si}$)

$$\begin{aligned}\varphi'_1 + \Sigma_a \varphi_0 &= S \\ \frac{2}{3} \varphi'_2 + \frac{1}{3} \varphi'_0 + \Sigma_{t1} \varphi_1 &= 0 \\ \frac{3}{5} \varphi'_3 + \frac{2}{5} \varphi'_1 + \Sigma_{t2} \varphi_2 &= 0 \\ \frac{3}{7} \varphi'_2 + \Sigma_{t3} \varphi_3 &= 0\end{aligned}\tag{8.44}$$

If we define

$$\Phi_0 = \varphi_0 + 2\varphi_2 \quad \text{and} \quad \Phi_1 = \varphi_1$$

we can rearrange the P_3 equations into the form

$$\begin{aligned}-D_1 \Phi_0'' + \Sigma_a \Phi_0 &= S + 2\Sigma_a \Phi_1 \\ -D_2 \Phi_1'' + \alpha \Phi_1 &= -\frac{2}{3} S + \frac{2}{3} \Sigma_a \Phi_0\end{aligned}$$

where we define

$$D_1 = (3\Sigma_{t1})^{-1}, \quad D_2 = (3/7\Sigma_{t3}), \quad \alpha = \frac{5}{3}\Sigma_{t2} + \frac{4}{3}\Sigma_a$$

But these are simply two coupled diffusion equations that can readily be solved with standard diffusion computer codes with appropriately defined diffusion coefficients. Unfortunately, this method cannot be applied in two-dimensional geometry because the resulting equations cannot be reduced to a second order equation in one moment (or a linear combination of moments such as Φ_0 above). However if one is willing to include the extra second order derivative terms as source terms within a source iteration solution technique, this problem can be avoided. In fact, this approach forms the basis for a second method for solving the P_N equations.^{39,40}

In the latter approach we do not attempt to derive diffusionlike equations for one moment alone. Again we illustrate the method with the P_3 equations (8.44). We begin by guessing an initial solution, $\varphi_0^{(0)}$, $\varphi_2^{(0)}$ (the odd moments are not computed). The following steps are then performed in an iterative fashion. (i) First differentiate the odd moment P_N equations [the second and fourth equations in the set (8.44)]. (ii) Eliminate the odd moments from the differentiated equations by using the equation for the preceding moment. (iii) Solve the resulting diffusionlike second order equations for the even moments by treating all unknown terms as source

terms. (iv) Continue this procedure until the even moments converge.

To be more explicit, step i yields for the P_3 equations (8.44):

$$\begin{aligned}\frac{2}{3}\varphi_2'' + \frac{1}{3}\varphi_0'' + \Sigma_{i1}\varphi_1' &= 0 \\ \frac{3}{7}\varphi_2'' + \Sigma_{i3}\varphi_3' &= 0\end{aligned}\quad (8.45)$$

But φ_1' in the first of these equations can be eliminated in Eq. 8.44

$$\varphi_1' = S - \Sigma_a\varphi_0$$

and therefore step ii has been completed. We now have

$$\frac{2}{3}\varphi_2'' + \frac{1}{3}\varphi_0'' + \Sigma_{i1}(S - \Sigma_a\varphi_0) = 0$$

or, rearranging,

$$-\frac{1}{3}\varphi_0'' + \Sigma_{i1}\Sigma_a\varphi_0 = \frac{2}{3}\varphi_2'' + \Sigma_{i1}S$$

which is the desired second order elliptic equation for φ_0 . This may be solved for φ_0 using a standard diffusion theory computer code. Note that we have included φ_2'' in the source term, since it is known either from the initial estimate $\varphi_2^{(0)}$ or the previous iteration. The next step is to solve for φ_3' in the third of Eqs. 8.44:

$$\varphi_3' = -\frac{5}{3}\left(\frac{2}{5}\varphi_1' + \Sigma_{i2}\varphi_2\right)$$

and then substitute for φ_1' from the first equation in this set

$$\varphi_3' = -\frac{5}{3}\left(\frac{2}{5}(S - \Sigma_a\varphi_0) + \Sigma_{i2}\varphi_2\right)$$

This is now used in the second of the differentiated equations (8.45) to obtain

$$-\frac{3}{7}\varphi_2'' + \frac{5}{3}\Sigma_{i3}\Sigma_{i2}\varphi_2 = -\frac{2}{3}\Sigma_{i3}S + \frac{2}{3}\Sigma_{i3}\Sigma_a\varphi_0$$

which may be solved for φ_2 . Since this is the last of the P_3 equations, we repeat the process until φ_0 and φ_2 converge to within some prescribed precision.

The attractive aspect of this scheme is that it can be applied to the two- and three-dimensional spherical harmonics equations. Interestingly enough, these spherical harmonics equations are so complicated that a

computer program has been used to differentiate the equations and perform the algebraic manipulations to arrive at the equations for the even flux moments.⁴⁰

8.3 □ THE FINITE ELEMENT METHOD □ The *finite element method* is the name commonly applied to the expansion of the solution to a set of partial differential equations in a set of local basis functions. Either variational or weighted residual methods are then used to arrive at a sparse matrix representation of the original problem. This method has received attention recently as a promising alternative to conventional techniques such as spherical harmonics or discrete ordinates for solving the transport equation. We have already considered one application of this approach when we expanded the spatial dependence of the angular flux in finite element basis functions to develop an alternative to the conventional finite difference–discrete ordinates equations. This section examines the more general application of finite element methods to both the space and angle variables in the transport equation.

The finite element method was first applied in the mid-1950s to a variety of problems in structural mechanics. Since that time finite element methods have been developed for such diverse areas as fluid mechanics, heat transfer, and neutron diffusion.^{41,42}

The success of the finite element method may be partially attributed to its versatility for treating quite general classes of partial differential equations. However it also presents decided advantages for handling complex, irregular geometries, and its firm theoretical foundation in approximation theory guarantees the convergence of the approximate solution in most applications of interest.⁴³

The application of the finite element method to transport problems has been a relatively recent venture. A variety of approaches have been studied, including finite element expansions in both the space and angle variables for both the traditional (non-self-adjoint)^{44–48} and the even and odd parity second-order forms of the transport equation.^{49–55} The combination of finite element and discrete ordinates methods was discussed in Section 8.1.4. These activities have led to the development of several production level and research transport computer codes based on such methods (e.g., ONETRAN,²¹ TRIDENT,²⁰ ZEPHYR,⁵⁶ FENT,⁵⁰ AND FTRAN⁴⁸).

This section investigates the application of finite element methods in space and angle variables to both the first and second order forms of the transport equation. We develop most of our analysis for the more conventional first order form, then contrast the differences that arise when

applying finite element methods to the second order, even-parity transport equation. We conclude with a summary of the relative advantages and disadvantages of finite element methods when compared with the more traditional finite difference–discrete ordinates approach.

8.3.1 □ Application of Finite Element Methods to the First Order Form of the Transport Equation □

The finite element method is always applied to an integral formulation of the original partial differential equation of interest. For example, one might introduce the finite element method as a suitable trial function in a variational principle having the original equation as its Euler equation. Alternatively, the solution of the weak (or integral) form of the partial differential equation can be expanded in a set of finite element basis functions.

For the case of a self-adjoint system such as the one-speed diffusion equation, these approaches are equivalent.⁵⁷ However since the first order transport equation is not self-adjoint, there is no extremum principle available. We have no choice but to apply the finite element method to the solution of the weak or integral law form of this equation. By way of contrast, the second order transport equations (even and odd parity forms) are self-adjoint, and one can proceed from a variational principle.

Integral Law (or Weak) Form of the Transport Equation □ Let us first consider the derivation of the integral law corresponding to the first order transport equation.^{46,48} The time-independent, one-speed form of this equation is as follows:

$$\hat{\Omega} \cdot \nabla \varphi + \Sigma_t(\mathbf{r})\varphi(\mathbf{r}, \hat{\Omega}) = \int d\hat{\Omega}' \Sigma_s(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega})\varphi(\mathbf{r}, \hat{\Omega}') + s(\mathbf{r}, \hat{\Omega}) \quad (8.46)$$

where, for simplicity, we assume inhomogeneous boundary conditions: $\varphi(\mathbf{r}_s, \hat{\Omega}) = \varphi_0(\mathbf{r}_s, \hat{\Omega})$, $\hat{\Omega} \cdot \hat{\mathbf{e}}_s < 0$. The following notation is introduced for convenience:

- R = spatial domain
- 4π = angular domain
- V = phase space domain $R \times 4\pi$
- ∂R = boundary of R
- Γ = boundary of $V = \partial R \times 4\pi$
- $\Gamma^\pm$ = outgoing (or ingoing) boundary [i.e., all $(\mathbf{r}, \hat{\Omega}) \in \Gamma$ such that $\hat{\Omega} \cdot \hat{\mathbf{e}}_s \gtrless 0$]

For the general analysis that follows, we introduce the space of allowable

solutions:

$$H_E = \left\{ \psi(\mathbf{r}, \hat{\Omega}) : \text{real } \psi(\mathbf{r}, \hat{\Omega}) \text{ such that } \int \int_V d\mathbf{r} d\hat{\Omega} [|\Psi|^2 + |\nabla \Psi|^2] < \infty \right\}$$

This class of functions is sometimes referred to as an “energy” or “Sobolev” space. The specific definition of the space is designed to ensure that phase space integrals that arise in the subsequent analysis will exist. Later we specialize this space of functions to be a finite element subspace, for example, the space of linear, piecewise polynomials defined on the interval $x \in [0, 1]$ and $\mu \in [-1, +1]$.

The derivation of the integral law is actually quite simple. We multiply Eq. 8.46 by an arbitrary $\psi(\mathbf{r}, \hat{\Omega}) \in H_E$ and integrate over the phase space V :

$$\begin{aligned} \int \int_V d\mathbf{r} d\hat{\Omega} \psi(\mathbf{r}, \hat{\Omega}) [\hat{\Omega} \cdot \nabla \varphi + \Sigma_t \varphi] \\ = \int \int_V d\mathbf{r} d\hat{\Omega} \psi(\mathbf{r}, \hat{\Omega}) \left[\int d\hat{\Omega}' \Sigma_s(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega}) \varphi(\mathbf{r}, \hat{\Omega}') + s \right] \end{aligned} \quad (8.47)$$

The general idea now is to manipulate this equation into a form that includes the boundary conditions by using integration by parts. To simplify the notation, we define the real inner product

$$(f, g) \equiv \int \int_V d\mathbf{r} d\hat{\Omega} f(\mathbf{r}, \hat{\Omega}) g(\mathbf{r}, \hat{\Omega})$$

where f and g are two elements of H_E . We also define an inner product that characterizes the boundary:

$$\langle f, g \rangle \equiv \int \int_{\Gamma} dS d\hat{\Omega} \hat{\Omega} \cdot \hat{\mathbf{e}}_s f(\mathbf{r}_s, \hat{\Omega}) g(\mathbf{r}_s, \hat{\Omega})$$

as well as inner products characterizing incoming (Γ^-) and outgoing (Γ^+) directions

$$\langle f, g \rangle \equiv \int \int_{\Gamma^\pm} dS d\hat{\Omega} |\hat{\Omega} \cdot \hat{\mathbf{e}}_s| f(\mathbf{r}_s, \hat{\Omega}) g(\mathbf{r}_s, \hat{\Omega})$$

It should be noted here that $\langle f, g \rangle = \langle f, g \rangle_+ - \langle f, g \rangle_-$. We will also define the collision operator K

$$K \circ \equiv \Sigma_t(\mathbf{r}) \circ - \int d\hat{\Omega}' \Sigma_s(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega}) \circ$$

Using these definitions, we can now rewrite Eq. 8.47 as follows:

$$(\hat{\Omega} \cdot \nabla \varphi, \psi) + (K\varphi, \psi) = (s, \psi) \quad (8.48)$$

If we now notice that

$$\psi \hat{\Omega} \cdot \nabla \varphi = \nabla \cdot \hat{\Omega}(\psi \varphi) - \varphi \nabla \cdot \hat{\Omega} \psi$$

we can integrate the streaming term in Eq. 8.48 by parts

$$(\hat{\Omega} \cdot \nabla \varphi, \psi) = \langle \varphi, \psi \rangle - (\varphi, \hat{\Omega} \cdot \nabla \psi)$$

so that Eq. 8.48 becomes

$$-(\varphi, \hat{\Omega} \cdot \nabla \psi) + \langle \varphi, \psi \rangle + (K\varphi, \psi) = (s, \psi) \quad (8.49)$$

But now we note that the boundary term can be decomposed as

$$\langle \varphi, \psi \rangle = \langle \varphi, \psi \rangle_+ - \langle \varphi, \psi \rangle_-$$

We are given that $\varphi(\mathbf{r}, \hat{\Omega}) = \varphi_0(\mathbf{r}, \hat{\Omega})$ on Γ^- , or

$$\langle \varphi, \psi \rangle_- = \langle \varphi_0, \psi \rangle_-$$

Therefore we can rewrite Eq. 8.49 as follows:

$$-(\varphi, \hat{\Omega} \cdot \nabla \psi) + \langle \varphi, \psi \rangle_+ + (K\varphi, \psi) = (s, \psi) + \langle \varphi_0, \psi \rangle_-$$

This is known as the *integral law* or *weak form*⁵⁷ of the transport equation (8.46). More precisely, we identify the integral law or weak formulation of the transport equation as follows: find a function $\varphi(\mathbf{r}, \hat{\Omega}) \in H_E$ such that for all $\psi(\mathbf{r}, \hat{\Omega}) \in H_E$

$$-(\varphi, \hat{\Omega} \cdot \nabla \psi) + \langle \varphi, \psi \rangle_+ + (K\varphi, \psi) = (s, \psi) + \langle \varphi_0, \psi \rangle_- \quad (8.50)$$

To demonstrate that Eqs. 8.50 and 8.46 are equivalent, assume that a solution $\tilde{\varphi}(\mathbf{r}, \hat{\Omega})$ has been found to Eq. 8.50. Now integrate Eq. 8.50 by parts to find

$$(\hat{\Omega} \cdot \nabla \tilde{\varphi}, \psi) + (K\tilde{\varphi}, \psi) + \langle \tilde{\varphi}, \psi \rangle_- = (s, \psi) + \langle \varphi_0, \psi \rangle_- \quad (8.51)$$

Since this equation is valid for all $\psi \in H_E$, it must be valid for the subspace H_E^B that consists of all $\psi \in H_E$ that vanish on Γ^- :

$$(\hat{\Omega} \cdot \nabla \tilde{\varphi} + K\tilde{\varphi} - s, \psi) = 0 \quad \text{for all } \psi \in H_E^B$$

But ψ is arbitrary; therefore,

$$\hat{\Omega} \cdot \nabla \tilde{\varphi} + K\tilde{\varphi} = s \quad (8.52)$$

which, of course, is just the original transport equation (8.46). To retrieve the boundary conditions, we can substitute Eq. 8.52 into Eq. 8.51 to find

$$\langle \tilde{\varphi} - \varphi_0, \psi \rangle_- = 0 \quad \text{for all } \psi \in H_E$$

But for this to be valid in general, it must hold that $\tilde{\varphi} = \varphi_0$ on Γ^- . Thus the equivalence of Eqs. 8.50 and 8.46 has been demonstrated.

Treatment of Boundary Conditions □ It is important to note that the boundary condition $\varphi = \varphi_0$ on Γ^- is included in the integral law (Eq. 8.50). It will be naturally satisfied by the solution $\varphi(\mathbf{r}, \hat{\Omega})$, even though we did not explicitly require the entire solution space H_E to satisfy it. This is an example of a *natural* boundary condition. Such boundary conditions are not imposed directly on the space of solutions, but rather result as a consequence of the integral law itself.

If we had not integrated Eq. 8.48 by parts, our integral law would have read: find $\varphi(\mathbf{r}, \hat{\Omega}) \in H_E^B$ such that for all $\psi(\mathbf{r}, \hat{\Omega}) \in H_E^B$,

$$(\hat{\Omega} \cdot \nabla \varphi, \psi) + (K\varphi, \psi) = (s, \psi)$$

where we have now restricted our allowable space of solutions to those φ in H_E that also satisfy the boundary condition, $\varphi = \varphi_0$ on Γ^- . In this case, we refer to the condition as an *essential* boundary condition. This formulation of the finite element method will not be considered further.

This is a general feature of the finite element method. An integration by parts is usually performed that will lead to natural boundary conditions. As we see when we analyze the second order form of the transport equation, the use of a variational principle reduces the order of the derivatives in addition to producing boundary terms.

It should be stressed that in the application of finite element methods to the first order form of the transport equation, all boundary conditions are treated as natural boundary conditions. That is, one simply substitutes the expression for φ on Γ^- into the surface term

$$\langle \varphi, \psi \rangle_- = \iint_{\Gamma^-} dS d\hat{\Omega} |\hat{\Omega} \cdot \hat{\mathbf{e}}_s| \varphi(\mathbf{r}, \hat{\Omega}) \psi(\mathbf{r}, \hat{\Omega})$$

If the boundary conditions are implicit, one substitutes the relation between φ on Γ^- to φ on Γ^+ into $\langle \varphi, \psi \rangle_{\pm}$. This becomes more evident when

we consider the specific case of one-dimensional plane symmetry in the next section.

The Approximate Integral Law □ The integral law is now in a form that is amenable to approximation by way of the finite element method. That is, rather than attempting to find a solution $\varphi(\mathbf{r}, \hat{\Omega})$ of Eq. 8.50 in the space H_E , we seek the solution in a “finite element” subspace $S^h \subset H_E$. More specifically, we will seek a solution $\varphi^h(\mathbf{r}, \hat{\Omega}) \in S^h$ such that Eq. 8.50 is satisfied for all $\psi^h(\mathbf{r}, \hat{\Omega}) \in S^h$. Here, h is a parameter that depends on the mesh spacing to be used in the approximate solution; S^h is a specially constructed subspace with basis functions $\psi_i^h(\mathbf{r}, \hat{\Omega})$, $i = 1, 2, \dots, N$, where N is the dimension of S^h (typically the number of nodes in the mesh). Details on the actual construction of such a subspace are deferred to the next section. However, it is worthwhile to note here that the basis functions are *local* in the sense that

$$\iint_V d\mathbf{r} d\hat{\Omega} \psi_i^h(\mathbf{r}, \hat{\Omega}) \psi_j^h(\mathbf{r}, \hat{\Omega})$$

is nonzero only when the nodes i and j are close together.

When we restrict ourselves to this subspace, we arrive at an approximate form of the integral law: find $\varphi^h(\mathbf{r}, \hat{\Omega}) \in S^h$ such that for all $\psi^h(\mathbf{r}, \hat{\Omega}) \in S^h$,

$$-(\varphi^h, \hat{\Omega} \cdot \nabla \psi^h) + \langle \varphi^h, \psi^h \rangle_+ + (K\varphi^h, \psi^h) = (s, \psi^h) + \langle \varphi_0, \psi^h \rangle_- \quad (8.53)$$

Since S^h is finite dimensional and $\varphi^h \in S^h$, we can expand φ^h in the basis functions

$$\varphi^h(\mathbf{r}, \hat{\Omega}) = \sum_{j=1}^N \varphi_j \psi_j^h(\mathbf{r}, \hat{\Omega})$$

and it is sufficient to require Eq. 8.53 to hold for all $\psi_i^h(\mathbf{r}, \hat{\Omega})$, $i = 1, 2, \dots, N$ to ensure that Eq. 8.53 is valid for all $\psi^h(\mathbf{r}, \hat{\Omega}) \in S^h$:

$$\begin{aligned} -\left(\sum_{j=1}^N \varphi_j \psi_j^h, \hat{\Omega} \cdot \nabla \psi_i^h\right) + \left\langle \sum_{j=1}^N \varphi_j \psi_j^h, \psi_i^h \right\rangle_+ + \left(K \sum_{j=1}^N \varphi_j \psi_j^h, \psi_i^h\right) \\ = (s, \psi_i^h) + \langle \varphi_0, \psi_i^h \rangle_- \end{aligned}$$

If we take the summation outside of the integrals, we arrive at the matrix system

$$A\varphi = S \quad (8.54)$$

where

$$\begin{aligned}
 A_{ij} &\equiv -(\psi_j^h, \hat{\Omega} \cdot \nabla \psi_i^h) + \langle \psi_j^h, \psi_i^h \rangle_+ + (K\psi_j^h, \psi_i^h) \\
 &= \iint_V d\mathbf{r} d\hat{\Omega} \psi_j^h (-\hat{\Omega} \cdot \nabla + \Sigma_i) \psi_i^h + \iint_{\Gamma^+} dS d\hat{\Omega} \hat{\Omega} \cdot \hat{\mathbf{e}}_s \psi_i^h \psi_j^h \\
 &\quad - \iint_V d\mathbf{r} d\hat{\Omega} \psi_i^h \int d\hat{\Omega}' \Sigma_s(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega}) \psi_j^h(\mathbf{r}, \hat{\Omega}') \\
 S_i &\equiv (s, \psi_i^h) = \iint_V d\mathbf{r} d\hat{\Omega} s(\mathbf{r}, \hat{\Omega}) \psi_i^h(\mathbf{r}, \hat{\Omega}) \\
 \boldsymbol{\varphi} &= \text{col}(\varphi_1, \varphi_2, \dots, \varphi_N)
 \end{aligned}$$

At this point we might note that the construction of the subspace S^h has not entered the discussion, and Eq. 8.54 could very well be applicable to any Galerkin formulation. However, it will be demonstrated that choosing a finite element basis considerably simplifies the calculations. More important, it will result in convergence to the actual solution as the mesh spacing is refined ($h \rightarrow 0$). That is, if $\varphi(\mathbf{r}, \hat{\Omega})$ is the actual solution, then $\lim_{h \rightarrow 0} \varphi^h(\mathbf{r}, \hat{\Omega}) \rightarrow \varphi(\mathbf{r}, \hat{\Omega})$ (in a suitable measure or norm).

Convergence of the Finite Element Solution □ Let us briefly examine the convergence properties of the finite element method.⁵⁸ Although the following remarks have been rigorously proved only for second order, self-adjoint systems (e.g., the one-speed diffusion equation), there is sufficient numerical evidence to indicate their more general validity for the first order, non-self-adjoint form of the transport equation.

In general, if the finite element method is applied to a second order, self-adjoint operator L [e.g., $L = -(d/dx) D(x) (d/dx) + \Sigma_a$], it can be shown that the L_2 error ϵ in the approximate solution $\varphi^h(\mathbf{r})$,

$$\epsilon = \left[\int d^3r |\varphi(\mathbf{r}) - \varphi^h(\mathbf{r})|^2 \right]^{1/2}$$

is less than the L_2 error for any other approximation that can be formed within the finite element subspace S^h

$$\left[\int d^3r |\varphi(\mathbf{r}) - \varphi^h(\mathbf{r})|^2 \right]^{1/2} \leq \left[\int d^3r |\varphi(\mathbf{r}) - \chi^h(\mathbf{r})|^2 \right]^{1/2}, \quad \text{for all } \chi^h \in S^h$$

(8.55)

But now we note that the finite element subspaces under consideration consist of piecewise polynomials. Therefore we can appeal to approximation theory to ascertain the degree to which the space of piecewise polynomials S^h can approximate an arbitrary function $f(\mathbf{r})$. In particular, if $f(\mathbf{r})$ has a square-integrable gradient over the domain R , there exists an approximation $f^h(\mathbf{r}) \in S^h$ such that

$$\left[\int d^3r |f(\mathbf{r}) - f^h(\mathbf{r})|^2 \right]^{1/2} \leq ch^{k+1}$$

where h is the mesh spacing, k the degree of the piecewise polynomials, and c is a constant independent of h or k . For example, $k=1$ for linear piecewise polynomials, and therefore for this case

$$\left[\int d^3r |f(\mathbf{r}) - f^h(\mathbf{r})|^2 \right]^{1/2} \leq ch^2$$

But from Eq. 8.55 we know that $\varphi^h(\mathbf{r})$ is at least as close to the true solution $\varphi(\mathbf{r})$ as this particular approximation. Therefore

$$\left[\int d^3r |\varphi(\mathbf{r}) - \varphi^h(\mathbf{r})|^2 \right]^{1/2} \leq ch^{k+1}$$

and as $h \rightarrow 0$, we conclude that $\varphi^h(\mathbf{r}) \rightarrow \varphi(\mathbf{r})$ (in the L_2 measure).

These remarks have yet to be proved for the first order transport equation, but numerical results^{47,48} substantiate the following claim for the error in the approximate solution of this equation:

$$\left[\iint_V d^3r d\hat{\Omega} |\varphi(\mathbf{r}, \hat{\Omega}) - \varphi^h(\mathbf{r}, \hat{\Omega})|^2 \right]^{1/2} \leq ch^{k+1}$$

Therefore the finite element method yields the “best” possible solution from the space of allowable trial functions. Since approximation theory tells us that the space of piecewise polynomials is capable of approximating the unknown solution to any degree of accuracy, we are assured that the finite element solution will be at least as accurate.

Specific Application to One-Dimensional Plane Geometry □ To illustrate this approach, we apply the finite element method to the one-dimensional transport equation in plane geometry. For simplicity, we consider the

transport equation for a homogeneous slab on the interval $0 \leq x \leq 1$

$$\mu \frac{\partial \varphi}{\partial x} + \Sigma_t(x) \varphi(x, \mu) = \sum_{l=0}^L \left(\frac{2l+1}{2} \right) \Sigma_{sl}(x) P_l(\mu) \int_{-1}^{+1} d\mu' P_l(\mu') \varphi(x, \mu') + s(x, \mu) \quad (8.56)$$

We chose an inhomogeneous boundary condition at $x=1$, $\varphi(1, \mu) = \varphi_0(x, \mu)$ for $\mu < 0$, and a reflecting boundary condition at $x=0$, $\varphi(0, \mu) = \varphi(0, -\mu)$. Figure 8.24 depicts the x - μ mesh structure. The finite element subspace S^h is spanned by the basis functions $\psi_i^h(x, \mu)$, $i=1, 2, \dots, N$. The subscript i refers to a particular space angle node.

We now multiply Eq. 8.56 by an arbitrary $\psi_i^h(x, \mu)$ and integrate over the x - μ phase space:

$$\begin{aligned} & \int_0^1 dx \int_{-1}^{+1} d\mu \psi_i^h(x, \mu) \left[\mu \frac{\partial \varphi}{\partial x} + \Sigma_t \varphi \right] \\ & - \int_0^1 dx \int_{-1}^{+1} d\mu \psi_i^h(x, \mu) \sum_{l=0}^L \left(\frac{2l+1}{2} \right) \Sigma_{sl} P_l(\mu) \int_{-1}^{+1} d\mu' P_l(\mu') \varphi(x, \mu') \\ & = \int_0^1 dx \int_{-1}^{+1} d\mu \psi_i^h(x, \mu) s(x, \mu) \end{aligned} \quad (8.57)$$

We can integrate the streaming term by parts to produce the boundary

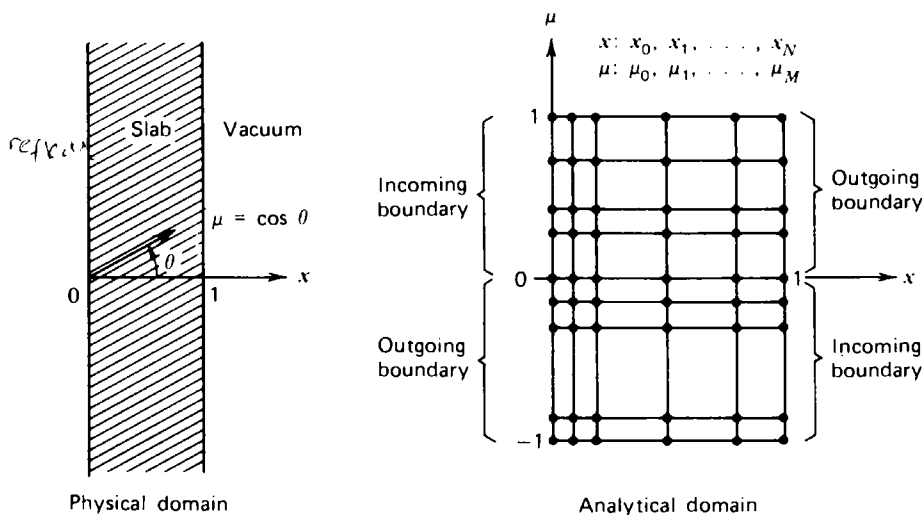


Fig. 8.24 □ One-dimensional plane geometry.

term:

$$\int_0^1 dx \int_{-1}^{+1} d\mu \psi_i^h \mu \frac{\partial \varphi}{\partial x} = - \int_0^1 dx \int_{-1}^{+1} d\mu \mu \frac{\partial \psi_i^h}{\partial x} \varphi(x, \mu) + \int_{-1}^{+1} d\mu \mu [\varphi(x, \mu) \psi_i^h(x, \mu)]_{x=0}^{x=1} \quad (8.58)$$

We can identify the second term in this equation as the boundary term (BT) and evaluate it at the endpoints $x = \pm 1$:

$$\text{BT} = \int_{-1}^{+1} d\mu \mu [\varphi(1, \mu) \psi_i^h(1, \mu) - \varphi(0, \mu) \psi_i^h(0, \mu)] \quad (8.59)$$

As in the more general case discussed in the previous section, we can now substitute the boundary conditions into Eq. 8.59. The boundary condition at $x = 1$ is easily included:

$$\begin{aligned} \text{BT} = & \int_{-1}^0 d\mu \mu \varphi_0(1, \mu) \psi_i^h(1, \mu) + \int_0^1 d\mu \mu \varphi(1, \mu) \psi_i^h(1, \mu) \\ & \text{incoming term (known)} \qquad \qquad \text{outgoing term (unknown)} \\ & - \int_{-1}^0 d\mu \mu \varphi(0, \mu) \psi_i^h(0, \mu) - \int_0^1 d\mu \mu \varphi(0, \mu) \psi_i^h(0, \mu) \\ & \qquad \qquad \text{outgoing term} \qquad \qquad \qquad \text{incoming term} \end{aligned} \quad (8.60)$$

The last two terms in this equation are related by the reflecting boundary condition at $x=0$. However it is not apparent how the reflecting condition should be included in Eq. 8.60. There are two possibilities: either eliminate $\varphi(0, \mu)$ in the third term of Eq. 8.60 or eliminate $\varphi(0, \mu)$ in the fourth term, using $\varphi(0, \mu) = \varphi(0, -\mu)$. Let us proceed by noting that the actual boundary condition sets the incoming angular flux at $x=0$ equal to the outgoing angular flux for the angle corresponding to spectral reflection. Therefore we should use $\varphi(0, \mu) = \varphi(0, -\mu)$, $\mu > 0$, and eliminate the incoming flux at $x=0$ in terms of the outgoing flux:

$$\begin{aligned} \text{BT} = & \int_{-1}^0 d\mu \mu \varphi_0(1, \mu) \psi_i^h(1, \mu) + \int_0^1 d\mu \mu \varphi(1, \mu) \psi_i^h(1, \mu) \\ & - \int_{-1}^0 d\mu \mu \varphi(0, \mu) \psi_i^h(0, \mu) + \int_{-1}^0 d\mu \mu \varphi(0, \mu) \psi_i^h(0, -\mu) \end{aligned}$$

where the range of the integration of the last integral has been transformed from μ to $-\mu$. It can be shown that this choice that corresponds to applying the reflecting boundary condition in the direction of particle

motion results in an effective source of particles for the nodes on the incoming boundary because of the corresponding nodes on the outgoing boundary. If we had chosen the alternative method to incorporate the reflecting boundary conditions, the matrix elements would have represented a negative source for the outgoing nodes because of the incoming flux, and this would lead to an ill-posed problem. Numerical results confirm that this approach yields incorrect results, probably because the natural reflecting boundary condition is imposed against the direction of particle motion.

The calculation of the remainder of the terms in Eq. 8.57 are straightforward. If we expand $\varphi^h(x, \mu)$ in terms of the finite element basis functions

$$\varphi^h(x, \mu) = \sum_{j=1}^N \varphi_j \psi_j^h(x, \mu)$$

and substitute this expansion into Eq. 8.57, we arrive at a system of algebraic equations

$$\sum_{j=1}^N A_{ij} \varphi_j = S_i, \quad i = 1, 2, \dots, N \quad (8.61)$$

where

$$\begin{aligned} A_{ij} = & - \int_0^1 dx \int_{-1}^{+1} d\mu \mu \psi_j^h \frac{\partial \psi_i^h}{\partial x} + \int_0^1 d\mu \mu \psi_i^h(1, \mu) \psi_j^h(1, \mu) \\ & - \int_{-1}^0 d\mu \mu \psi_i^h(0, \mu) \psi_j^h(0, \mu) + \int_{-1}^0 d\mu \mu \psi_i^h(0, -\mu) \psi_j^h(0, \mu) \\ & + \int_0^1 dx \int_{-1}^{+1} d\mu \Sigma_l \psi_i^h \psi_j^h - \sum_{l=0}^L \left(\frac{2l+1}{2} \right) \int_0^1 dx \Sigma_l \int_{-1}^{+1} d\mu \psi_i^h P_l \\ & \quad \times \int_{-1}^{+1} d\mu' \psi_j^h P_l \\ S_i = & \int_0^1 dx \int_{-1}^{+1} d\mu s(x, \mu) \psi_i^h(x, \mu) - \int_{-1}^0 d\mu \mu \psi_i^h(1, \mu) \varphi_0(1, \mu) \end{aligned}$$

Therefore we have derived a system of algebraic equations that can be solved by standard methods for the expansion coefficients φ_j . Before we consider the construction of the finite element subspace S^h and the solution of this set of equations, we develop the alternative formulation of the finite element method using the second-order form of the transport equation.

8.3.2 □ Application of Finite Element Methods to the Second Order Form of the Transport Equation □

It is possible to give an integral formulation of the second order transport equation in terms of a self-adjoint variational principle. Before we demonstrate how finite element methods can be applied to this formulation, we present a brief derivation of the second order form of the transport equation.⁵⁹

Derivation of the Second Order Form of the Transport Equation □ We begin with the one-speed transport equation

$$\hat{\Omega} \cdot \nabla \varphi + \Sigma_s \varphi = \int d\hat{\Omega}' \Sigma_s(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega}) \varphi(\mathbf{r}, \hat{\Omega}') + s(\mathbf{r}, \hat{\Omega}) \quad (8.62)$$

where, for convenience, we assume vacuum boundary conditions on the boundary ∂R , $\varphi(\mathbf{r}, \hat{\Omega}) = 0$, $\mathbf{r} \in \partial R$ and $\hat{\Omega} \cdot \hat{\mathbf{e}}_s < 0$. Since this equation also holds for $-\hat{\Omega}$

$$-\hat{\Omega} \cdot \nabla \varphi + \Sigma_s \varphi(\mathbf{r}, -\hat{\Omega}) = \int d\hat{\Omega}' \Sigma_s(\mathbf{r}, -\hat{\Omega}' \cdot \hat{\Omega}) \varphi(\mathbf{r}, \hat{\Omega}') + s(\mathbf{r}, -\hat{\Omega}) \quad (8.63)$$

it is apparent that we can add and subtract these equations to obtain

$$\begin{aligned} \hat{\Omega} \cdot \nabla [\varphi(\mathbf{r}, \hat{\Omega}) - \varphi(\mathbf{r}, -\hat{\Omega})] + \Sigma_s [\varphi(\mathbf{r}, \hat{\Omega}) + \varphi(\mathbf{r}, -\hat{\Omega})] \\ = \int d\hat{\Omega}' [\Sigma_s(\hat{\Omega}' \cdot \hat{\Omega}) + \Sigma_s(-\hat{\Omega}' \cdot \hat{\Omega})] \varphi(\mathbf{r}, \hat{\Omega}') + [s(\mathbf{r}, \hat{\Omega}) + s(\mathbf{r}, -\hat{\Omega})] \end{aligned} \quad (8.64)$$

and

$$\begin{aligned} \hat{\Omega} \cdot \nabla [\varphi(\mathbf{r}, \hat{\Omega}) + \varphi(\mathbf{r}, -\hat{\Omega})] + \Sigma_s [\varphi(\mathbf{r}, \hat{\Omega}) - \varphi(\mathbf{r}, -\hat{\Omega})] \\ = \int d\hat{\Omega}' [\Sigma_s(\hat{\Omega} \cdot \hat{\Omega}') - \Sigma_s(-\hat{\Omega}' \cdot \hat{\Omega})] \varphi(\mathbf{r}, \hat{\Omega}') + [s(\mathbf{r}, \hat{\Omega}) - s(\mathbf{r}, -\hat{\Omega})] \end{aligned} \quad (8.65)$$

We now introduce the following definitions

$$\psi(\mathbf{r}, \hat{\Omega}) = \frac{1}{2} [\varphi(\mathbf{r}, \hat{\Omega}) + \varphi(\mathbf{r}, -\hat{\Omega})], \quad \text{even-parity flux}$$

$$\chi(\mathbf{r}, \hat{\Omega}) = \frac{1}{2} [\varphi(\mathbf{r}, \hat{\Omega}) - \varphi(\mathbf{r}, -\hat{\Omega})], \quad \text{odd-parity flux}$$

$$s^\pm(\mathbf{r}, \hat{\Omega}) = \frac{1}{2} [s(\mathbf{r}, \hat{\Omega}) \pm s(\mathbf{r}, -\hat{\Omega})]$$

$$\Sigma_s^\pm(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega}) = \frac{1}{2} [\Sigma_s(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega}) \pm \Sigma_s(\mathbf{r}, -\hat{\Omega}' \cdot \hat{\Omega})]$$

so that we can identify Eqs. 8.64 and 8.65 as two coupled equations for the even- and odd-parity fluxes, $\psi(\mathbf{r}, \hat{\Omega})$ and $\chi(\mathbf{r}, \hat{\Omega})$ (noting that the integral vanishes if it is odd):

$$\hat{\Omega} \cdot \nabla \chi + \Sigma_t \psi = \int d\hat{\Omega}' \Sigma_s^+(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega}) \psi(\mathbf{r}, \hat{\Omega}') + s^+(\mathbf{r}, \hat{\Omega}) \quad (8.66)$$

$$\hat{\Omega} \cdot \nabla \psi + \Sigma_t \chi = \int d\hat{\Omega}' \Sigma_s^-(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega}) \chi(\mathbf{r}, \hat{\Omega}') + s^-(\mathbf{r}, \hat{\Omega}) \quad (8.67)$$

We now obtain second order equations for $\psi(\mathbf{r}, \hat{\Omega})$ and $\chi(\mathbf{r}, \hat{\Omega})$ separately. First rearrange Eq. 8.67 as

$$\Sigma_t \chi - \int d\hat{\Omega}' \Sigma_s^-(\hat{\Omega}' \cdot \hat{\Omega}) \chi(\mathbf{r}, \hat{\Omega}') = s^- - \hat{\Omega} \cdot \nabla \psi \quad (8.68)$$

Consider first the case that $\Sigma_s^-(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega}) = 0$. Then we can immediately solve for

$$\chi(\mathbf{r}, \hat{\Omega}) = \Sigma_t^{-1}(\mathbf{r}) [s^-(\mathbf{r}, \hat{\Omega}) - \hat{\Omega} \cdot \nabla \psi(\mathbf{r}, \hat{\Omega})]$$

This expression for $\chi(\mathbf{r}, \hat{\Omega})$ can be substituted into Eq. 8.66 to yield

$$-\hat{\Omega} \cdot \nabla [\Sigma_t^{-1} \hat{\Omega} \cdot \nabla \psi] + \Sigma_t \psi = \int d\hat{\Omega}' \Sigma_s^+(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega}) \psi(\mathbf{r}, \hat{\Omega}') + s^+ - \hat{\Omega} \cdot \nabla [\Sigma_t^{-1} s^-] \quad (8.69)$$

Therefore if there is isotropic scattering (or no odd moments in the scattering kernel), the second order, even-parity transport equation takes the form of Eq. 8.69.

In the more general case in which $\Sigma_s^-(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega})$ is nonzero, we must explicitly invert the operator

$$G \circ \equiv \Sigma_t \circ - \int d\hat{\Omega}' \Sigma_s^-(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega}) \circ$$

so that

$$\chi = G^{-1} [s^- - \hat{\Omega} \cdot \nabla \psi] \quad (8.70)$$

To this end, consider the action of G on an arbitrary function $f(\mathbf{r}, \hat{\Omega})$

$$Gf = \Sigma_t(\mathbf{r}) f(\mathbf{r}, \hat{\Omega}) - \int d\hat{\Omega}' \Sigma_s^-(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega}) f(\mathbf{r}, \hat{\Omega}') \equiv g(\mathbf{r}, \hat{\Omega}) \quad (8.71)$$

If we now expand the scattering kernel in spherical harmonics [noting that $\Sigma_s^-(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega})$ is an odd function of $\hat{\Omega}' \cdot \hat{\Omega}$]

$$\Sigma_s^-(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega}) = \sum_{l \text{ odd}}^{\infty} \left(\frac{2l+1}{4\pi} \right) \Sigma_{sl}(\mathbf{r}) P_l(\hat{\Omega}' \cdot \hat{\Omega})$$

and use the addition theorem for spherical harmonics, Eq. 8.71 becomes

$$\Sigma_l f - \sum_{l \text{ odd}}^{\infty} \sum_{m=-l}^l \Sigma_{sl}(\mathbf{r}) Y_{lm}(\hat{\Omega}) \int d\hat{\Omega}' Y_{lm}^*(\hat{\Omega}') f(\mathbf{r}, \hat{\Omega}') = g \quad (8.72)$$

In the usual way we can multiply by $Y_{lm}^*(\hat{\Omega})$, integrate over angle, and use orthogonality to solve for

$$\int d\hat{\Omega} f(\mathbf{r}, \hat{\Omega}) Y_{lm}^*(\hat{\Omega}) = [\Sigma_l - \Sigma_{sl}]^{-1} \int d\hat{\Omega} g(\mathbf{r}, \hat{\Omega}) Y_{lm}^*(\hat{\Omega})$$

This can be substituted back into Eq. 8.72 to find

$$f(\mathbf{r}, \hat{\Omega}) = \frac{1}{\Sigma_l} g(\mathbf{r}, \hat{\Omega}) + \frac{1}{\Sigma_l} \sum_{l \text{ odd}}^{\infty} \left(\frac{\Sigma_{sl}}{\Sigma_l - \Sigma_{sl}} \right) \sum_{m=-l}^l Y_{lm}(\hat{\Omega}) \int d\hat{\Omega}' Y_{lm}^*(\hat{\Omega}') g(\mathbf{r}, \hat{\Omega}')$$

Therefore we can identify our inverse collision operator as

$$G^{-1} \circ = \frac{1}{\Sigma_l} \circ + \frac{1}{\Sigma_l} \sum_{l \text{ odd}}^{\infty} \left(\frac{\Sigma_{sl}}{\Sigma_l - \Sigma_{sl}} \right) \sum_{m=-l}^l Y_{lm}(\hat{\Omega}) \int d\hat{\Omega}' Y_{lm}^*(\hat{\Omega}') \circ \quad (8.73)$$

Finally, substituting Eqs. 8.73 and 8.70 into Eq. 8.66, we find the more general second order, even-parity form of the transport equation

$$\begin{aligned} -\hat{\Omega} \cdot \nabla \left[\frac{1}{\Sigma_l} \hat{\Omega} \cdot \nabla \psi \right] + \Sigma_l \psi &= \int d\hat{\Omega}' \Sigma_s^+(\hat{\Omega}' \cdot \hat{\Omega}) \psi(\mathbf{r}, \hat{\Omega}') \\ &+ \hat{\Omega} \cdot \nabla \left[\int d\hat{\Omega}' g(\hat{\Omega}' \cdot \hat{\Omega}) \hat{\Omega}' \cdot \nabla \psi \right] + s^+ - \hat{\Omega} \cdot \nabla \left[\frac{1}{\Sigma_l} s^- \right] \\ &- \hat{\Omega} \cdot \nabla \left[\int d\hat{\Omega}' g(\hat{\Omega}' \cdot \hat{\Omega}) s^-(\mathbf{r}, \hat{\Omega}') \right] \end{aligned} \quad (8.74)$$

where

$$g(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega}) = \frac{1}{\Sigma_l(\mathbf{r})} \sum_{l \text{ odd}}^{\infty} \left(\frac{\Sigma_{sl}(\mathbf{r})}{\Sigma_l(\mathbf{r}) - \Sigma_{sl}(\mathbf{r})} \right) \sum_{m=-l}^l Y_{lm}(\hat{\Omega}) Y_{lm}^*(\hat{\Omega}')$$

The boundary conditions can be transformed in a very similar manner. In particular, vacuum boundary conditions for the incoming boundary fluxes can be expressed in terms of the even- and odd-parity fluxes as

$$\varphi(\mathbf{r}_s, \hat{\Omega}) = \psi(\mathbf{r}_s, \hat{\Omega}) + \chi(\mathbf{r}_s, \hat{\Omega}) = 0, \quad \hat{\Omega} \cdot \hat{\mathbf{e}}_s < 0$$

But the vacuum boundary condition can also be written as

$$\varphi(\mathbf{r}_s, -\hat{\Omega}) = \psi(\mathbf{r}_s, \hat{\Omega}) - \chi(\mathbf{r}_s, \hat{\Omega}) = 0, \quad \hat{\Omega} \cdot \hat{\mathbf{e}}_s > 0$$

Therefore, using our earlier evaluation of the inverse G^{-1} , we can rewrite the vacuum boundary condition for the even-parity flux alone as

$$\begin{aligned} \psi(\mathbf{r}_s, \hat{\Omega}) + \Sigma_i^{-1} [s^-(\mathbf{r}, \hat{\Omega}) - \hat{\Omega} \cdot \nabla \psi(\mathbf{r}, \hat{\Omega})] \\ + \int d\hat{\Omega}' g(\mathbf{r}, \hat{\Omega}' \cdot \hat{\Omega}) [s^-(\mathbf{r}, \hat{\Omega}') - \hat{\Omega}' \cdot \nabla \psi(\mathbf{r}, \hat{\Omega}')] = 0, \quad \hat{\Omega} \cdot \hat{\mathbf{e}}_s \geq 0 \end{aligned}$$

The Variational Principle Associated with the Second Order Form □ It can be shown that a functional that yields Eq. 8.74 as its Euler equation is⁵⁹

$$\begin{aligned} F[\psi] = \int \int d\mathbf{r} d\hat{\Omega} \left\{ \Sigma_i^{-1} [\hat{\Omega} \cdot \nabla \psi]^2 + \Sigma_i \psi^2 - \psi \int d\hat{\Omega}' \Sigma_s^+ (\hat{\Omega}' \cdot \hat{\Omega}) \psi(\hat{\Omega}') \right. \\ + [\hat{\Omega} \cdot \nabla \psi] \int d\hat{\Omega}' g(\hat{\Omega}' \cdot \hat{\Omega}) \hat{\Omega}' \cdot \nabla \psi - 2\psi s^+ - 2\Sigma_i^{-1} s^- \hat{\Omega} \cdot \nabla \psi \\ \left. - 2\hat{\Omega} \cdot \nabla \psi \int d\hat{\Omega}' g(\hat{\Omega}' \cdot \hat{\Omega}) s^-(\hat{\Omega}') \right\} + 2 \int \int_{\Gamma^+} dS d\hat{\Omega} \psi^2 \end{aligned}$$

where we have assumed vacuum boundary conditions on Γ^- . [If reflecting boundary conditions are also imposed, the surface term is only over that portion of the boundary (if any) where vacuum boundary conditions apply.] The vacuum boundary conditions appear as natural boundary conditions, and reflecting boundary conditions appear as essential boundary conditions.

The finite element method can be applied by expanding the even-parity flux in terms of the finite element basis functions

$$\psi(\mathbf{r}, \hat{\Omega}) = \sum_{j=1}^N \varphi_j \psi_j^h(\mathbf{r}, \hat{\Omega})$$

The functional $F[\psi]$ is then minimized with respect to variations in the expansion coefficients φ_j , $j=1, 2, \dots, N$ to arrive at a matrix equation for $\boldsymbol{\varphi} = \text{col}[\varphi_1, \varphi_2, \dots, \varphi_N]$

$$\mathbf{A}\boldsymbol{\varphi} = \mathbf{S}$$

where the detailed definition of the matrix elements are left to the references.^{50,51} If it had been necessary to start with the integral law form of the second order, even-parity transport equation, we would have obtained the same system of equations in the end by following a procedure similar to that in the preceding section. Thus the variational approach and the integral law approach are equivalent for the second order, self-adjoint form of the transport equation.

Therefore we have arrived once again at a system of algebraic equations that represents the original transport equation on the finite element subspace S^h . We now turn our attention to the construction of this subspace and the solution of these equations.

8.3.3 □ Construction of the Finite Element Subspace □ To illustrate how to construct a suitable finite element subspace S^h , we provide specific details for one-dimensional plane geometry. In general the finite element method is employed in a nodal fashion. That is, the expansion coefficients for the solution are nodal parameters that are typically the value of the solution or one of its derivatives at a node of the space angle mesh. We speak of a “Lagrangian finite element scheme” as one that employs Lagrange interpolation polynomials over each local mesh or finite element. The values of the solution at the nodes are the expansion coefficients, hence the unknowns in the system of equations. We could also employ Hermite interpolation polynomials on a given finite element mesh; however in this case each node would include additional parameters representing the values of both the solution and its derivatives. Lagrange finite element schemes typically result in continuity of the solution everywhere in the mesh, although derivatives are generally discontinuous across interelement boundaries. Hermitian schemes typically result in continuity of one or more partial derivatives everywhere in the mesh.

Since the transport equation is only of first order, one can expect at most continuity of the angular flux. Even this may be too restrictive for the angular variable. Therefore the use of Lagrangian elements that preserve continuity in the solution but not its derivatives would appear to be a proper choice for transport problems. Lagrangian elements may be determined for a specific element type or may be formulated for multidimensional elements in terms of direct products of two or more one-dimensional Lagrangian basis functions.

The more general method is to shape the basis functions to the particular element. For example, a triangular element with three nodes can uniquely represent a linear polynomial over a two-dimensional surface, with each node contributing a piece of data. That is, a general linear polynomial in two variables $p(x,y) = a_0 + a_1x + a_2y$ requires the value of three parameters to be uniquely determined. If the values of the solution at

the nodes of a triangle are taken to be the three parameters, the linear polynomial is uniquely determined within the triangle. With Lagrangian elements, where the nodal parameters are the values of the unknown solution, a convenient basis for a triangle consists of three linear polynomials, each of which is unity at one node and zero at the other nodes. This will result in the expansion coefficients being identical to the value of the solution at the nodes. This concept of choosing a basis consisting of functions that are unity at a particular node and zero at all other nodes is typical of Lagrangian elements, and it is used for the direct product basis functions discussed below as well as for quite general multidimensional schemes. Section 8.1.4 gave explicit formulas for the three linear polynomials over a triangle that are unity at one vertex and zero at the other two vertices. However it should be noted that these particular basis functions are discontinuous across element boundaries because common vertices of different triangles have different solution values for each triangle, whereas the usual Lagrangian triangular element scheme employs continuous functions.

For multidimensional elements one can also formulate basis functions that are direct products of simple one-dimensional basis functions. This can be illustrated for the x - μ mesh for the plane geometry transport equation. Figure 8.25 illustrates a typical mesh and indicates the global numbering for the nodes. Let us denote the global numbering index as n and the spatial and angular indices as i and j , respectively. For example, $n = 12$ corresponds to $i = 2$ and $j = 5$ in Figure 8.25.

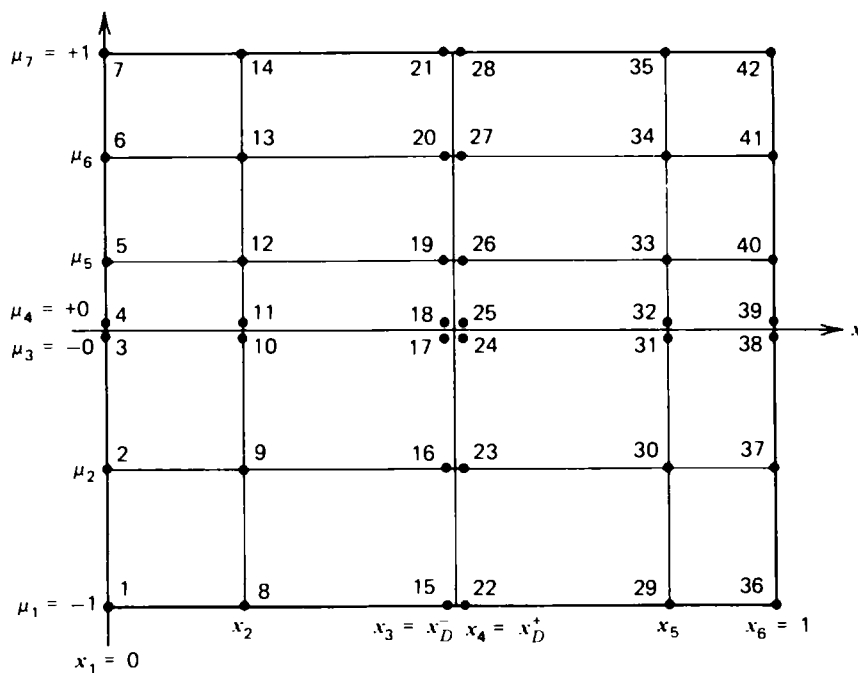
A basis function for a global node n is then defined as a direct product of one-dimensional basis functions for the corresponding spatial node i and angular node j :

$$\psi_n(x, \mu) = \psi_i(x) \psi_j(\mu)$$

The one-dimensional basis functions are the standard “tent” functions (see Figure 8.26), which are expressed as follows:

$$\psi_i(x) = \begin{cases} \frac{x - x_{i-1}}{x_i - x_{i-1}}, & x_{i-1} \leq x \leq x_i \\ \frac{x_{i+1} - x}{x_{i+1} - x_i}, & x_i \leq x \leq x_{i+1} \\ 0, & \text{otherwise} \end{cases}$$

$$\psi_j(\mu) = \begin{cases} \frac{\mu - \mu_{j-1}}{\mu_j - \mu_{j-1}}, & \mu_{j-1} \leq \mu \leq \mu_j \\ \frac{\mu_{j+1} - \mu}{\mu_{j+1} - \mu_j}, & \mu_j \leq \mu \leq \mu_{j+1} \\ 0, & \text{otherwise} \end{cases}$$



Note:



Discontinuous angular
elements at $\mu = 0$



Discontinuous spatial
elements at $x = x_D$

Fig. 8.25 □ Nodal numbering.



Fig. 8.26 □ "Tent" finite element basis functions (continuous).

Then $\psi_n(x, \mu)$ is easily expressed for each quadrant of the x - μ finite element mesh (see Figure 8.27).

A convenient consequence of the direct product basis functions is that the components of the matrix elements A_{ij} are separable into products of spatial and angular integrals. For example, the contribution to A_{ij} in Eq. 8.61 due to the streaming term becomes

$$\int_0^1 dx \int_{-1}^{+1} d\mu \mu \psi_j \frac{\partial \psi_i}{\partial x} = \int_0^1 dx \frac{d\psi_{ix}(x)}{dx} \psi_{jx}(x) \int_{-1}^{+1} d\mu \mu \psi_{i\mu}(\mu) \psi_{j\mu}(\mu)$$

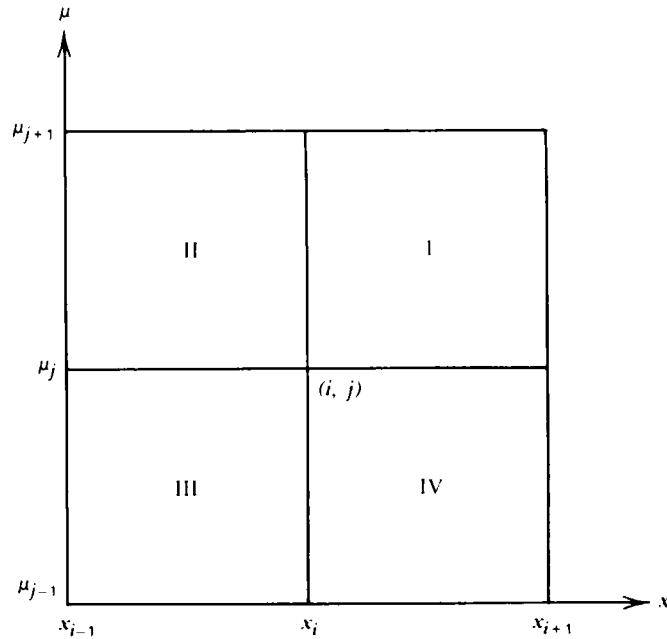


Fig. 8.27 □ Direct product basis functions; $\psi_{ij}(x, \mu)$ is as follows:

$$\begin{aligned} \psi_{ij}(x, \mu) &= \left(\frac{x_{i+1} - x}{x_{i+1} - x_i} \right) \left(\frac{\mu_{j+1} - \mu}{\mu_{j+1} - \mu_j} \right), & (x, \mu) \in I \\ &= \left(\frac{x - x_{i-1}}{x_i - x_{i-1}} \right) \left(\frac{\mu_{j+1} - \mu}{\mu_{j+1} - \mu_j} \right), & (x, \mu) \in II \\ &= \left(\frac{x - x_{i-1}}{x_i - x_{i-1}} \right) \left(\frac{\mu - \mu_{j-1}}{\mu_j - \mu_{j-1}} \right), & (x, \mu) \in III \\ &= \left(\frac{x_{i+1} - x}{x_{i+1} - x_i} \right) \left(\frac{\mu - \mu_{j-1}}{\mu_j - \mu_{j-1}} \right), & (x, \mu) \in IV \end{aligned}$$

where ix is the x node corresponding to node i . This greatly simplifies the calculation of the integrals because the spatial and angular integrals may be performed independent of one another.

Although the ranges of integration of the integrals in Eq. 8.61 for A_{ij} are given over the full spatial and angular ranges, in fact the local definition of the basis functions greatly reduces the range of integration, and the components of A_{ij} generally vanish if nodes i and j are not adjacent (for linear elements). There is one notable exception, however. The scattering contribution to A_{ij}

$$\sum_{l=0}^L \left(\frac{2l+1}{2} \right) \int_0^1 dx \sum_s \psi_{ix} \psi_{jx} \int_{-1}^{+1} d\mu P_l \psi_{i\mu} \int_{-1}^{+1} d\mu' P_l \psi_{j\mu}$$

is a product of integrals of basis functions rather than an integral of a product of basis functions. Therefore scattering couples all the angular nodes (although the spatial coupling is unaffected). This would be expected on physical grounds, since there is a finite probability of scattering from one direction into any other direction.

One can also define higher order basis functions, either as a higher order polynomial over a general element such as a triangle or as a direct product of higher order one-dimensional polynomials. To construct higher order elements, one introduces additional nodes (e.g., one additional node for quadratic basis functions) and defines the higher order polynomials over several nodes (vs. two nodes for linear elements). This results in a coupling of nodes that would not be coupled by linear elements. This is not a concern with the angular elements because all nodes are coupled by scattering in any event. But this increased coupling does present severe problems if higher order elements are used in space.⁴⁸ Figure 8.28 illustrates quadratic basis functions on a typical mesh, and it can be seen that a quadratic basis function can interact with its two nearest neighbors on either side. For cubic elements, the interaction would extend over the three nearest neighbors on either side. This increased coupling is undesirable because the bandwidth of the coefficient matrix A is increased in proportion to the increased spatial coupling. For example, linear elements will cause three columns in the x - μ plane to interact (all angular nodes interact because of scattering); therefore the length of a typical row in the matrix A is $3N_\mu$, where N_μ is the number of μ nodes. Since there are $N_x \times N_\mu$ equations (rows of the matrix A), one must store $3N_x \times N_\mu^2$ matrix

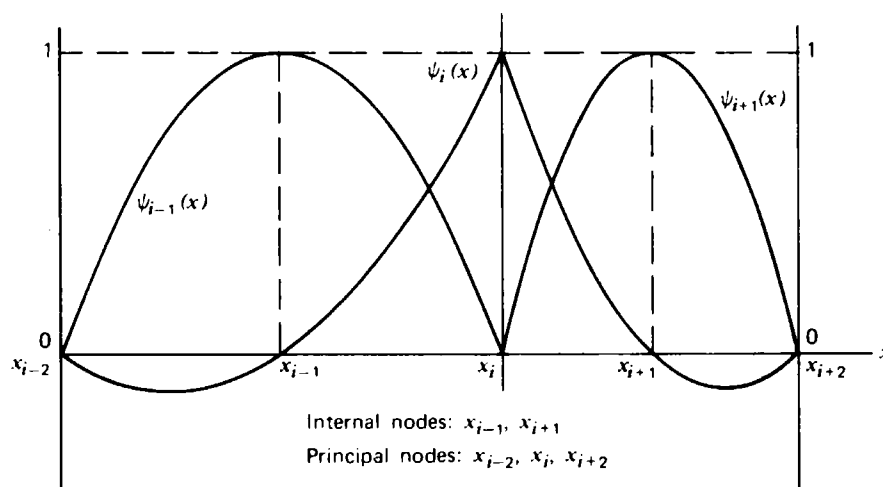


Fig. 8.28 □ Quadratic basis functions, where $\psi_i(x)$ are the separate basis functions for discontinuous elements at $x = x_i$.

elements, regardless of the degree of the angular element. For quadratics, this becomes $5N_x \times N_\mu^2$ and for cubics, $7N_x \times N_\mu^2$.

Although the matrix elements are relatively simple to compute analytically, the sheer number of integrals for even moderate sized problems forces one to simplify the work even further. For example, all integrals can be done on the standard interval $[-1, +1]$ by Gaussian quadrature, then mapped into the particular mesh interval by a simple linear transformation. For an integral over the interval x_i to x_{i+1} (or μ_j to μ_{j+1}) one would employ the transformation

$$x = \frac{1}{2}(x_{i+1} - x_i)\xi + \frac{1}{2}(x_{i+1} + x_i)$$

so that

$$\int_{x_i}^{x_{i+1}} dx \psi_i(x) \psi_{i+1}(x) = \frac{1}{2}(x_{i+1} - x_i) \int_{-1}^{+1} d\xi \psi_a(\xi) \psi_b(\xi)$$

or for an angular integral

$$\begin{aligned} \int_{\mu_i}^{\mu_{i+1}} d\mu \mu \psi_i(\mu) \psi_{i+1}(\mu) \\ = \frac{1}{2}(\mu_{i+1} - \mu_i) \int_{-1}^{+1} d\xi \left[\frac{1}{2}(\mu_{i+1} - \mu_i)\xi + \frac{1}{2}(\mu_{i+1} + \mu_i) \right] \psi_a(\xi) \psi_b(\xi) \end{aligned}$$

Here $\psi_a(\xi)$ and $\psi_b(\xi)$ are generic basis functions that can be used to construct all other finite element basis functions. There are only $k+1$ such basis functions for the entire system, where k is the order of the polynomials used as finite elements.

8.3.4 □ Discontinuous Phase Space Finite Elements □

Discontinuous Angular Finite Elements □ In plane geometry it is well known that the transport equation may have discontinuities in the angular flux at $\mu=0$ at interfaces or boundaries. In fact this behavior at $\mu=0$ was the primary motivation behind the double P_N method and the double S_N quadrature sets introduced earlier. In each of these cases the discontinuity at $\mu=0$ was avoided by considering separately the flux in each half-range, $-1 \leq \mu \leq 0$ and $0 \leq \mu \leq 1$.

We now consider a method for handling this discontinuity within the framework of the finite element scheme.⁴⁸ Since the finite element scheme we have developed thus far assumes continuity of the angular flux in both space and angle, some extensions of our earlier treatment are necessary.

For the angular variable, continuity is not required during the derivation of the integral law. However use of Lagrange basis functions (see Section 8.3.3) will result in an approximate solution that is continuous throughout the angular domain, even though the actual solution may be discontinuous. Thus the actual discontinuous solution is being approximated by a continuous function, and poor results will probably occur, particularly near interfaces or strong absorbers.

But the presence of an angular flux discontinuity in the angular domain does not affect the validity of the integral law formulation of the transport equation in one-dimensional plane geometry. Analytically this is expected because the transport equation in plane geometry (or orthogonal geometries in general) has no angular derivatives; hence continuity of the solution in the angular domain is not a requirement. Second, the derivation of the integral law involves (for the angular variable) only simple integrations that are valid in the presence of discontinuities as long as the integrals are evaluated in a piecewise fashion.

Therefore the use of discontinuous angular elements is simply a matter of constructing basis functions that are discontinuous at $\mu=0$ (for plane geometry) and being careful to evaluate the integral in a piecewise fashion. This is easily accomplished by splitting the basis function at $\mu=0$ into two basis functions, one for $\mu=0^-$ and the other for $\mu=0^+$. Thus there is a double node at $\mu=0$, as illustrated in Figure 8.25 for a typical finite element mesh. For a multidimensional problem where two angles are needed, one could use direct product basis functions of these discontinuous one-dimensional functions.

Discontinuous Spatial Finite Elements □ Although analytically the solution to the transport equation must be everywhere continuous in the spatial domain, there may be points at which the solution exhibits a near discontinuity. For example, the simple problem of a strong source of neutrons in a strong absorber surrounded by a vacuum will result in an angular flux with nearly discontinuous spatial dependence at the vacuum boundaries. This is because the analytic solution is a constant everywhere in the interior of the slab, but near an incoming boundary the spatial dependence of the flux must drop to zero within a few mean free paths to meet the vacuum boundary condition. However it is difficult for the approximate solution to follow this discontinuous behavior because it is constrained to be continuous by the choice of the approximating subspace (Lagrange basis functions).

In order to allow the treatment of strong spatial variations in the flux, one can proceed as with the angular variable and simply construct discontinuous basis functions at the desired spatial positions, thus allowing the

approximate solution to be discontinuous. However the presence of the spatial derivative in the streaming term $\mu \partial \varphi / \partial x$ necessitates care when the transport equation is integrated over the spatial domain. That is, the integration across the discontinuity will yield surface terms which must be carefully incorporated into the integral law.

These interface terms can be properly accounted for in the following manner that allows the use of discontinuous basis functions in such a way that the regions are coupled by transport. We illustrate the procedure with the one-dimensional transport equation

$$\mu \frac{\partial \varphi}{\partial x} + \Sigma_t(x) \varphi(x, \mu) = \frac{1}{2} \Sigma_s(x) \int_{-1}^{+1} d\mu' \varphi(x, \mu') + s(x, \mu)$$

with arbitrary boundary conditions. We consider in detail only the transport term $\mu \partial \varphi / \partial x$, since the other terms are treated in an identical manner to our earlier analysis. If we multiply this term by an arbitrary $\psi^h \in S^h$ and integrate over phase space, taking care to split up the integral to avoid the discontinuity in $\psi^h(x, \mu)$, we find

$$T = \int_0^{x_D^-} dx \int_{-1}^{+1} d\mu \mu \frac{\partial \varphi}{\partial x} \psi^h(x, \mu) + \int_{x_D^+}^1 dx \int_{-1}^{+1} d\mu \mu \frac{\partial \varphi}{\partial x} \psi^h(x, \mu)$$

We then integrate each term by parts to obtain

$$\begin{aligned} T = & - \int_0^1 dx \int_{-1}^{+1} d\mu \mu \varphi \frac{\partial \psi^h}{\partial x} + \int_{-1}^{+1} d\mu \mu [\varphi(1, \mu) \psi^h(1, \mu) - \varphi(0, \mu) \psi^h(0, \mu)] \\ & - \int_{-1}^{+1} d\mu \mu [\varphi(x_D^+, \mu) \psi^h(x_D^+, \mu) - \varphi(x_D^-, \mu) \psi^h(x_D^-, \mu)] \end{aligned} \quad (8.75)$$

Here we note that Eq. 8.75 is identical to the transport term plus boundary terms derived earlier in Eq. 8.58, except for the last term, which we denote by I . It is this interface term that must be carefully treated to allow use of discontinuous spatial elements.

The objective now is to use known information to reduce the interface term in a manner similar to the reduction of the boundary terms by explicitly substituting in the known boundary conditions. Since the only known condition at an interface is that the solution $\varphi(x, \mu)$ is continuous, albeit strongly varying, let us use this condition in the direction of particle motion (similar to the reflecting boundary case)

$$\varphi(x_D^+, \mu) = \varphi(x_D^-, \mu), \quad \mu \geq 0$$

$$\varphi(x_D^-, \mu) = \varphi(x_D^+, \mu), \quad \mu \leq 0$$

(Note the similarity to the definition of the cell edge flux in the finite element-discrete ordinate method of Section 8.1.4.) These substitutions are made in Eq. 8.75 for I and $\varphi(x, \mu)$ is expanded in terms of the basis functions

$$\varphi^h(x, \mu) = \sum_{j=1}^N \varphi_j \psi_j^h(x, \mu)$$

If we now require the new integral law (with the extra term I) to hold for all $\psi_j^h(x, \mu)$, $j = 1, 2, \dots, N$, we obtain the matrix element

$$\begin{aligned} I_{ij} = & - \int_{-1}^0 d\mu \mu \psi_j^h(x_D^+, \mu) [\psi_i^h(x_D^+, \mu) - \psi_i^h(x_D^-, \mu)] \\ & - \int_0^1 d\mu \mu \psi_j^h(x_D^-, \mu) [\psi_i^h(x_D^+, \mu) - \psi_i^h(x_D^-, \mu)] \end{aligned}$$

which is additive to the earlier matrix element A_{ij} defined in Eq. 8.61.

Since the space of trial functions S^h is no longer continuous at the specified spatial discontinuity, but continuity in the direction of particle travel is imposed within the integral law, the net result is that continuity of the angular flux in the direction of particle motion is a natural interface condition. Although there was no need to mention it earlier, the previous formulation treats continuity of the angular flux as an essential condition because continuity was imposed on the space S^h . Therefore the discontinuous element scheme allows more flexibility for the approximate solution to match the actual solution. This has been verified in a number of numerical studies.⁴⁸

There is a close relationship between the method discussed in this section and the methods used to incorporate spatial discontinuities in the discrete ordinates-finite element schemes treated in Section 8.1.3. Both the ONETRAN/TRIDENT approach and the approach above allow the incoming flux on a boundary of an element to be different from the corresponding outgoing flux of the adjacent element. Conservation of particles is then ensured by use of surface terms. In TRIDENT this is accomplished by explicitly expressing the jump in the angular flux at the incoming boundaries, and when this term is differentiated (because of the transport term), Dirac δ -functions result. Then when this resulting equation is integrated with some weighting function, the Dirac δ -functions kick out the appropriate surface terms, and these terms are similar to the terms obtained in the foregoing analysis.

The slightly different formulation in ONETRAN yields the same results in that the angular flux on the incoming boundary is allowed to contribute to the effective source of particles within the element as a surface term when discontinuities are allowed.

To implement the discontinuous finite element method one can utilize one-dimensional spatial basis functions similar to the discontinuous angular basis functions. However in this case discontinuities would be allowed at arbitrary locations rather than at a specific location such as $\mu=0$ for the angular elements. One could also use the discontinuous triangular elements implemented in the TRIDENT scheme (see Section 8.1.3).

8.3.5 □ Eigenvalue Problems □ The finite element method is readily adapted to solve eigenvalue problems. For example, if we wish to determine the number of secondary particles per collision c for criticality in a given configuration, the integral law corresponding to Eq. 8.50 would become: find $\varphi^h(\mathbf{r}, \hat{\Omega}) \in S^h$ and the lowest value of c such that for all $\psi^h(\mathbf{r}, \hat{\Omega}) \in S^h$

$$-(\varphi^h, \hat{\Omega} \cdot \nabla \psi^h) + \langle \varphi^h, \psi^h \rangle_+ + (\Sigma_t \varphi^h, \psi^h) = c \left(\int d\hat{\Omega}' \Sigma_s(\hat{\Omega}' \rightarrow \hat{\Omega}) \varphi^h(\hat{\Omega}'), \psi^h \right) \quad 8.76)$$

After expanding the solution in terms of the basis functions and requiring Eq. 8.76 to hold for $\{\psi_i^h\}$, the generalized matrix eigenvalue problem is obtained

$$A\varphi = cM\varphi$$

where M is the scattering matrix and A is the same as the matrix of coefficients given previously except that M has been subtracted. This matrix equation is readily solved by standard eigenvalue iteration methods such as the inverse power method.⁴⁸

8.3.6 □ Comments on the Finite Element Method □ We have considered the application of the finite element method to both the first and second order transport equations. We also examined hybrid schemes such as the finite element–discrete ordinates method. The discrete ordinates method has also been combined with a triangular finite element solution of the second order transport equation.⁵⁵

At this point there is no question that the highly developed finite element–discrete ordinates method^{19,21} (for the first order transport equation) is the most attractive from the standpoint of computing economy. However it is susceptible to the ray effect; and although measures can be taken to mitigate this phenomenon by converting the discrete ordinates form of the equations to spherical harmonics form, this procedure is quite costly.²⁷

The successful application of the finite element method to the first order transport equation in space and angle has been demonstrated.⁴⁸ However the need to solve the resulting asymmetric system of equations using direct matrix inversion methods has a severe impact on computer time and memory requirements. At present these penalties outweigh such advantages of the first order approach as ease of incorporating anisotropic scattering, mitigation of the ray effect, and convenient treatment of all boundary conditions as natural boundary conditions.

On the other hand, the second order finite element scheme does result in symmetric, banded matrices that are positive definite, hence amenable to iterative solution techniques such as the block successive overrelaxation method combined with a coarse mesh rebalance.⁶⁰ This feature, when viewed in conjunction with the demonstrated success of the second order method for alleviating the ray effect⁶¹ and the reduction of the angular domain due to symmetry of the even-parity angular flux, seems to indicate the potential success of this approach. However computing times still do not compare well with the production level discrete ordinates codes, and it appears that anisotropic scattering is extremely difficult to implement in multidimensional geometry. In addition, voids may present a problem because of the $(\Sigma_r)^{-1}$ term in the second order equation (although thus far this problem has been avoided).⁴ Finally, if the angular flux is desired, apparently it will be necessary in general to solve both the even- and odd-parity equations simultaneously.⁶² (The scalar flux is known once the even-parity angular flux has been calculated.)

8.4 □ INTEGRAL TRANSPORT METHODS □ The preceding sections of this chapter have all been concerned with the solution of the integrodifferential form of the transport equation, although in the case of the finite element method this was masked in the guise of an equivalent integral formulation (i.e., variational or Galerkin forms). However, as noted in Section 2.1.5, the transport equation can be integrated along its characteristics to yield an integral equation form.

A variety of specific numerical methods have been developed for solving the integral transport equation. We consider the traditional "collision probability" method, then develop an alternative approach based on a discretized formulation of the integral transport equation. Both these methods can lead to exorbitant computing effort for even moderate sized problems because the various mesh regions are strongly coupled. Therefore we develop interface current and response matrix methods that avoid this full coupling by coupling larger regions to one another by way of their respective partial currents.

8.4.1 □ Collision Probability Method □ The *collision probability method*⁶³⁻⁶⁶ is commonly regarded as an approach that discretizes the integral transport equation directly to yield matrix elements (the “collision probabilities”), which then must be calculated. To illustrate this method, we begin with the one-speed form of the integral transport equation assuming isotropic sources and scattering for convenience:

$$\phi(\mathbf{r}) = \int d^3\mathbf{r}' \frac{e^{-\alpha(\mathbf{r},\mathbf{r}')}}{4\pi|\mathbf{r}-\mathbf{r}'|^2} \psi(\mathbf{r}') \quad (8.77)$$

where $\psi(\mathbf{r}) \equiv \Sigma_s(\mathbf{r})\phi(\mathbf{r}) + S(\mathbf{r})$ is the emission density (see Section 2.1.5) and $\alpha(\mathbf{r},\mathbf{r}')$ is the optical thickness between $\mathbf{r}$ and $\mathbf{r}'$

$$\alpha(\mathbf{r},\mathbf{r}') \equiv \int_0^{|\mathbf{r}-\mathbf{r}'|} ds \Sigma_t\left(\mathbf{r}-s\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}\right)$$

For a homogeneous medium, $\alpha(\mathbf{r},\mathbf{r}') = \Sigma_t|\mathbf{r}-\mathbf{r}'|$ is simply the number of mean free paths between $\mathbf{r}$ and $\mathbf{r}'$. The integral in Eq. 8.77 is taken over all space. Our goal is to solve this equation numerically.

In principle at least, this task is quite straightforward. Let us assume that we have a finite volume V of interest with vacuum boundary conditions on all sides. In this case the integration in Eq. 8.77 can be taken over the volume V only. Then we split V into N regions, $V_1, V_2, \dots, V_N$, where the V_i are distinct and $V = \sum_{i=1}^N V_i$. After multiplication by $\Sigma_i(\mathbf{r})$ and integration over an arbitrary region V_i , Eq. 8.77 becomes

$$\int_{V_i} d^3\mathbf{r} \Sigma_i(\mathbf{r})\phi(\mathbf{r}) = \int_{V_i} d^3\mathbf{r} \Sigma_i(\mathbf{r}) \sum_{j=1}^N \int_{V_j} d^3\mathbf{r}' \frac{e^{-\alpha(\mathbf{r},\mathbf{r}')}}{4\pi|\mathbf{r}-\mathbf{r}'|^2} \psi(\mathbf{r}') \quad (8.78)$$

Next we introduce the definitions

$$\begin{aligned} \phi_i &\equiv \frac{1}{V_i} \int_{V_i} d^3\mathbf{r} \phi(\mathbf{r}), & \psi_i &\equiv \frac{1}{V_i} \int_{V_i} d^3\mathbf{r} \psi(\mathbf{r}) \\ \Sigma_i^j &\equiv \frac{\int_{V_i} d^3\mathbf{r} \Sigma_i(\mathbf{r})\phi(\mathbf{r})}{\int_{V_i} d^3\mathbf{r} \phi(\mathbf{r})} \\ P_{ij} &\equiv \frac{\int_{V_i} d^3\mathbf{r} \Sigma_i(\mathbf{r}) \int_{V_j} d^3\mathbf{r}' \frac{e^{-\alpha(\mathbf{r},\mathbf{r}')}}{4\pi|\mathbf{r}-\mathbf{r}'|^2} \psi(\mathbf{r}')}{\int_{V_j} d^3\mathbf{r}' \psi(\mathbf{r}')} \end{aligned}$$

and substitute these into Eq. 8.78 to obtain

$$\sum_i \phi_i V_i = \sum_{j=1}^N P_{ij} \psi_j V_j, \quad i = 1, 2, \dots, N \quad (8.79)$$

If we note that $\psi_j = \sum_s \phi_s + S_j$, Eq. 8.79 becomes

$$\sum_i \phi_i V_i = \sum_{j=1}^N P_{ij} V_j [\sum_s \phi_s + S_j] \quad (8.80)$$

which is a system of algebraic equations for the average scalar fluxes $\phi_i, i = 1, 2, \dots, N$. Since the left-hand side of Eq. 8.80 corresponds to $\sum_i \phi_i V_i$ = number of collisions per second in V_i , and the right-hand side contains a term $V_j \psi_j$ = number of particles produced per second in V_j , evidently we can associate P_{ij} with the average probability that a particle appearing isotropically in region j will make its first collision in region i . If we assume uniform material properties and emission densities ψ_i in all regions V_i , the P_{ij} simplifies to

$$P_{ij} = \sum_i \frac{V_i}{V_j} \int_{V_j} d^3r' \frac{e^{-\alpha(r, r')}}{4\pi |r - r'|^2}$$

If we now interchange i and j in the definition for P_{ij} , we obtain

$$\sum_i V_i P_{ji} = \sum_i V_j P_{ij}$$

which is the discretized form of the reciprocity principle (see Section 2.1.4).

Thus it would appear that we are finished. We need only solve the system of equations (8.80), and this does not appear to be a formidable task. However we still must evaluate the collision probabilities P_{ij} , and this presents the major difficulty in the collision probabilities method. First we note that the matrix $\mathbf{P} = [P_{ij}]$ will be full in general because there is a finite (although perhaps small) probability of transport from any volume V_j to any other volume V_i . Thus there will be $N^2/2$ collision probabilities (due to reciprocity) to compute and store for the resulting matrix inversion. Second, the collision probabilities are difficult to compute, as we now demonstrate for a general two-dimensional geometry.

We consider the calculation of collision probabilities for geometries that are uniform in one direction. In this instance we can reduce the problem to the computation of planar collision probabilities by integrating over the direction of symmetry. We assume that particles are emitted isotropically and uniformly within each discrete volume. This is known as the *flat flux*

approximation.⁶⁴ (The next section considers a method of relaxing this approximation by using Gaussian quadrature to evaluate the P_{ij} integrals.) The flat flux approximation places a restriction on the mesh: if the flux varies rapidly within a region, the mesh should be refined sufficiently to ensure that the flux is well approximated by a piecewise-constant function.

Before we consider the actual computation of the P_{ij} terms, let us consider some basic concepts for the attenuation of particles in a geometry with plane symmetry. First we note that if two points i and j are separated by a distance τ measured in mean free paths (i.e., τ = optical thickness), the probability that a particle leaving point i in the direction of point j will not suffer a collision before point j is $e^{-\tau}$. Now consider the case of two parallel lines l_i and l_j of infinite extent in the z direction separated by a distance τ (in mfp). We wish to compute the average probability $P(l_j \rightarrow l_i)$ that a particle emitted uniformly and isotropically from l_j in the direction of l_i will not suffer a collision before it reaches l_i . That is, we average the probability over all possible paths between l_i and l_j . We describe a particular path by the angle θ which it subtends with the z -axis and define $P(l_j \rightarrow l_i, \theta)$ as the probability that a particle will travel from l_j to l_i along the path at an angle θ to the z -axis without making a collision. Clearly $P(l_j \rightarrow l_i, \theta) = \exp(-\tau/\sin \theta)$. But since we have assumed an isotropic emission of particles from l_j , the probability of the particle being in the angle element $d\theta$ is proportional to $\sin \theta d\theta$. Therefore the average probability is (see Fig. 8.29)

$$P(l_j \rightarrow l_i) = \int_0^\pi d\theta \sin \theta P(l_j \rightarrow l_i, \theta) \left[\int_0^\pi d\theta \sin \theta \right]^{-1} = \frac{1}{2} \int_0^\pi d\theta \sin \theta e^{-\tau/\sin \theta} \quad (8.81)$$

Equation 8.81 can be put in a more standard form with the substitution $\cosh u = (\sin \theta)^{-1}$:

$$P(l_j \rightarrow l_i) = \int_0^\infty du [(\cosh u)^{-2} \exp(-\tau \cosh u)] = Ki_2(\tau)$$

where $Ki_2(\tau)$ is the Bickley-Naylor function⁶⁷ of order 2. In general the n th Bickley-Naylor function is defined by

$$Ki_n(x) = \int_0^\infty du [(\cosh u)^{-n} \exp(-x \cosh u)]$$

Note that $P(l_j \rightarrow l_i)$ is simply P_{ij} to two points i and j in a planar geometry (i.e., a geometry with axial symmetry) if we assume isotropic emission of particles. Therefore for geometries with planar symmetry we

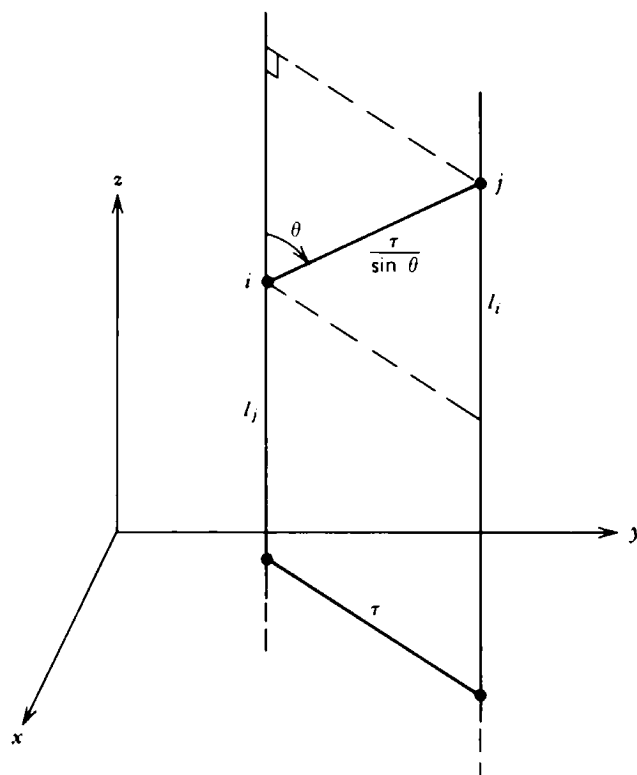


Fig. 8.29 □ Line source geometry for two-dimensional collision probability calculation.

can replace the usual $e^{-\tau}$ linear attenuation factor with the planar attenuation factor $Ki_2(\tau)$, where τ is the distance (in mfp) separating i and j in the plane. This correspondence serves to simplify the calculation of collision probabilities in quite general two-dimensional geometries, as we now demonstrate.⁶⁴

Consider the general two-dimensional geometry illustrated in Figure 8.30. We wish to compute the average probability P_{ij} that a particle emitted uniformly and isotropically in V_j will suffer its first collision in V_i . Note that we can split up the probability P_{ij} as

$$P_{ij} = (\text{probability particle will not suffer a collision before it reaches } V_i) \times (\text{probability that particle will suffer a collision in } V_i)$$

To compute this average, we lay down a grid of paths between V_j and V_i and simply average P_{ij} over all possible paths. This is conveniently done by

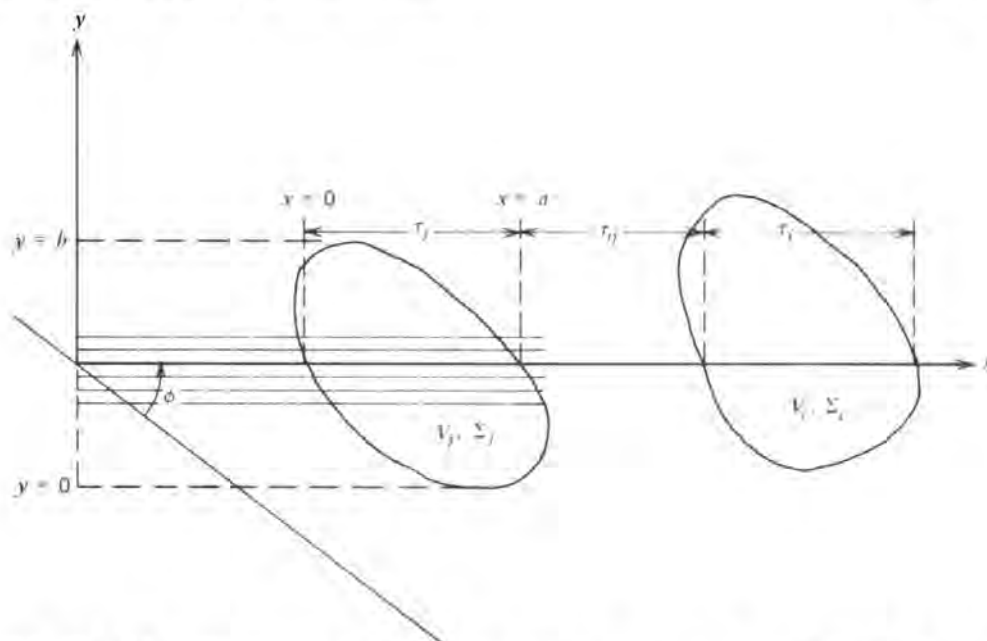


Fig. 8.30 □ Cell geometry for discrete integral transport method (after Carlvik⁶⁴).

placing several parallel lines at some reference angle ϕ , as illustrated in Figure 8.30. The number of these lines is determined by their separation distance and the number of discrete directions ϕ considered. Let us define the probability

$$P_{ij}(x, y, \phi) = \text{probability that a particle emitted at } x \text{ in a direction along the line } (y, \phi) \text{ in volume } V_j \text{ will have its first collision somewhere in the volume } V_i$$

[Note that by definition this first collision occurs along the line (y, ϕ) .]

But from our discussion of the attenuation in plane geometries, we immediately note with the aid of Figure 8.30 that

$$Ki_2[\Sigma_j(a-x) + \tau_{ij}] = \text{probability of traveling from } x \text{ to boundary of } V_i \text{ without a collision}$$

$$1 - Ki_2(\tau_i) = \text{probability of a particle having a collision somewhere in } V_i \text{ if it starts at the boundaries}$$

Therefore by multiplying these terms and then expanding, we have

$$P_{ij}(x, y, \phi) = Ki_2[\Sigma_j(a - x) + \tau_{ij}] - Ki_2[\Sigma_j(a - x) + \tau_{ij} + \tau_i]$$

Then if we average over all x , we find

$$\begin{aligned} P_{ij}(y, \phi) &= \frac{\int_0^a dx P(x, y, \phi)}{\int_0^a dx} \\ &= (a\Sigma_j)^{-1} [Ki_3(\tau_{ij}) - Ki_3(\tau_{ij} + \tau_j) - Ki_3(\tau_{ij} + \tau_i) + Ki_3(\tau_{ij} + \tau_j + \tau_i)] \end{aligned}$$

Finally we average over all y and ϕ , noting that since we have assumed uniform and isotropic emission of particles in V_j , the number of particles in a volume element $a dy$ is proportional to $d\phi$

$$P_{ij} = \frac{\int_0^{2\pi} d\phi \int_0^b dy a P_{ij}(y, \phi)}{\int_0^{2\pi} d\phi \int_0^b dy a}$$

But $V_j = \int_0^{b(x)} dy a(y)$. Therefore our final result is

$$\begin{aligned} P_{ij} &= (2\pi V_j \Sigma_j)^{-1} \int d\phi \int dy [Ki_3(\tau_{ij}) - Ki_3(\tau_j + \tau_{ij}) \\ &\quad - Ki_3(\tau_{ij} + \tau_i) + Ki_3(\tau_{ij} + \tau_i + \tau_j)] \end{aligned} \quad (8.82)$$

where we should keep in mind that all the path lengths τ_i , τ_j , and τ_{ij} are functions of y and ϕ .

Since the volumes V_i are of finite extent, it is possible for some of the particles emitted in V_i to suffer their first collision in V_i . In other words, we need to compute the self-collision probability P_{ii} . This can be written as

$$P_{ii} = (2\pi V_i)^{-1} \int d\phi \int a dy \int_0^a dx P_{ii}(x, y, \phi)$$

where $P_{ii}(x, y, \phi) = 1 - Ki_2[\Sigma_i(a - x)]$. Integrating, we obtain

$$P_{ii} = 1 - (2\pi V_i \Sigma_i)^{-1} \int dy \int d\phi [Ki_3(0) - Ki_3(\tau_i)]$$

We have now computed, in principle at least, all the collision probabilities P_{ij} needed to solve Eq. 8.80. As noted earlier with the general

expression for P_{ij} in Eq. 8.79, Eq. 8.82 results in the reciprocity condition $V_j \sum_i P_{ij} = V_i \sum_j P_{ji}$.

Equation 8.82 is a general formula for P_{ij} in any two-dimensional geometry. However it still represents a significant amount of computing effort because of the need to evaluate the Bickley functions as well as the large number of collision probabilities that must be computed for realistic configurations. Also, the form of Eq. 8.82 may be somewhat misleading in that a significant amount of effort must be expended just to identify the various regions that the chosen paths will intersect. Even with the use of fast, rational approximations to the Bickley functions, the computation of the P_{ij} 's may still be prohibitive for many typical configurations.⁶⁵

If the geometry being analyzed is annular, such as a pin cell calculation for a reactor lattice analysis, the P_{ij} calculation can be simplified considerably. For example, the THERMOS code,⁶³ which was the forerunner of collision probability codes for reactor analysis, uses annular symmetry to simplify the integrations considerably. Another successful approach is the FLURIG scheme,⁶⁴ wherein a specially chosen Gaussian quadrature set is used to compute approximate collision probabilities. This scheme avoids the restrictive flat flux approximation and is generally more accurate for a given number of mesh points. Instead of considering these specific applications, however, we proceed to an alternative method for solving the integral transport equation.

8.4.2 □ Discrete Integral Transport □ An alternative method for solving the integral transport equation is the *discrete integral transport* method of Carlvik.⁶⁸ This method offers significant advantages over the traditional collision probabilities method with respect to computing efficiency and accuracy for a given mesh. It is particularly useful for configurations in which strongly varying fluxes are expected, although in the limit of a black absorber the flat flux approximation may be more efficient due to the decoupling of the Gauss points. (For a black absorber there will always be a finite probability of travelling from one region to another, but not necessarily from one point to another point.) In addition this method is readily generalized to include surface sources and can be cast into an interface current technique that is capable of treating relatively large configurations with a considerable savings in computing effort.

The discrete integral transport method differs from the conventional collision probabilities method in the following ways. (i) It is applied to the general angle-dependent integral transport equation. (ii) The angular flux and emission density are first expanded in spherical harmonics in angle and Fourier series in space (azimuth), and the expansion coefficients are

treated as unknowns in the calculation. (iii) Transport coefficients (similar to collision probabilities) are computed by way of Gaussian quadrature because they are formulated in terms of a discrete pointwise representation in space rather than a regionwise representation.

We consider only a few of the more interesting features of the discrete integral transport method, following closely the development of Carlvik.⁶⁸ (Consult the original work for more details.)

We begin with the angle-dependent integral transport equation, which we write as follows:

$$\varphi(\mathbf{r}, \hat{\Omega}) = \int_0^\infty dR e^{-\alpha} \psi(\mathbf{r}', \hat{\Omega}) \quad (8.83)$$

where $\psi(\mathbf{r}, \hat{\Omega})$ is the emission density, and α is the optical thickness (see Section 2.1.5). We consider the case of an annular geometry depicted in Figure 8.31. We first expand the angular flux in terms of spherical harmonics in angle (see Section 4.2.2) and Fourier series in the spatial azimuthal angle φ (not to be confused with the azimuthal angle ϕ in the

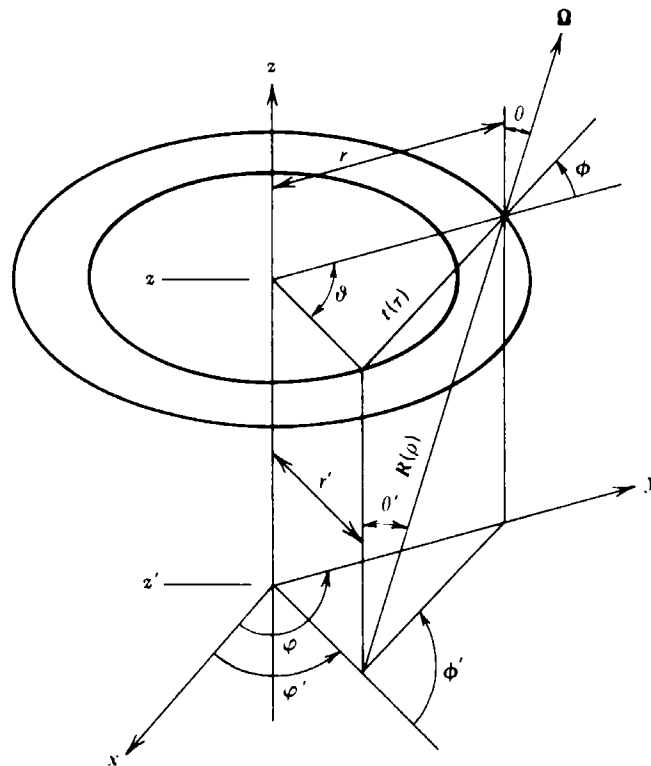


Fig. 8.31 □ Coordinate system for annular geometry (after Carlvik⁶⁷).

direction space):

$$\varphi(\mathbf{r}, \hat{\Omega}) = (2\pi)^{-1} \sum_{k=-\infty}^{\infty} \sum_{\nu=0}^{\infty} \sum_{\mu=-\nu}^{\nu} \varphi_{\nu k}^{\mu}(\mathbf{r}) e^{ik\varphi} Y_{\nu\mu}(\theta, \phi)$$

where by orthogonality

$$\varphi_{\nu k}^{\mu}(\mathbf{r}) = \int_0^{2\pi} d\phi' \int d\hat{\Omega} e^{-ik\phi} Y_{\nu\mu}^*(\theta, \phi) \varphi(\mathbf{r}, \hat{\Omega})$$

Here we have implicitly assumed that there is no z -dependence. Using a similar expansion for the emission density $\psi(\mathbf{r}, \hat{\Omega})$, we substitute these expansions into Eq. 8.83, multiply by $Y_{nm}^*(\theta, \phi) e^{-ik\phi}$, and integrate over all $\hat{\Omega}$ and φ :

$$\begin{aligned} \varphi_{nk}^m(\mathbf{r}) &= \int_0^{2\pi} d\varphi \int d\hat{\Omega} \int_0^{\infty} dR e^{-\alpha R} e^{ik\varphi} Y_{nm}^*(\theta, \phi) \\ &\times \sum_{\kappa=-\infty}^{\infty} \sum_{\nu=0}^{\infty} \sum_{\mu=-\nu}^{\nu} \psi_{\nu\kappa}^{\mu}(\mathbf{r}') (2\pi)^{-1} e^{ik\varphi'} Y_{\nu\mu}(\theta', \phi') \end{aligned} \quad (8.84)$$

Our goal is to transform Eq. 8.84 into the following system of equations:

$$\varphi_{nk}^m(\mathbf{r}_i) = \sum_{j=1}^J \sum_{\nu=0}^N \sum_{\mu=-\nu}^{\nu} T_{n\nu k}^{m\mu}(\mathbf{r}_i, \mathbf{r}_j) V_j \psi_{\nu k}^{\mu}(\mathbf{r}_j)$$

This system is quite similar to the set (8.80) obtained earlier for the more conventional collision probabilities method. In this case the transport coefficients $T_{n\nu k}^{m\mu}(\mathbf{r}_i, \mathbf{r}_j)$ give the angular flux moments φ_{nk}^m at $\mathbf{r}_i$ due to a unit source at $\mathbf{r}_j$ emitting particles with an angular distribution $Y_{\nu\mu}(\theta, \phi)$.

To simplify Eq. 8.84, we note that the integrals $\int d\hat{\Omega} \int dR$ are taken over all space. Therefore we can change the variable of integration to the more convenient volume element:

$$d\hat{\Omega} dR \rightarrow \frac{R^2}{R^2} dR d\hat{\Omega} \rightarrow \left(\frac{1}{R^2} \right) dV \rightarrow r' dr' d\varphi' d \frac{(z-z')}{R^2}$$

If we define t as the distance between $\mathbf{r}$ and $\mathbf{r}'$ measured in the xy plane (see Figure 8.31), then $R = [(z-z')^2 + t^2]^{1/2}$ and $\sin \theta = t/R$. Now we make the same change in variable, $\cosh u = (\sin \theta)^{-1}$, as we did when we integrated Eq. 8.81, causing the integrals to become

$$\int d\hat{\Omega} \int dR [] = \int_0^{\infty} dr' r' \int_0^{2\pi} d\varphi' \int_{-\infty}^{\infty} d(z-z') t^{-2} \cosh^{-2} u$$

But now we define τ as the distance (in mfp) corresponding to t and note that $d(z - z') = t \cosh u du$. With these changes, Eq. 8.84 becomes (noting $\cos \theta = \tanh u$)

$$\begin{aligned} \varphi_{nk}^m(r) = & \int_0^\infty r' dr' \sum_{\kappa=-\infty}^\infty \sum_{\nu=0}^\infty \sum_{\mu=-\nu}^\nu \psi_{\nu\kappa}^\mu(r') (2\pi)^{-1} \int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' e^{i(\kappa\varphi' - k\varphi)} \\ & \times t^{-1} \int_{-\infty}^\infty du Y_{nm}(\tanh u, \phi) Y_{\nu\mu}(\tanh u, \phi') \frac{e^{-\tau \cosh u}}{\cosh u} \end{aligned}$$

Using the explicit form of the $Y_{nm}(\hat{\Omega})$ functions, we can reduce this to

$$\begin{aligned} \varphi_{nk}^m(r) = & \int_0^\infty 2\pi r' dr' \sum_{\kappa=-\infty}^\infty \sum_{\nu=0}^\infty \sum_{\mu=-\nu}^\nu \psi_{\nu\kappa}^\mu(r') (2\pi^2)^{-1} A_\nu^\mu \\ & \times \int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' e^{i(\kappa\varphi' - k\varphi + \mu\phi' - m\phi)} t^{-1} G_{n\nu,1}^{m\mu}(\tau) \quad (8.85) \end{aligned}$$

where $G_{n\nu,1}^{m\mu}(\tau)$ is related to the Bickley-Naylor functions [$G_{0,0,1}^{0,0}(\tau) = Ki_1(\tau)$] and defined by

$$G_{n\nu,l}^{m\mu}(\tau) \equiv \frac{1}{2} \int_{-\infty}^\infty du P_n^m(\tanh u) P_\nu^\mu(\tanh u) \frac{e^{-\tau \cosh u}}{\cosh u}$$

Furthermore

$$A_\nu^\mu = \left(\frac{2\nu+1}{4\pi} \right) \left[\frac{(\nu-\mu)!}{(\nu+\mu)!} \right]$$

Equation 8.85 can be simplified even further if the material properties do not depend on the azimuthal angle φ . In this case τ is a function only of $\vartheta = \varphi - \varphi'$ and it is easy to show that

$$\begin{aligned} \int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' e^{i(\kappa\varphi' - k\varphi)} t^{-1} e^{i(\mu\phi' - m\phi)} G_{n\nu,1}^{m\mu}(\tau) \\ = 2\pi \delta_{\kappa k} \int_0^{2\pi} d\vartheta e^{ik\vartheta} t^{-1} e^{i(\mu\phi' - m\phi)} G_{n\nu,1}^{m\mu}(\tau) \end{aligned}$$

With this simplification, Eq. 8.85 becomes

$$\varphi_{nk}^m(r) = \int_0^\infty 2\pi r' dr' \sum_{\nu=0}^\infty \sum_{\mu=-\nu}^\nu \psi_{\nu k}^\mu(r') A_\nu^\mu \int_0^{2\pi} d\vartheta (\pi t)^{-1} e^{i(k\vartheta - \mu\phi' + m\phi)} G_{n\nu,1}^{m\mu}(\tau)$$

Finally, we choose a discrete radial mesh at the points r_i , $i = 1, 2, \dots, I$ and evaluate the integral with Gaussian quadrature. For example, an arbitrary integral over r becomes

$$\int_0^a dr' 2\pi r' f(r') = \sum_{i=1}^N v_i f(r_i)$$

where v_i contains the appropriate weight ($\times 2\pi$). We now have the final expression for $\varphi_{nk}^m(r)$

$$\varphi_{nk}^m(r_i) = \sum_{j=1}^I \sum_{\nu=0}^N \sum_{\mu=-\nu}^{\nu} T_{n\nu,k}^{m\mu}(r_i, r_j) V_j \psi_{\nu k}^{\mu}(r_j)$$

where

$$T_{n\nu,k}^{m\mu}(r_i, r_j) = A_{\nu}^{\mu} \int_0^{2\pi} d\vartheta (\pi l)^{-1} e^{i(k\vartheta + \mu\varphi' - m\phi)} G_{n\nu,l}^{m\mu}(\tau) \quad (8.86)$$

Concerning this result, note that the azimuthal (“pole” mode) terms do not interact. This is a consequence of our assumption that the material properties were azimuthally symmetric. The diagonal terms ($r_i = r_j$) present a problem because they diverge in general. However they can be calculated on the basis of particle conservation over the entire cell.⁶⁷

The analysis has assumed that the spatial integration was extended over all space, or if there were boundaries, they were of a vacuum nature. For other boundary conditions, such as the usual “white” boundary condition for a pin cell calculation, one can modify the matrix elements $T(r_i, r_j)$ on the basis of conservation and reciprocity arguments.

In practice, the calculation of the matrix elements $T(r_i, r_j)$ can be made simpler by transforming the ϑ integration to a more convenient variable, then using a specially tailored Gaussian set that takes into account the properties of the integrand.^{68,69}

We complete our coverage of discrete integral transport calculations with a brief discussion of its generalization to include surface sources in the next section.

8.4.3 □ Interface Coupling Methods □ The traditional approach to solving the integral transport equation proceeds by calculating the collision probabilities (or transport coefficients) that relate a given spatial region to all other spatial regions in the domain of interest. This approach, which we refer to simply as the “ P_{ij} method,” was seen to be somewhat time-consuming because of the full coupling of the collision probability terms.

We now turn to an alternative method based on coupling spatial regions with incoming and outgoing partial currents between the regions. By definition, this implies that a region will be coupled only to its adjacent neighbors. This feature has obvious implications for drastically reducing the computational effort associated with the standard P_{ij} techniques. There have been a variety of applications of this basic approach, and we refer collectively to these methods as “interface coupling” methods or “ $J_{\pm}$ ” methods. Such schemes include the interface current,^{70–74} discrete integral coupling,^{75,76} and response matrix methods.^{77–81}

The interface current and the discrete integral coupling methods are based on a mesh structure consisting of relatively coarse regions that are further subdivided into finer mesh regions. Within a coarse mesh region or node, the fine mesh regions are all coupled together by way of the traditional collision probabilities method (or the discrete integral transport method). These regions are also coupled to any incoming fluxes on the boundaries of their respective coarse regions. The nodes are coupled together by way of incoming or outgoing partial currents, which, of course, are the same quantities for adjacent nodes. Therefore fine mesh regions corresponding to different nodes are not related directly as they would be with the traditional P_{ij} methods, but rather are related indirectly through the interface currents. Thus the interface currents and the fine mesh fluxes are the unknowns in the corresponding system of equations.

The response matrix method is similar except that the fine mesh fluxes are not computed as unknowns along with the incoming and outgoing partial currents. Instead, one computes the response matrices that relate the outgoing partial current of a node (the response) to a given incoming partial current (the input). Thus the fine mesh calculation is used to compute the response matrices beforehand, not during the actual solution of the equations. Once the response matrices have been computed by way of standard collision probabilities methods, or Monte Carlo or diffusion theory methods, for example, one solves for the distribution of partial currents that results in a self-consistent system (i.e., $J_I^{\text{in}} = J_J^{\text{out}}$ for adjacent regions I and J). Once the partial current distribution is known, the detailed within-node flux distribution can be calculated with another response matrix generated during the fine mesh computations.

The interface coupling methods are derived from the following generalization of the integral transport equation:

$$\varphi(\mathbf{r}, \hat{\Omega}) = \int_0^{R_{\max}} dR \psi(\mathbf{r}', \hat{\Omega}) e^{-\alpha(\mathbf{r}, \mathbf{r}')} + \varphi_{-}(\mathbf{r}_s, \hat{\Omega}) e^{-\alpha(\mathbf{r}, \mathbf{r}_s)} \quad (8.87)$$

where $\psi(\mathbf{r}, \hat{\Omega})$ is the usual emission density, $\alpha(\mathbf{r}, \mathbf{r}')$ is the optical thickness between $\mathbf{r}$ and $\mathbf{r}' = \mathbf{r} - R\hat{\Omega}$, $\alpha(\mathbf{r}, \mathbf{r}_s)$ is the optical thickness between $\mathbf{r}$ and

$\mathbf{r}_s = \mathbf{r} - |\mathbf{r} - \mathbf{r}_s| \hat{\Omega}$, and $\varphi_-(\mathbf{r}_s, \hat{\Omega})$ is the incoming angular flux at $\mathbf{r}_s$ [i.e., $\varphi_-(\mathbf{r}_s, \hat{\Omega}) = \varphi(\mathbf{r}_s, \hat{\Omega})$ for $\hat{\Omega} \cdot \hat{\mathbf{e}}_s < 0$, and zero otherwise]. Note that the integration in Eq. 8.87 is taken over a finite region, and the contribution from the boundary is explicitly included. If the region of interest had vacuum boundaries, $\varphi_-(\mathbf{r}_s, \hat{\Omega})$ would be zero and Eq. 8.87 would reduce to an earlier version of the integral transport equation (8.83). Equation 8.87 is the starting point for the various interface coupling methods.

Interface Current Method □ Let us integrate Eq. 8.87 over all $\hat{\Omega}$ and introduce the following changes in the variables of integration⁷⁰:

$$\begin{aligned}
 d^3r' &= dV' = |\mathbf{r} - \mathbf{r}'|^2 dR d\hat{\Omega} \\
 d^2r_s &= dS = |\mathbf{r} - \mathbf{r}_s|^2 d\hat{\Omega} |\hat{\Omega} \cdot \hat{\mathbf{e}}_s|^{-1}
 \end{aligned}$$

to obtain

$$\phi(\mathbf{r}) = \int_V d^3r' \frac{e^{-\alpha(\mathbf{r}, \mathbf{r}')}}{|\mathbf{r} - \mathbf{r}'|^2} \psi(\mathbf{r}', \hat{\Omega}) + \int_S d^2r_s \frac{e^{-\alpha(\mathbf{r}, \mathbf{r}_s)}}{|\mathbf{r} - \mathbf{r}_s|^2} |j_{\text{in}}(\mathbf{r}_s, \hat{\Omega}) \cdot \hat{\mathbf{e}}_s| \quad (8.88)$$

Here we have identified the inward partial angular current $j_{\text{in}} = \hat{\Omega} \varphi_-(\mathbf{r}_s, \hat{\Omega})$. Next we partition the volume V and surface S into regions $V_i, i = 1, \dots, N$ and $S_a, a = 1, \dots, M$. If we now multiply Eq. 8.88 by $\Sigma_i(\mathbf{r})$ and integrate over V_i , we find

$$V_i \Sigma_i \phi_i = \sum_{j=1}^N V_j \psi_j P_{ij} + \sum_{a=1}^M J_{\text{in}}^a P_{ia} \quad (8.89)$$

where

$$\begin{aligned}
 \phi_i &\equiv \frac{1}{V_i} \int d^3r \phi(\mathbf{r}), & \psi_i &\equiv \frac{1}{V_i} \int d\hat{\Omega} \int d^3r \psi(\mathbf{r}, \hat{\Omega}) \\
 J_{\text{in}}^a &\equiv \int_{\hat{\Omega} \cdot \hat{\mathbf{e}}_s < 0} d\hat{\Omega} \int_{S_a} d^2r_s |j_{\text{in}}(\mathbf{r}_s, \hat{\Omega}) \cdot \hat{\mathbf{e}}_s|, & \Sigma_i^j &\equiv \frac{1}{\phi_i} \int_{V_i} d^3r \Sigma_i(\mathbf{r}) \phi(\mathbf{r}) \\
 P_{ij} &\equiv \frac{1}{V_j \psi_j} \int_{V_i} d^3r \int_{V_j} d^3r' \frac{e^{-\alpha(\mathbf{r}, \mathbf{r}')}}{|\mathbf{r} - \mathbf{r}'|^2} \Sigma_i(\mathbf{r}) \psi(\mathbf{r}', \hat{\Omega}) \\
 P_{ia} &\equiv \frac{1}{J_{\text{in}}^a} \int_{S_a} d^2r_s \int_{V_i} d^3r \Sigma_i(\mathbf{r}) \frac{e^{-\alpha(\mathbf{r}, \mathbf{r}_s)}}{|\mathbf{r} - \mathbf{r}_s|^2} |j_{\text{in}}(\mathbf{r}_s, \hat{\Omega}) \cdot \hat{\mathbf{e}}_s|
 \end{aligned}$$

Note that P_{ia} is just the first-flight collision probability characterizing

particles entering the system at S_a that make their first collision in V_i .

Equation 8.89 is the generalization of Eq. 8.80 to include surface sources. At this point, if we knew the incoming current distributions $j_{\text{in}}(\mathbf{r}_s, \hat{\Omega})$, we could treat the terms $\sum_{a=1}^N J_{\text{in}}^a P_{ia}$ as an effective source and directly solve Eq. 8.89. Suppose we treat the volume V as one node, call it V_I , in the overall domain of interest. Then we require Eq. 8.89 to be satisfied for each such volume:

$$V_i \sum_{ii} \phi_i = \sum_{j \in V_I} V_j \psi_j P_{ij} + \sum_{a \in S_I} J_{\text{in}}^a P_{ia}, \quad \begin{matrix} i = 1, 2, \dots, N_I \\ I = 1, 2, \dots, N \end{matrix} \quad (8.90)$$

At this point we note that J_{in}^a for a volume V_I will be the same as J_{out}^b for an adjacent volume V_J . However we still need additional equations to solve for the ϕ 's and J 's, since Eq. 8.90 is not sufficient by itself. We obtain these additional equations by multiplying Eq. 8.87 by $\hat{\Omega} \cdot \hat{\mathbf{e}}_s$ and integrating over the surface S_a and the angular domain $\hat{\Omega} \cdot \hat{\mathbf{e}}_s > 0$:

$$\begin{aligned} \int_{S_a} d^2 r_s \int_{\hat{\Omega} \cdot \hat{\mathbf{e}}_s > 0} d\hat{\Omega} \hat{\Omega} \cdot \hat{\mathbf{e}}_s \varphi(\mathbf{r}_s, \hat{\Omega}) &= \int_{S_a} d^2 r_s \int_{\hat{\Omega} \cdot \hat{\mathbf{e}}_s > 0} d\hat{\Omega} \hat{\Omega} \cdot \hat{\mathbf{e}}_s \int dR \psi(\mathbf{r}', \hat{\Omega}) e^{-\alpha(\mathbf{r}, \mathbf{r}')} \\ &+ \int_{S_a} d^2 r_s \int_{\hat{\Omega} \cdot \hat{\mathbf{e}}_s > 0} d\hat{\Omega} \hat{\Omega} \cdot \hat{\mathbf{e}}_s \varphi(\mathbf{r}'_s, \hat{\Omega}) e^{-\alpha(\mathbf{r}_s, \mathbf{r}'_s)} \end{aligned} \quad (8.91)$$

Now we note that the integrations over $\hat{\Omega}$ on the right-hand side can be transformed into volume and surface integrals as before to yield

$$J_{\text{out}}^a = \sum_{i \in V_I} V_i \psi_i P_{ai} + \sum_{b \in S_I} J_{\text{in}}^b P_{ab}, \quad \text{for } a \in S_I, \quad I = 1, 2, \dots, N \quad (8.92)$$

Here P_{ai} is the first-flight escape probability for a particle to escape through surface S_a if it is emitted in region V_i ,

$$P_{ai} \equiv \frac{1}{\psi_i} \int_{S_a} d^2 r_s \int_{V_i} d^3 r' \frac{e^{-\alpha(\mathbf{r}_s, \mathbf{r}')}}{|\mathbf{r}_s - \mathbf{r}'|^2} |\hat{\Omega} \cdot \hat{\mathbf{e}}_s| \psi(\mathbf{r}', \hat{\Omega})$$

and P_{ab} is the first-flight escape probability for a particle that enters S_b to escape through S_a

$$P_{ab} \equiv \frac{1}{J_{\text{in}}^b} \int_{S_a} d^2 r_s \int_{S_b} d^2 r'_s \frac{e^{-\alpha(\mathbf{r}_s, \mathbf{r}'_s)}}{|\mathbf{r}_s - \mathbf{r}'_s|^2} |\hat{\Omega} \cdot \hat{\mathbf{e}}_s| |j'_{\text{in}}(\mathbf{r}_s, \hat{\Omega}) \cdot \hat{\mathbf{e}}'_s|$$

Equations 8.91 and 8.92 are the interface current equations to be solved for the fluxes and currents. Of course we thus far have only formal definitions of the various collision and escape probabilities, and these remain to be calculated. This task requires a significant effort, but it is nevertheless considerably less time-consuming than the work of calculating the standard collision probabilities. In practice, one generally assumes the flat flux approximation to simplify the P_{ij} and P_{ai} computations and a cosine current (corresponding to an isotropic incoming flux) distribution at the boundaries. The cosine current approximation yields poor results for small mesh spacings since anisotropic angular distributions can be significant on the scale of a lattice calculation, and this results in poor predictions if a cosine distribution is assumed.^{66,70}

One can also express the interface flux in a P_1 expansion instead of the cosine current (P_0 expansion). However it has been noted that this assumption still results in significant errors for some applications. An interesting remedy to this problem involves expressing the angular flux at a boundary in terms of a P_1 expansion relative to an arbitrary direction rather than the normal to the surface.⁷³ In essence this method determines iteratively the predominant direction of particle flow and then expands the flux in a P_1 expansion about this direction.

Discrete Integral Coupling □ The discrete integral transport method discussed in Section 8.4.2 is readily generalized to include surface sources. It can therefore be cast into an interface coupling method quite similar to the interface current method discussed in the preceding section. Since many of the steps are similar to either the earlier development of the method (cf. Section 8.4.2) or the interface current method, we present only the principal results.^{75,76}

The generalization consists of replacing Eq. 8.83 with the following integral equations:

$$\varphi(\mathbf{r}, \hat{\Omega}) = \int_0^{R_{\max}} dR \psi(\mathbf{r}', \hat{\Omega}) e^{-\alpha(\mathbf{r}, \mathbf{r}')} + \varphi_-(\mathbf{r}_s', \hat{\Omega}) e^{-\alpha(\mathbf{r}, \mathbf{r}_s')} \quad (8.93)$$

$$\varphi_+(\mathbf{r}_s, \hat{\Omega}) = \int_0^{R_{\max}} dR \psi(\mathbf{r}', \hat{\Omega}) e^{-\alpha(\mathbf{r}_s, \mathbf{r}')} + \varphi_-(\mathbf{r}_s', \hat{\Omega}) e^{-\alpha(\mathbf{r}_s, \mathbf{r}_s')} \quad (8.94)$$

where Eq. 8.94 is simply the outgoing angular flux at $\mathbf{r}_s$ due to uncollided particles from within the volume as well as uncollided particles entering the surface elsewhere. (We could have used Eq. 8.94 to derive Eq. 8.91 in the preceding section.)

Equations 8.93 and 8.94 are then manipulated in the same manner as Eq. 8.83. That is, we expand $\varphi(r, \hat{\Omega})$, $\varphi_+(r, \hat{\Omega})$, and $\varphi_-(r, \hat{\Omega})$ as follows:

$$\begin{aligned}\varphi(r, \hat{\Omega}) &= \sum_{\kappa=-\infty}^{\infty} \sum_{\nu=0}^{\infty} \sum_{\mu=-\nu}^{\nu} \varphi_{\nu\kappa}^{\mu}(r) (2\pi)^{-1} e^{i\kappa\varphi} Y_{\nu\mu}(\theta, \phi) \\ \varphi_{\pm}(r, \hat{\Omega}) &= \sum_{\kappa=-\infty}^{\infty} \sum_{\nu=0}^{\infty} \sum_{\mu=-\nu}^{\nu} \varphi_{\nu\kappa\pm}^{\mu} (2\pi)^{-1} e^{i\kappa\varphi} Y_{\nu\mu}(\theta, \phi)\end{aligned}$$

and integrate Eqs. 8.93 and 8.94 over all space and angle. If we follow the same steps as in Section 8.4.2, we arrive at a set of coupled matrix equations similar to Eq. 8.86 for the angular flux moments $\varphi_{nk}^m(r_i)$ and $\varphi_{nk+}^m(r_b)$, where r_i is an interior point and r_b is a boundary point. (The detailed equations and matrix elements may be found in Reference 75.)

Finally, we observe again that an outgoing flux for one cell is an incoming flux for the adjacent cell to derive supplemental equations relating the incoming and outgoing angular nodes φ_{nk-}^m and φ_{nk+}^m , respectively. These equations result in a coupling of the pole order modes (different k), but not the angular moments.

The result, as in the interface current method, is a system of algebraic equations that are solved for the flux moments φ_{nk}^m and $\varphi_{nk\pm}^m$.

Response Matrix Methods □ Consider again Eq. 8.89, which relates the outgoing partial current of a particular node V_l with its internal emission density and its incoming partial currents:

$$J_{\text{out}}^a = \sum_{i \in V_l} V_i \psi_i P_{ai} + \sum_{b \in S_l} J_{\text{in}}^b P_{ab} \quad (8.89)$$

where P_{ai} and P_{ab} are the first-flight escape probabilities described earlier. Note that for a given configuration, the outgoing current is a linear function (response) of the incoming current. If we define a vector of outgoing currents $\mathbf{J} = \text{col}(J_1, J_2, \dots, J_N)$, where N is the number of surfaces S_a being considered, we can represent this linear relationship as follows:

$$\mathbf{J}^{\text{out}} = \mathbf{R} \mathbf{J}^{\text{in}}$$

where $\mathbf{R}$ is the *response matrix*. For example, if $J^{\text{out}}(i, n)$ is the outward partial current in node i (corresponding to a given angular, energy, and spatial indexing scheme) on face n due to an incoming current $J^{\text{in}}(j, m)$, the response coefficient is computed as follows:

$$R(i, n; j, m) = \frac{J^{\text{out}}(i, n)}{J^{\text{in}}(j, m)}$$

Thus the entries of $\mathbf{R}$ are determined by setting all incoming currents to zero on all faces, except node j and face m , then computing the ratio above given the partial response $J^{\text{out}}(i, n)$. For a given distribution of incoming current $\mathbf{J}^{\text{in}}$, we then sum up over all the partial responses to find the total response $\mathbf{J}^{\text{out}}$.

The response matrix $\mathbf{R}$ may be viewed as the discretization of the surface-to-surface Green's function defined by

$$j_+(\mathbf{r}_s, \hat{\Omega}) = \int_S d^2r'_s \int d\hat{\Omega}' G(\mathbf{r}_s, \hat{\Omega}; \mathbf{r}'_s, \hat{\Omega}') j_-(\mathbf{r}'_s, \hat{\Omega}')$$

The response matrix $\mathbf{R}$ may be a function of the system multiplication $k = k_{\text{eff}}$ [i.e., $\mathbf{R} = \mathbf{R}(k)$], and it is necessary to account for this in practice. Thus the response coefficients must be determined with k as a parameter.^{78, 79}

We can express mathematically the fact that the incoming current vector is merely a rearrangement of the outgoing current vector, or

$$\mathbf{J}^{\text{in}} = \mathbf{P} \mathbf{J}^{\text{out}}$$

where $\mathbf{P}$ is a permutation matrix that reorders $\mathbf{J}^{\text{out}}$. But we know that

$$\mathbf{J}^{\text{out}} = \mathbf{R}(k) \mathbf{J}^{\text{in}}$$

Therefore

$$\mathbf{J}^{\text{in}} = \mathbf{P}(\mathbf{R}(k) \mathbf{J}^{\text{in}})$$

and now we can solve for $\mathbf{J}^{\text{in}}$ and k such that this equation is satisfied. This can be accomplished iteratively by estimating k and $\mathbf{J}^{\text{in}}$, then computing $\mathbf{R}(k) \mathbf{J}^{\text{in}}$. But since we have already computed $\mathbf{R}(k)$, the amount of computational effort is substantially reduced.

Once $\mathbf{J}^{\text{in}}$ has been determined, the local flux distributions within each cell may be determined by way of Eq. 8.89. Again this equation may be expressed in terms of a response equation

$$\phi = \mathbf{R}^{\text{cell}} \mathbf{J}^{\text{in}}$$

where the entries of $\mathbf{R}^{\text{cell}}$ are computed in a manner similar to that employed for the current response matrix.

Clearly the response matrix method should result in substantial improvements in computational efficiency once the response matrices have been calculated. However, this task may be formidable, and it is difficult to judge the relative efficiencies of the response matrix method, the interface current method, and the discrete integral coupling method.

8.5 □ TIME-DEPENDENT TRANSPORT □ The relative simplicity of the time derivative term, $v^{-1}\partial\varphi/\partial t$, that appears in the transport equation allows the application of numerical schemes that are essentially straightforward extensions of the methods used to solve the time-independent transport equation. In this section we will describe a general method for treating time-dependent transport processes that is independent of the method used to treat the remaining spatial and angular variables. Then we develop particular examples of time-differencing schemes that are compatible with either discrete ordinate or finite element transport methods.

8.5.1 □ Direct Time-Differencing Methods □ Consider the time-dependent transport equation written in abstract notation as follows:

$$\frac{1}{v} \frac{\partial \varphi}{\partial t} + L\varphi = s \quad (8.95)$$

Here, we take L to be the one-speed transport operator

$$L \circ \equiv \hat{\Omega} \cdot \nabla \circ + \Sigma_t(\mathbf{r}) \circ - \int d\hat{\Omega}' \Sigma_s(\hat{\Omega}' \rightarrow \hat{\Omega}) \circ$$

and assume that the appropriate initial conditions and boundary conditions are specified on the angular flux $\varphi(\mathbf{r}, \hat{\Omega}, t)$. The most direct approach to solving Eq. 8.95 consists of discretizing the time variable into time steps $t_0, t_1, \dots, t_n$, then approximating the time derivative in Eq. 8.95 with a simple forward difference formula

$$\left. \frac{1}{v} \frac{\partial \varphi}{\partial t} \right|_{t_n} \cong \frac{1}{v} \frac{\varphi(\mathbf{r}, \hat{\Omega}, t_{n+1}) - \varphi(\mathbf{r}, \hat{\Omega}, t_n)}{t_{n+1} - t_n}$$

We could then evaluate the remaining terms in the transport equation at the advanced time step t_{n+1}

$$\frac{\varphi^{n+1} - \varphi^n}{v \Delta t_n} + L\varphi^{n+1} = s^{n+1}$$

where $\Delta t_n \equiv t_{n+1} - t_n$ and $\varphi^n(\mathbf{r}, \hat{\Omega}) \equiv \varphi(\mathbf{r}, \hat{\Omega}, t_n)$. This can be rearranged as

$$\tilde{L}\varphi^{n+1} = \tilde{s} \quad (8.96)$$

where we define $\tilde{L} \equiv L + (v\Delta t_n)^{-1}$ and $\tilde{s}(\mathbf{r}, \hat{\Omega}) \equiv s^{n+1}(\mathbf{r}, \hat{\Omega}) +$

$(v\Delta t_n)^{-1}\varphi^n(\mathbf{r}, \hat{\Omega})$. Since the right-hand side of Eq. 8.96 will be known from the n th time or the initial condition, we can identify Eq. 8.96 as just the steady-state transport equation with a modified total cross section

$$\tilde{\Sigma}_t \equiv \Sigma_t + (v\Delta t_n)^{-1}$$

Therefore this fully implicit scheme allows us to solve the time-dependent transport equation by simply redefining the total cross section and source at each time step and applying a standard time-independent transport method to invert $\tilde{L}$. For example, the TIMEX⁸² computer code employs the ONETRAN²¹ finite element-discrete ordinates method to solve the time-dependent transport equation in this fashion.

8.5.2 □ Weighted Difference Schemes □ One can treat the time variable in a manner more analogous to conventional discrete ordinates methods by discretizing the time derivative using cell-centered difference formulas, then relating the cell-cornered fluxes to the cell-centered fluxes by weighted arithmetic relations. For example, with a one-dimensional spherical discrete ordinates method, the time derivative at time t_n would be expressed as

$$\left. \frac{\partial \varphi}{\partial t} \right|_{t_n} \cong \frac{\varphi_{im}^{n+1/2} - \varphi_{im}^{n-1/2}}{\Delta t}$$

and the “cell-cornered” (in time) terms $\varphi_{im}^{n+(1/2)}$ and $\varphi_{im}^{n-(1/2)}$ would be related to the cell-centered flux with a weighted diamond difference expression

$$\varphi_{im}^n = (1 - \alpha)\varphi_{im}^{n-1/2} + \alpha\varphi_{im}^{n+1/2}$$

For $\alpha = \frac{1}{2}$ we arrive at the usual diamond difference scheme. This has been employed for the solution of the unsteady radiative transfer equation.⁸³ The case $\alpha = 1$ corresponds to the fully implicit scheme used in the TIMEX code. A time-dependent version of ANISN, TDA,⁸⁴ uses the weighted difference approach, as does the two-dimensional time-dependent discrete ordinates code TRANZIT.⁸⁵ Both these codes have built-in provisions for modifying α (and the weights for the other variables as well) to ensure a positive solution.

8.5.3 □ Time-Dependent Finite Element Methods □ The general approach of solving the time-dependent transport equation by inverting the effective steady-state transport operator L at each time step is well suited

for discrete ordinates methods. However a somewhat different approach is more convenient when phase space finite element methods are employed. We can derive the integral law characterizing the time-dependent transport equation as follows:

find $\varphi(\mathbf{r}, \hat{\Omega}, t) \in H_E$ such that for all $\psi(\mathbf{r}, \hat{\Omega}) \in H_E$

$$\frac{1}{v} \frac{d}{dt} (\varphi, \psi) - (\varphi, \hat{\Omega} \cdot \nabla \psi) + \langle \varphi, \psi \rangle_+ + (K\varphi, \psi) = (s, \psi) + \langle \varphi_B, \psi \rangle_- \quad (8.97)$$

where $s = s(\mathbf{r}, \hat{\Omega}, t)$ and $\varphi_B(\mathbf{r}, \hat{\Omega}, t)$ is a time-dependent incoming flux on the boundary.

Note here that we have kept our space H_E the same as for the time-independent problem. The variable t is simply a parameter as far as the space H_E is concerned. As we did for the steady-state case, we can seek a solution from a finite element subspace $S^h \subset H_E$ and expand the approximate solution in terms of the basis functions for S^h

$$\varphi^h(\mathbf{r}, \hat{\Omega}, t) = \sum_{j=1}^N \phi_j(t) \psi_j^h(\mathbf{r}, \hat{\Omega})$$

—except that now the expansion coefficients $\phi_j(t)$ are allowed to be time dependent. It is straightforward to demonstrate that when this expansion is substituted into Eq. 8.97 and the weighting function $\psi(\mathbf{r}, \hat{\Omega})$ is chosen as each of the basis functions $\psi_i^h(\mathbf{r}, \hat{\Omega})$, one arrives at a matrix equation

$$\frac{1}{v} M \dot{\phi} + A \phi = S \quad (8.98)$$

where A , ϕ , and S are identical to their earlier definitions in Eq. 8.54, and $M_{ij} = (\psi_j^h, \psi_i^h)$.

Standard time-stepping methods can now be used to solve Eq. 8.98. For example, if we choose the Crank-Nicholson scheme, Eq. 8.98 would be discretized as follows:

$$\frac{1}{v} M \left[\frac{\phi^{(n+1)} - \phi^{(n)}}{\Delta t} \right] + A \left[\frac{\phi^{(n+1)} + \phi^{(n)}}{2} \right] = \frac{1}{2} [S^{(n+1)} + S^{(n)}]$$

where we have assumed that the matrix A is not a function of time. This equation can be rearranged to yield

$$\left[M + \left(\frac{v \Delta t}{2} \right) A \right] \phi^{(n+1)} = \left[M - \left(\frac{v \Delta t}{2} \right) A \right] \phi^{(n)} + (S^{(n+1)} + S^{(n)}) \left(\frac{v \Delta t}{2} \right) \quad (8.99)$$

Since we know $\phi^{(0)}$ from the initial conditions, Eq. 8.99 can be solved for all later times $t_n, n = 1, 2, \dots$. If A does not depend on time, it is convenient to use an LU decomposition scheme to invert $M + (v\Delta t/2)A$

$$M + \left(\frac{v\Delta t}{2}\right)A = LU$$

since for time steps after the first step, only back substitutions are required to solve for $\phi^{(n)}$. The matrices L and U are saved from the first time step, and then

$$\phi^{(n+1)} = U^{-1}L^{-1}\tilde{S}$$

where

$$\tilde{S} = \left[M - \left(\frac{v\Delta t}{2}\right)A \right] \phi^{(n)} + (S^{(n+1)} + S^{(n)}) \left(\frac{v\Delta t}{2}\right)$$

It should be apparent that the numerical solution of the time-dependent transport equation can be achieved by a relatively straightforward extension of the finite element method developed for steady state problems. Whether discrete ordinate or finite element methods are used to attack time-dependent problems, it is clear that the burden of the effort involved in developing efficient and accurate solution methods centers on the particular scheme used to solve the steady state transport equation at each time step.

□ PROBLEMS □

8.1 Derive the form of the one-speed transport equation in plane geometry by expanding the scattering kernel in a Legendre polynomial expansion of order L .

8.2 Many numerical transport codes solve the criticality eigenvalue problem for the number of secondaries per collision c which makes the given configuration critical. Relate this parameter to the more conventional criticality eigenvalue k_{eff} for a homogeneous slab geometry, assuming one-speed transport and isotropic scattering.

8.3 Derive the discrete ordinates equations in one-dimensional slab geometry for the case of $N=2$ (e.g., the S_2 equations). Assume isotropic scattering and choose $\mu_1 = -\mu_2, w_1 = w_2$. Compare the structure of these equations with the P_1 equations. Assume steady state and a homogeneous medium for convenience.

8.4 Using the S_2 equations developed in Problem 8.3, derive equations satisfied by the sum and difference of the two angular flux components, $\varphi(x, \mu_1)$ and $\varphi(x, \mu_2)$. Then show that with an appropriate choice of μ_1 , the flux will have the exact asymptotic diffusion length ν_0 . (See Reference 9 for further details.)

8.5 By using forward difference approximations for the derivatives in the plane geometry S_N equations, that is,

$$\left. \frac{\partial \varphi}{\partial x} \right|_{x_k} \cong \frac{\varphi^{k+1} - \varphi^k}{\Delta x}$$

show that difference equations can be obtained from which φ will always be positive, no matter what the mesh spacing. (Such difference equations are, however, less accurate than the central difference equations, which can lead to negative values of the angular flux.)

8.6 Derive the original form of the S_N equations in spherical coordinates by using linear angular interpolation to develop numerical differentiation and quadrature formulas.

8.7 Obtain and run a discrete ordinates code such as ANISN for a one-speed slab of thickness 2.0 mfp. In particular, compute the critical number of secondaries per collision c , using Gaussian quadrature sets for $N=2, 4$, and 8 and a mesh spacing $\Delta x = (2N)^{-1}$, $\Sigma_t = 1.0$, $\nu \Sigma_f = 0.5$, and $\Sigma_s = 0.5$. Compute the eigenvalue $c = \frac{1}{2}(1 + k^{-1})$ and compare this with the benchmark value $c = 1.277101824$. Plot the error ε versus mesh spacing Δx and determine the order of convergence p , where $\varepsilon \sim (\Delta x)^p$.

8.8 The standard Gaussian (P_N) quadrature set is defined on the interval $[-1, 1]$ and is normalized to $\int_{-1}^{+1} dx = \sum_n w_n = 2$. Therefore an arbitrary integral can be written as follows:

$$\int_{-1}^{+1} dx f(x) = \sum_{n=1}^N f(x_n) w_n$$

Assume we would like to perform a P_N quadrature over the intervals $[-1, a]$ and $[a, 1]$ separately. Express the two separate quadrature sets $\{y_n, u_n\}$ and $\{z_n, v_n\}$ for $[-1, a]$ and $[a, 1]$, respectively, in terms of the original set $\{x_n, w_n\}$.

8.9 Consider the classical Milne problem for a semi-infinite scattering ($c=1$) medium. Choose an S_N quadrature set (at least S_4) and a DP_N quadrature with the same total number of points (e.g., S_4 and S_2 on each half-range). Then run a standard discrete ordinates code (e.g., ANISN) to compute the emergent angular flux $\varphi(0, \mu)$ and compare this with the exact

angular distribution as given by Case, de Hoffmann, and Placzek.⁸⁶ Extrapolate the asymptotic scalar flux $\phi(x)$ to zero and determine the extrapolation length graphically and compare this with the exact value. In order to simulate the semi-infinite geometry, choose a slab thickness of several mean free paths with an incoming source on one face to simulate the infinite source at infinity. If the slab is thick enough, the scalar flux will reach its asymptotic form within the interior and will not depend on your choice of the incoming source.

8.10 Compare the asymptotic flux in the interior of the slab generated in Problem 8.9 with the exact flux from Case, de Hoffman, and Placzek.⁸⁶ (Hint: the choice of $c = 1$ yields a particularly convenient asymptotic flux.)

8.11 Demonstrate that a direct finite differencing of the conservative form of the one-dimensional spherical geometry transport equation results in the same difference equations that are obtained using the particle balance approach. In particular, demonstrate that the $\alpha_{m \pm 1/2}$ terms are the same, and that they satisfy the usual recursion relation if a certain condition on the quadrature set $\{\mu_m, w_m\}$ is satisfied.

8.12 Prove that the weighting scheme used in Section 8.1.4 for the discontinuous finite element–discrete ordinates scheme is equivalent to Galerkin weighting (i.e., that one implies the other).

8.13 Show that the coupled diffusionlike equations that resulted from the first method of solution of the P_3 equations, Eq. 8.44, are formally identical to the two-group diffusion equations by identifying each of the coefficients as one of the two-group cross sections.

8.14 The finite element formulation of the first order transport equation (assuming vacuum boundaries)

$$-(\varphi, \hat{\Omega} \cdot \nabla \psi) + \langle \varphi, \psi \rangle_+ + (K\varphi, \psi) = (s, \psi)$$

can be written compactly with the introduction of the bilinear form

$$a(\varphi, \psi) = -(\varphi, \hat{\Omega} \cdot \nabla \psi) + \langle \varphi, \psi \rangle_+ + (K\varphi, \psi)$$

as follows:

$$a(\varphi, \psi) = (s, \psi)$$

Show that $a(\varphi, \psi)$ is positive definite, that is,

$$a(\varphi, \varphi) = 0 \Rightarrow \varphi = 0$$

if the system is characterized by $c < 1$ and isotropic scattering.

8.15 Show that the matrix of coefficients A resulting from the finite element approach to the first order transport equation is nonsingular. That is, show that if $A\mathbf{c}=0$, where $\mathbf{c}$ is arbitrary, then $\mathbf{c}=0$. (*Hint.* Premultiply by $\mathbf{c}^*$ and expand in the basis functions for S^h .)

8.16 Under what conditions will the collision operator be symmetric, that is,

$$(K\varphi, \psi) = (K\psi, \varphi)$$

where K is defined by Eq. 8.48?

8.17 Prove the reciprocity relation

$$\sum_i V_i P_{ji} = \sum_j V_j P_{ij}$$

using the notation from Eq. 8.79.

8.18 Demonstrate that

$$Ki_{n+1}(x) = \int_x^\infty dx' Ki_n(x')$$

8.19 Prove the surface reciprocity theorem

$$S_\alpha P_{i\alpha} = 4V_i \sum_l P_{\alpha l}$$

under the assumptions of the flat flux and cosine current approximation.

8.20 Show that if an annular geometry with azimuthal symmetry is being considered, Eq. 8.85 can be simplified to the form of Eq. 8.86.

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Computer Simulation of Particle Transport

Thus far our concern has been the solution of the transport equation (using either analytical or numerical methods) to determine the particle phase space density $n(\mathbf{r}, \mathbf{v}, t)$ or various weighted integrals of this quantity. However we can adopt a totally different approach and attempt to simulate the particle transport process directly on a computer without even referring to the transport equation.

Since particle collision events are usually described statistically, particle transport takes on a highly stochastic nature, that of a random walk in which particles stream freely between random interaction events. Therefore it is natural to utilize statistical methods for simulating transport processes. The most common methods, referred to aptly enough as *Monte Carlo techniques*, estimate the expected characteristics of the particle population as statistical averages over a large number of case histories of particle lives that are simulated by a computer. Such random sampling techniques can also be used to generate solutions to the transport equation directly.

Random sampling or Monte Carlo methods are most appropriate for test particle (linear) transport processes such as those characterizing neutron diffusion or radiation transport. Collective particle (nonlinear) transport is more commonly simulated using deterministic methods in which the microscopic equations of motion (e.g., Newton's laws) characterizing the dynamics of the many particle system are solved directly. Such particle dynamics simulations are commonly used today in studying dense fluids such as liquids or plasmas.

This chapter discusses both statistical and deterministic methods for simulating particle transport processes and introduces some of the more popular computational tools used in transport simulations.

9.1 □ STATISTICAL SIMULATION (MONTE CARLO) METHODS

□ One commonly encounters transport problems in practical applications too complex to allow direct numerical solutions of the transport equation (e.g., three-dimensional geometries, time-dependent transport phenomena). In these situations, one is usually forced to rely on Monte Carlo or

statistical sampling methods to simulate the transport process. That is, one develops a statistical analogue description of a particle's life history on the computer, using random sampling methods. Then by running off a large number of such case histories, these results can be averaged to obtain estimates of the expected behavior of the particle population. Particle transport processes are quite amenable to such a treatment, since the individual interaction events (collisions) are usually described in terms of statistical characteristics (mean free paths or cross sections).

In this sense, then, the Monte Carlo method may be defined as a method of statistical simulation of some probabilistic model or analogue of a given problem.¹⁻⁷ However, as we demonstrate momentarily, Monte Carlo methods can also be used to solve deterministic problems such as the evaluation of definite integrals or the solution of integral or differential equations. Indeed, both approaches have been applied with some success to particle transport problems that can be characterized either as a random walk process (by specifying the relevant interaction probabilities), or as a deterministic problem (described by the particle transport equation characterizing the phase space particle density).

The application of Monte Carlo methods to the direct simulation of particle transport phenomena is conceptually rather simple (although the programming logic of even a simple "physical analogue" Monte Carlo computer code can become quite complex). One need merely model the relevant physics of each particle interaction event as closely as possible, allowing the particles to stream freely between interactions. Unfortunately, this direct simulation approach fails in a large number of problems of practical interest; therefore many modern Monte Carlo methods are based instead on the transport equation for the development of random sampling procedures.

Although a primitive form of Monte Carlo method was applied to the Boltzmann equation as long ago as 1901, the major stimulus for the development of Monte Carlo techniques came from the complicated neutron diffusion problems that were encountered in the early work on atomic energy. Fermi was among the first to apply random sampling methods to study neutron moderation.⁷ The major development of computer-oriented Monte Carlo methods for transport problems was provided by N. Metropolis and S. Ulam⁸ (who also coined the name) at Los Alamos during the 1940s. The application of Monte Carlo methods to the solution of integral equations was developed by Albert⁹ and Spanier,¹⁰ and the development of variance-reduction schemes was initiated with the work of von Neumann, Ulam, and Kahn¹¹ during the early 1950s.

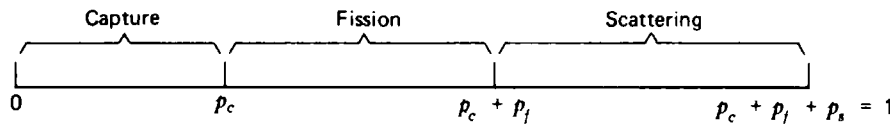
To illustrate the various ideas involved in the use of Monte Carlo methods to simulate particle transport, consider how we might apply random sampling techniques to describe neutron transport.⁵ The essential

idea is to trace out a number of neutron histories, using a table of random numbers to determine whether and what type of interactions occur along a neutron's flight path.

For example, suppose we know that a neutron of energy E has suffered a collision at a point $\mathbf{r}$. To determine the type of collision event, we first compute the probabilities for capture, fission, and scattering, p_c , p_f , and p_s , respectively, using the appropriate cross section data:

$$p_c = \frac{\Sigma_c(\mathbf{r}, E)}{\Sigma_t(\mathbf{r}, E)}, \quad p_f = \frac{\Sigma_f(\mathbf{r}, E)}{\Sigma_t(\mathbf{r}, E)}, \quad p_s = \frac{\Sigma_s(\mathbf{r}, E)}{\Sigma_t(\mathbf{r}, E)}$$

Since $p_c + p_f + p_s = 1$, we can divide up the real interval $[0, 1]$ into segments proportioned as these probabilities



Now we just select a “random number”, call it ξ_i , from a sequence or table of positive real numbers distributed uniformly (equally likely) on the interval $[0, 1]$. If this number ξ_i lies in the range $0 \leq \xi_i < p_c$, we choose a capture event; if $p_c \leq \xi_i < p_c + p_f$, we say that a fission event has occurred; and if $p_c + p_f \leq \xi_i \leq 1$, we identify the interaction as a scattering event. In this way we have managed to randomly select the type of interaction event in a manner consistent with the known probabilities of occurrence for each type of event.

If we choose a capture event, we terminate the neutron history. But if either fission or scattering occurs, we must perform an additional “sampling” process to determine the number and characteristics of neutrons resulting from these interactions. Once again we would implement a random sampling process that is biased as the known probabilities for fission neutron emission or neutron scattering.

Once having determined the consequences of a collision event, we then compute the distance the neutron will travel before suffering its next collision. Again this involves a random sampling procedure. But now we must be a bit more sophisticated, since the probability of a neutron interaction is not distributed uniformly along the neutron path length (i.e., the collision probability is larger close to the origin point).

To illustrate, recall that for a uniform medium, the probability that a neutron will suffer an interaction in an interval dx about x is given by

$$p(x)dx = \Sigma_t \exp(-\Sigma_t x) dx \quad (9.1)$$

[This probability $p(x)$ is an example of what is known as a probability “distribution” or “density” function. As such, its integral over all x must obviously be equal to 1.]

Let us also calculate the probability $P(x)$ that the neutron will suffer an interaction before traveling a distance x by integrating $p(x)$ from 0 to x :

$$P(x) \equiv \int_0^x dx' p(x') = 1 - \exp(-\Sigma_t x) \quad (9.2)$$

[$P(x)$ is referred to as a “cumulative” distribution function.] Now note that $P(x)$ is a monotonically increasing function of x that ranges from 0 to 1 as x ranges from 0 to ∞ (see Figure 9.1). Therefore for each neutron path length x_i , there is a unique interaction probability P_i (and vice versa). That is, it should be possible (in principle, at least) to invert $P(x)$ to determine x as a function of P .

The latter feature is quite important. Since the values of P_i are distributed over the interval $[0, 1]$, we are tempted to use a table of random numbers distributed uniformly on the interval $[0, 1]$ to sample for values of P_i , then calculate the corresponding point of interaction x_i . In fact, we can easily demonstrate that if the point of interaction x_i is distributed according to $p(x)$, the corresponding values P_i are distributed uniformly in $[0, 1]$. First define the probability distribution for P as

$$\mathcal{P}(P)dP = \text{probability that } P \text{ lies in } dP \text{ about } P$$

Since there is a one-to-one relationship between P and x [i.e., since $P(x)$ is a monotonically increasing function of x], we can write

$$\mathcal{P}(P)dP = p(x)dx$$

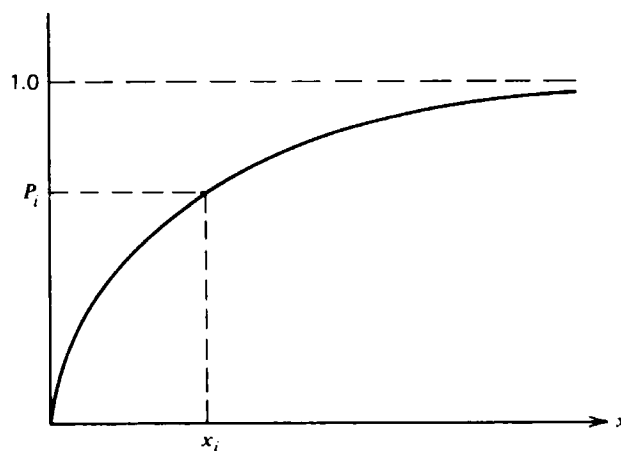


Fig. 9.1 □ Sampling P_i from the cumulative distribution function.

But we recall from the definition given by Eq. 9.2 that

$$p(x) = \frac{dP}{dx}$$

or

$$dP = \left(\frac{dP}{dx} \right) dx = p(x) dx$$

so that

$$\mathfrak{P}(P) = 1$$

—that is, the values P_i are distributed uniformly on the interval $[0, 1]$.

Hence we can just use our table of random numbers to select a value for P_i and determine

$$x_i = -\Sigma_i^{-1} \ln(1 - P_i) = -\Sigma_i^{-1} \ln(1 - \xi_i)$$

Actually, since the quantity $(1 - P_i)$ is also distributed uniformly on the interval $[0, 1]$, we might as well just determine x_i using

$$x_i = -\Sigma_i^{-1} \ln \xi_i$$

In many cases, the functional form of $P(x)$ is too complicated to invert explicitly—in fact, it may be available only in a tabulated form. Then interpolation methods can be used to obtain $x = x(P)$. The next section discusses sampling from probability distributions in more detail.

We have given two examples of how one can sample from the probability laws governing a physical process (e.g., the type of interaction or the probability that an interaction will occur). However one can also implement a variety of sampling procedures of other types in simulating a neutron life history. Suppose, for example, that we wish to determine the location at which a source neutron first appears.⁵ To be more precise, let us consider a two-dimensional problem in which a source is distributed uniformly across a circular area of radius R (e.g., fission neutrons appearing in a fuel element). Then to sample the initial position of a source neutron, we can choose two random numbers $\xi_1, \xi_2 \in [0, 1]$ and calculate coordinates x_i, y_i as

$$x_i = 2(\xi_1 - 0.5)R, \quad y_i = 2(\xi_2 - 0.5)R$$

But of course not all such coordinates will lie in the circular area. Therefore we simply reject any points x_i, y_i for which $x_i^2 + y_i^2 > R^2$. In this

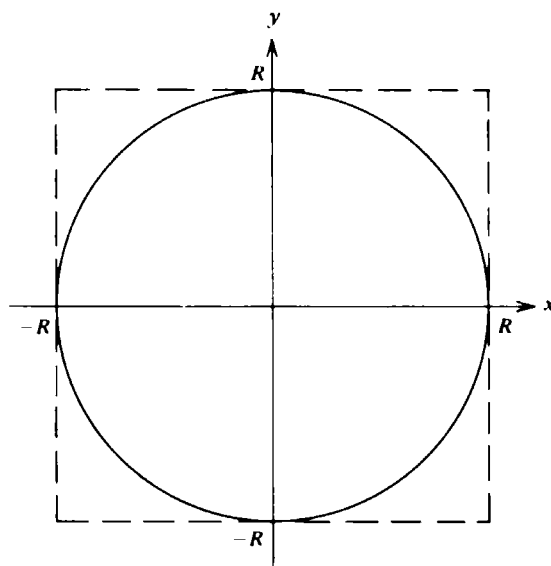


Fig. 9.2 □ Sampling from a circular area using the rejection method.

manner we can sample from a uniform distribution confined to the area (see Figure 9.2).

Thus we can track the neutron history by determining its point of birth as a source neutron, then finding the positions and types of interactions, allowing the neutron to stream freely between interactions until a capture or leakage event terminates the life of the neutron. We continue in this fashion to simulate the case histories of a large number of neutrons using such random sampling techniques. Then we estimate the quantities of interest (e.g., detector responses or leakage rates) as averages over this batch of case histories.

Through the use of sophisticated sampling algorithms and clever programming methods, Monte Carlo computer codes have been developed that can process tens of thousands of particle histories in complicated geometries to allow a detailed treatment of space, energy, angle, and time-dependent transport phenomena.¹²⁻¹⁵ Unfortunately, however, various other transport problems cannot be studied using such direct analogue simulation methods because they involve events that occur with very low probability. For example, in shielding problems, the events of most interest (e.g., neutron penetration through a shield) occur very infrequently (sometimes with a probability as low as 10^{-10}). The direct simulation of such events would require an enormous number of case histories (10^{10} at least) and would be unthinkable even on the most sophisticated computer.¹⁶

In such problems, direct physical analogue simulations are simply not sufficient. Instead, one must employ one of a variety of “variance-reduc-

tion" schemes in which the original problem is modified so that the event of interest occurs more frequently. In this way most of the computation time and cost are spent on cases leading to the event of interest and are not wasted on uninteresting cases.

To develop these schemes, one must turn away from physical analogues to an alternative application of Monte Carlo methods as a stochastic method for solving the deterministic transport equation. That is, Monte Carlo methods may be implemented not only as a stochastic method to simulate stochastic processes, but as a stochastic method to solve deterministic equations, as well.^{1,3,9} It is this dual capability that makes Monte Carlo methods so very useful in transport problems, since these are amenable either to a stochastic analogue or to deterministic transport equation descriptions.

In both approaches the key feature of a Monte Carlo calculation involves the selection of random samples from specified probability distributions. Therefore we first discuss more thoroughly the ways of constructing such sampling schemes, the performance and interpretation of averages over such sample populations, and the biasing of such sampling procedures to facilitate the study of low probability events.

9.1.1 □ Random Sampling Methods □ We have noted that the key aspect of Monte Carlo simulation involves the use of random sampling to generate statistical estimates of the solution to physical or mathematical problems. Therefore we begin with a brief discussion of random sampling methods.

Random Number Generation □ Of course we first need a large supply of random numbers, ξ_i , distributed uniformly on the interval $[0, 1]$. A variety of methods can be used to generate tables of (approximately) random numbers. These range from the sophisticated random number generators used in modern computer programs¹⁷⁻¹⁹ to more primitive methods such as selecting the last digit from the list of phone numbers in a New York City telephone directory (this approach apparently was used by some scientists who worked on the Manhattan Project).

A typical Monte Carlo calculation usually requires so many random numbers that an adequate random number table would far exceed computer memory. Therefore Monte Carlo computer codes generate random numbers as they are needed, using arithmetic operations such as the congruential multiplicative method.¹⁹ Such schemes actually generate only pseudorandom numbers, that is, sequences of random numbers that will repeat themselves after a large number of samples. For example, the RANDU random number generator in the IBM Scientific Subroutine

Package has a period of 10^9 . This should be kept in mind when running very large Monte Carlo problems (which may require several hours of central processing unit time), since these may generate enough case histories to run the risk of repeating the sequence of random numbers, thereby generating correlated samples.

For our further discussion, we assume that we can generate a sequence of random numbers ξ_i distributed uniformly on the interval $0 \leq \xi_i \leq 1$.

Probability Distribution Functions^{1,3} □ Consider a random variable x defined on the interval $a \leq x \leq b$. Since we cannot predict with certainty what value this variable will assume, we introduce the concept of the *probability distribution* or *probability density function* $p(x)$ governing the random variable, which is defined such that:

$$p(x)dx = \text{probability that } x \text{ assumes a value between } x \text{ and } x + dx$$

For example, our random number table has the probability distribution function

$$p(\xi) = 1 \quad \text{for } 0 \leq \xi \leq 1$$

that is, the probability distribution is uniform on the interval $[0, 1]$. More generally, we are interested in distributions of random variables that are not uniform. For example, recall that the probability of neutron interaction in a distance dx about x is given by

$$p(x)dx = \Sigma_t \exp(-\Sigma_t x) dx$$

The probability that a random variable assumes a value less than some number x is given by the *cumulative distribution function* $P(x)$:

$$P(x) \equiv \int_a^x dx' p(x') \quad (9.3)$$

Notice from this definition that $P(x)$ is a monotonically increasing function of x and is restricted to the interval $0 \leq P(x) \leq 1$. In particular, $P(a) = 0$ and $P(b) = 1$. In a very similar manner one can define probability distribution functions and cumulative distribution functions of several random variables (see Figure 9.3).

We use such distribution functions to characterize the probability of different “events” in particle transport.^{3,5} To be more precise, we define an

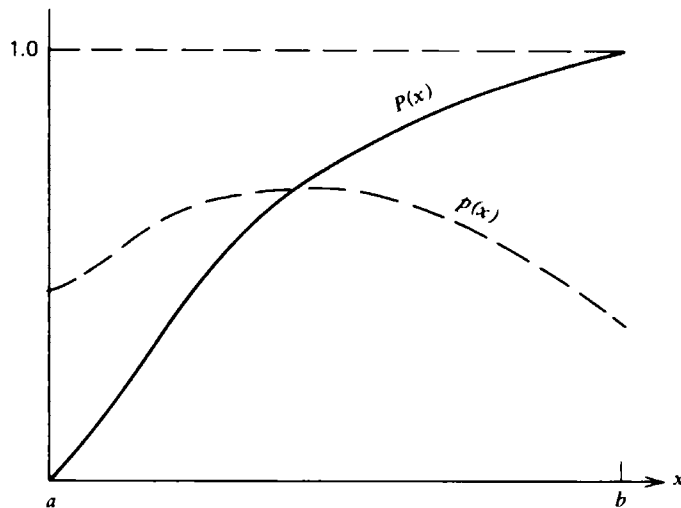
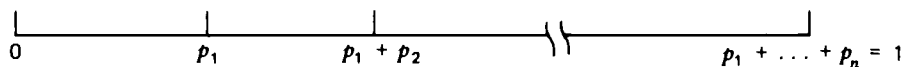


Fig. 9.3 □ The probability distribution function and cumulative distribution function.

event as something that happens to a particle (e.g., a collision event or leakage through a surface). A *case history* or *sample* then is a sequence of such events, beginning and ending with some preselected criterion (e.g., particles emitted from a source or particle capture).

We can easily specialize the concept of a probability distribution function to characterize a set of discrete, independent (mutually exclusive) events. Suppose we assign to each such event $E_1, E_2, \dots, E_n$ a probability $p_1, p_2, \dots, p_n$. Then we construct a probability distribution function of a random variable x to characterize these events as follows: First break up the interval $[0, 1]$ as shown below:



Now if $x \in [0, p_1)$, we say that event E_1 occurs, and so on. Hence we can define the probability distribution function as a “step” function

$$p(x) = p_i, \quad p_1 + p_2 + \dots + p_{i-1} \leq x < p_1 + \dots + p_i$$

Recall that in our previous example, we used this prescription to sample particle interaction events by noting $p_c = \Sigma_c / \Sigma_t$, $p_f = \Sigma_f / \Sigma_t$, and $p_s = \Sigma_s / \Sigma_t$. The corresponding cumulative distribution function is a sequence of ramps as shown in Figure 9.4.

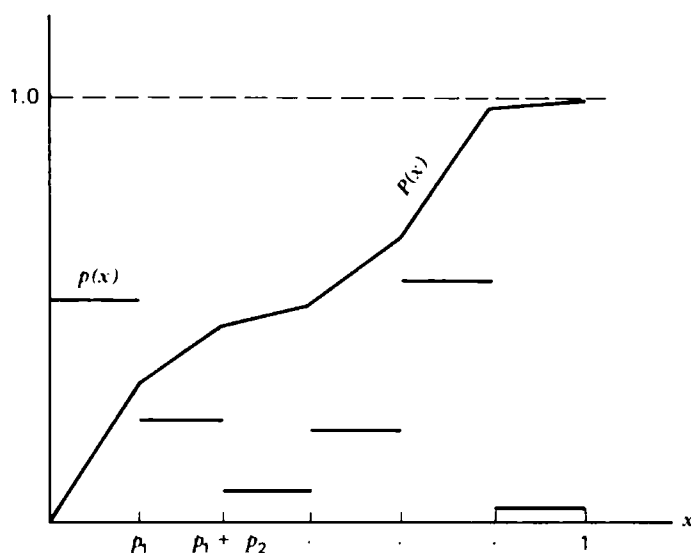
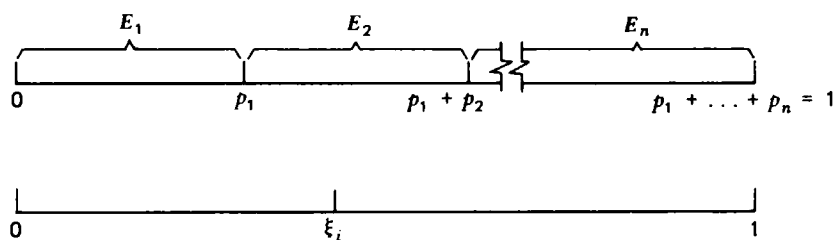


Fig. 9.4 □ The probability distribution function and cumulative distribution function characterizing discrete events.

Sampling from Probability Distribution Functions □ The selection of the value of a random variable distributed according to a given probability distribution plays a central role in Monte Carlo calculations. There are several methods for performing this random sampling.

i *Sampling from discrete probability distributions.* To sample from the probability distribution characterizing a set of discrete events, we can merely associate a sequence of uniformly distributed random numbers, $\xi_i \in [0, 1]$, to the range of x as shown below:



Then depending on the value chosen from the random number set, we can choose an event E_i .

ii *Sampling from continuous probability distributions.* To sample from a continuous probability distribution function $p(x)$, we note the following fundamental principle.^{1,3}

If $p(x)$ is a probability distribution function defined on the interval $a \leq x \leq b$, then

$$\xi = P(x) = \int_a^x dx' p(x')$$

determines x uniquely as a function of ξ . If ξ is uniformly distributed on $0 \leq \xi \leq 1$, the random variable x falls with frequency $p(x)dx$ on the interval $(x, x + dx)$.

The demonstration of this result is straightforward. As we noted earlier, the probability distributions of P and x can be related as follows:

$$\mathcal{P}(P)dP = p(x)dx$$

But from the definition Eq. 9.3 of the cumulative distribution function, we can write

$$dP = \left(\frac{dP}{dx} \right) dx = p(x)dx$$

to find that P is distributed uniformly on $[0, 1]$ (see Figure 9.5):

$$\mathcal{P}(P) = 1$$

Therefore we can use a random number table of values $\xi_i \in [0, 1]$ to sample from an arbitrary distribution $p(x)$ by “inverting” its cumulative

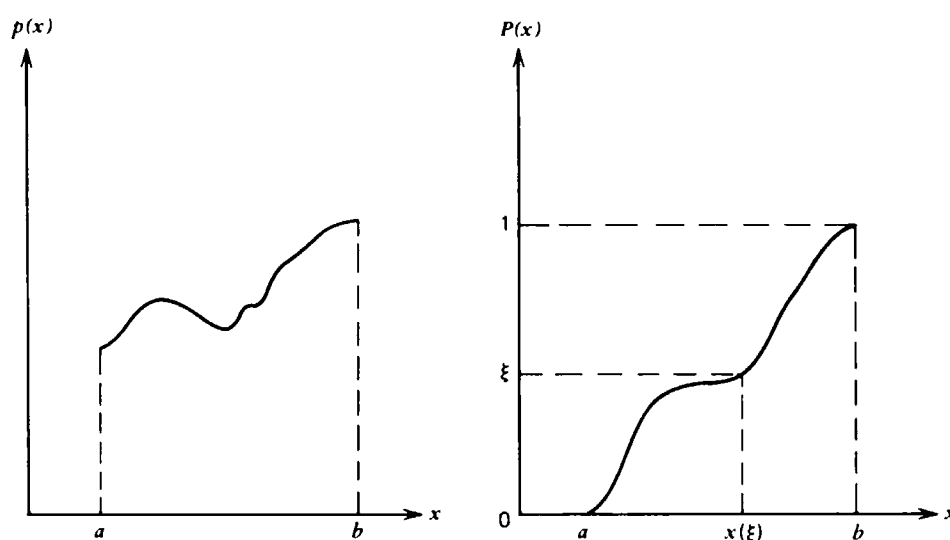


Fig. 9.5 □ Sampling from the cumulative distribution function.

distribution function $P(x)$ to find

$$x_i = P^{-1}(\xi_i)$$

Example. To sample the distance to collision of a particle traveling through a medium characterized by a total cross section Σ_t , we note

$$p(x) dx = \Sigma_t \exp(-\Sigma_t x) dx$$

Hence

$$\xi = P(x) = 1 - \exp(-\Sigma_t x)$$

or

$$x = P^{-1}(\xi) = -\Sigma_t^{-1} \ln(1 - \xi)$$

Therefore we can select random numbers ξ_i and sample the distance to collision as follows:

$$x_i = -\Sigma_t^{-1} \ln \xi_i$$

Example. Suppose we wish to sample the direction of a particle emitted from an isotropic source distribution. We can separate the probability distribution functions for each of the angles θ and ϕ as follows:

$$\begin{aligned} \frac{1}{4\pi} d\hat{\Omega} &= \frac{\sin \theta}{2} d\theta \frac{1}{2\pi} d\phi = p_1(\theta) d\theta p_2(\phi) d\phi \\ &= \frac{1}{2} d\mu \frac{1}{2\pi} d\phi = p_1(\mu) d\mu p_2(\phi) d\phi \end{aligned}$$

where we have identified $\mu = \cos \theta$. Since μ and ϕ are independent random variables, we can sample them separately using the cumulative distribution functions:

$$\begin{aligned} \xi_1 = P_1(\mu) &= \int_{-1}^{\mu} d\mu' \frac{1}{2} = \frac{1}{2}(\mu + 1) \\ \xi_2 = P_2(\phi) &= \int_0^{\phi} d\phi' \frac{1}{2\pi} = \frac{1}{2\pi} \phi \end{aligned}$$

Therefore we can invert to find

$$\begin{aligned} \cos \theta = \mu &= 2\xi_1 - 1 \\ \phi &= 2\pi\xi_2 \end{aligned}$$

and then determine the direction cosines of the source particle as follows:

$$\Omega_x = \sin \theta \cos \phi, \quad \Omega_y = \sin \theta \sin \phi, \quad \Omega_z = \cos \theta$$

iii *Indirect sampling methods.* Frequently the cumulative distribution is too complex or unwieldy to allow a direct analytical inversion to obtain $x = P^{-1}(\xi)$. Then we must revert to numerical methods. For example, we could use an iterative method such as the Newton-Raphson technique to invert $P(x)$. However it is more common to simply construct a table of values of $P(x_i) = P_i$ and use linear interpolation to invert:^{1,6}

$$x = x_i - \frac{P_i - \xi}{P_i - P_{i-1}} (x_i - x_{i-1}), \quad \text{for } P_{i-1} \leq \xi \leq P_i$$

iv *Rejection methods.* Another indirect method for sampling from distribution functions is the *rejection method*. Consider a given distribution function $p(x)$ defined on the interval $a \leq x \leq b$. We begin by normalizing this function as follows:

$$p^*(x) = \frac{p(x)}{\sup[p(x)]}$$

so that $p^*(x)$ lies in the interval $0 \leq p^*(x) \leq 1$. Now we select a pair of random numbers (ξ, η) and define

$$x' = a + \xi(b - a)$$

If $p^*(x') > \eta$, we accept x' as a sample value. Otherwise we reject the pair (ξ, η) and try again. In this way, all the points (x', η) retained are uniformly distributed below the curve $p^*(x)$ (see Figure 9.6). After many such trials, the fraction of points x' retained in the interval $(x, x + dx)$ will be the ratio of the areas:¹

$$\frac{\int_a^b p^*(x) dx}{\int_a^b p^*(x) dx} = \frac{\int_a^b p(x) dx}{\int_a^b p(x) dx} = p(x) dx$$

Hence we can use this rejection method to sample points x' distributed according to $p(x)$.

The efficiency of the rejection method can be defined as follows:

$$\text{efficiency} = \frac{\text{number of values of } x' \text{ selected}}{\text{total number of trials}} = \frac{\int_a^b p(x) dx}{(b - a) \sup[p]}.$$

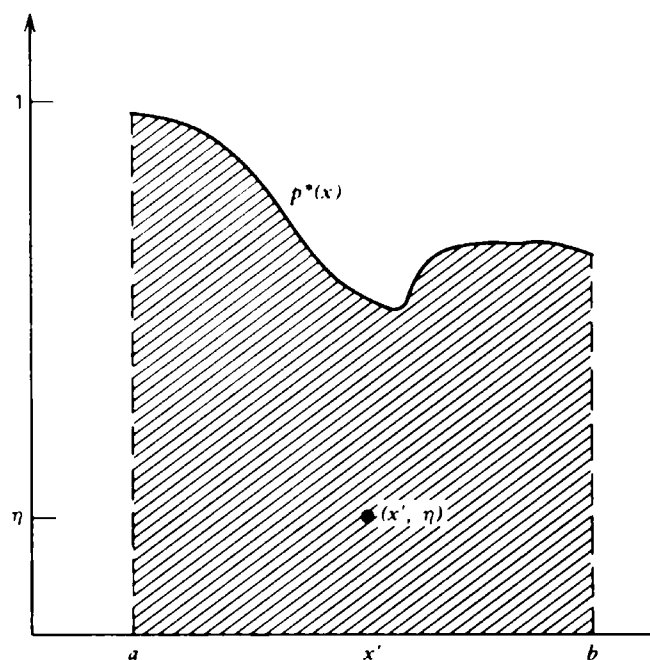


Fig. 9.6 □ Sampling using the rejection method.

Rejection methods are usually employed only if this efficiency is relatively large (e.g., greater than $\frac{1}{2}$).

Example. Suppose we wish to sample the random functions $\cos\theta$ and $\sin\theta$. We first choose a pair of random numbers (ξ_1, ξ_2) defined on the interval $[0, 1]$ and compute

$$x_1 = 2\xi_1 - 1, \quad x_2 = 2\xi_2 - 1$$

We then reject all points (x_1, x_2) that fall outside the unit circle (see Figure 9.7) so that θ will be sampled uniformly between 0 and 2π . Finally we calculate

$$\cos\theta = \frac{x_1}{(x_1^2 + x_2^2)^{1/2}}, \quad \sin\theta = \frac{x_2}{(x_1^2 + x_2^2)^{1/2}}$$

In this case, the efficiency of the rejection method can be calculated as the ratio $\bigcirc/\square = \pi/4$.

Other approaches. A variety of ingenious methods have been developed for sampling from specific distribution functions such as the Maxwell-Boltzmann distribution or the black body spectrum. The interested reader should refer to Carter and Cashwell¹ for examples and further references.

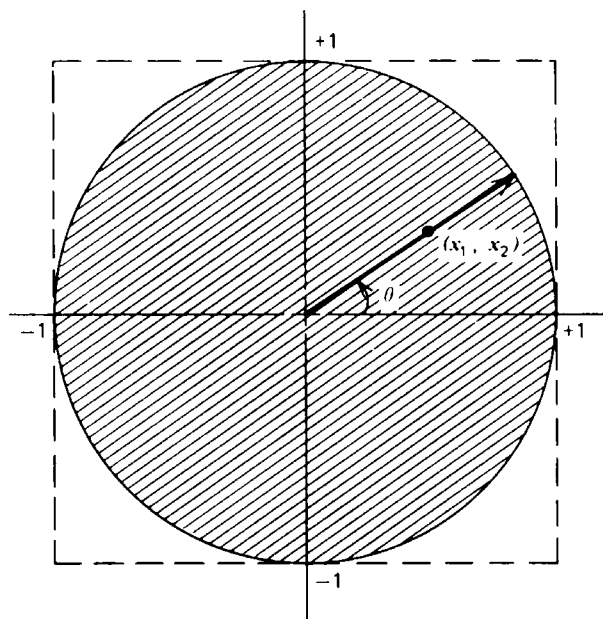


Fig. 9.7 □ Sampling for $\sin \theta$ and $\cos \theta$ using rejection methods.

The Use of Monte Carlo Techniques to Evaluate Deterministic Mathematical Expressions □ We can also use Monte Carlo (random sampling) methods to evaluate mathematical expressions such as integrals or to solve deterministic (nonrandom) equations.

i *Evaluation of integrals.* Consider the integral

$$I = \int_a^b dx f(x)$$

Since the value of this integral is just the area under the curve $f(x)$, if we could sample from a set of points distributed uniformly over the rectangle bounding $f(x)$ (see Figure 9.8), it is apparent that the probability that these points will land below $f(x)$ is just given by the ratio of the area below $f(x)$ to the total area.

Therefore we choose a pair of random numbers (ξ_i, η_i) distributed uniformly on the interval $[0, 1]$ and scale these to determine a point (x_i, y_i) from a set distributed uniformly on the bounding area:

$$x_i = a + (b - a)\xi_i$$

$$y_i = f_{\max} \eta_i$$

We next test to see whether this point falls below $f(x)$: keep (x_i, y_i) if $f(x_i) > y_i$ —otherwise, reject the point.

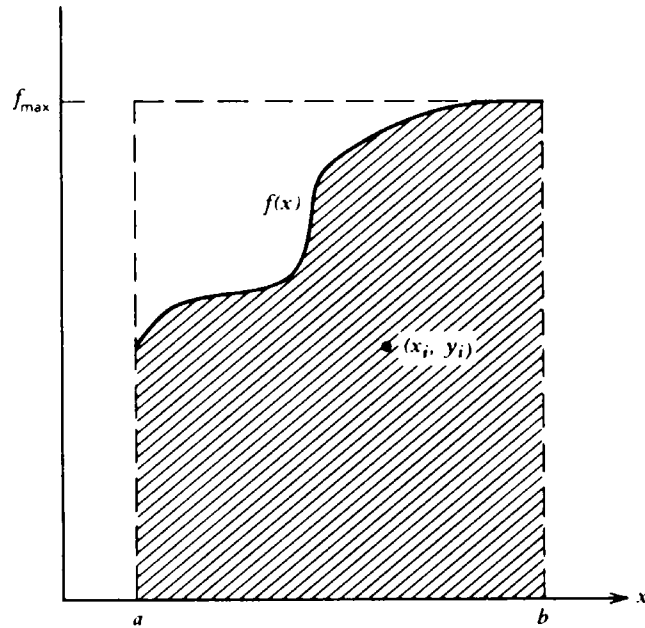


Fig. 9.8 □ Use of sampling methods to evaluate definite integrals.

We continue on and note that the ratio of points selected to the total number of points sampled is approximately equal to the ratio of the area under the curve to the area of the bounding rectangle:

$$\frac{\text{number selected}}{\text{number sampled}} \cong \frac{\int_a^b dx f(x)}{(b-a)f_{\max}}$$

Hence we can use this procedure to estimate the value of the integral in a straightforward manner. It should be noted that no conditions on the smoothness of $f(x)$ are required for this procedure aside from measurability and boundedness. It should also be noted that this use of random sampling to evaluate integrals is just an application of the rejection method we discussed in the preceding section.

ii *Evaluation of averages (expectation values).* Frequently we are interested in calculating the mean or expected value of a function $\psi(x)$ of a random variable x . If x is described by a probability distribution function $p(x)$, we define the *expectation value* $E[\psi]$ by

$$E[\psi] \equiv \int_a^b dx \psi(x) p(x) \quad (9.4)$$

But we also note that ψ itself can be interpreted as a random variable. That

is, one can select a sequence of N values x_i distributed according to $p(x)$ using random sampling methods, then evaluate the average

$$\bar{\psi}_N = \frac{1}{N} \sum_{i=1}^N \psi(x_i) \equiv \frac{1}{N} \sum_{i=1}^N \psi_i$$

A fundamental result from the theory of probability^{1,3} (the “law of large numbers”) states that $\bar{\psi}_N$ approaches the true expectation value $E[\psi]$ for large N

$$\bar{\psi}_N \xrightarrow{\text{large } N} E[\psi]$$

Therefore by taking more and more samples, we expect our estimate of $E[\psi]$ to become more and more accurate. (We make this discussion more precise momentarily by appealing to the central limit theorem.)

We can also apply this approach to evaluate integrals by factoring the integrand $f(x)$ into two functions $\psi(x)$ and $p(x)$

$$I = \int_a^b dx f(x) = \int_a^b dx \psi(x) p(x)$$

where $p(x)$ is chosen such that

$$\int_a^b dx p(x) = 1, \quad p(x) \geq 0$$

Since $p(x)$ now has the properties of a distribution function, we can identify I as an expectation value

$$I = E[\psi]$$

and therefore compute it by sampling $\psi(x)$ at random points x_i distributed according to $p(x)$:

$$I \sim \bar{\psi}_N = \frac{1}{N} \sum_{i=1}^N \psi(x_i)$$

Here we note that our earlier procedure for evaluating integrals using random sampling is obviously just a special case with

$$p(x) = (b-a)^{-1}$$

$$\psi(x) = (b-a)f(x)$$

However in this method we “scored” a value of 0 or 1, depending on whether the random variable was greater or less than $f(x_i)$. In the second method, a score of $\psi(x_i)$ is tallied for every point x_i selected from a distribution $p(x)$.

iii *Solution of integral equations.* Consider the inhomogeneous integral equation

$$f(x) = \int dx' k(x', x) f(x') + s(x) \quad (9.5)$$

Suppose further that we are interested in evaluating a functional of the solution to this equation that can be written in the form

$$J = \int dx g(x) f(x)$$

For example, Eq. 9.5 might be the integral transport equation and J a detector response.

To estimate J using random sampling methods, we first normalize the inhomogeneous source term $s(x)$ and the kernel $k(x', x)$ such that

$$\int dx s(x) = 1, \quad \int dx k(x', x) = 1$$

[This can always be accommodated by rescaling $g(x)$.]

To identify a random sampling scheme, let us first formally solve for the unknown f and therefore for J using a Neumann expansion (assuming for the moment that the kernel $k(x', x)$ is suitably well behaved):

$$f = \sum_{n=0}^{\infty} f_n, \quad f_0 = s, \quad f_n = \int dx' k(x', x) f_{n-1}(x')$$

or

$$J = \int dx g(x) \left[\sum_{n=0}^{\infty} f_n(x) \right]$$

Now notice something: we can interpret $s(x)$ as a probability distribution characterizing a source, and $k(x', x)$ as a “transition” probability distribution characterizing the distribution of x resulting from an event that occurs at x' . In this sense, then, each of the $f_n(x)$ can be interpreted as the probability distribution of x after n events. In this manner we can interpret J as the sum of the expectation values of $g(x)$, each calculated with respect

to a different number of events:

$$J = \sum_{n=0}^{\infty} \int dx g(x) f_n(x) = \sum_{n=0}^{\infty} E_n[g]$$

But we can see how to estimate this quantity using random sampling techniques. We merely simulate a number of random multiple event histories. For each such history, we begin by sampling for a value of x_0 from $s(x)$, then sampling for x_1 from $k(x_0, x)$, for x_2 from $k(x_1, x)$, ..., for x_n from $k(x_{n-1}, x)$, and so on. After simulating a number of such histories, we can estimate the contributions to J from n events by averaging over the histories, then sum over the number of events to estimate

$$J \cong \sum_{n=0}^{\infty} \left[\frac{1}{N} \sum_i g(x_n^i) \right]$$

Of course, since it is necessary only to simulate an individual history until its "score" $g(x_n^i)$ —that is, its contribution to J —is negligible, the summation over event number n is limited to a finite value M_i (dependent on the individual case history):

$$J \cong \frac{1}{N} \sum_i \sum_{n=0}^{M_i} g(x_n^i)$$

We discuss this particular application of Monte Carlo methods in more detail in the next section as we turn to the solution of the integral transport equation.

Statistical Analysis □ Let us return for a moment to the question of how accurately we can expect to be able to estimate an expectation value $E[\psi]$ by averaging the values of ψ for N case histories. We can appeal to a very important theorem from probability theory^{1,3,5} (which we state here in a simplified form).

The Central Limit Theorem. The probability that the error in the estimate of an expectation value by an average over N case histories $|E[\psi] - \bar{\psi}_N|$ is less than an amount ϵ approaches

$$P\{|E[\psi] - \bar{\psi}_N| < \epsilon\} \xrightarrow{N \rightarrow \infty} \left(\frac{2}{\pi}\right)^{1/2} \int_0^{\epsilon\sqrt{N}/\sigma} dt \exp\left(-\frac{t^2}{2}\right) \quad (9.6)$$

for large N . Here, σ^2 is the *variance* of ψ defined by

$$\sigma^2 \equiv E[\psi^2] - E^2[\psi] \equiv \text{var}[\psi]$$

(and σ is referred to as the *standard deviation*).

That is, the central limit theorem implies that the statistical distribution of values assumed by $\bar{\psi}_N$ about $E[\psi]$ will approach a normal or Gaussian distribution for large N . Furthermore, the statistical uncertainty associated with this estimate depends on both the sample size N and the variance σ^2 . This theorem has a number of extremely important implications for Monte Carlo calculations. First note that although $P \rightarrow 1$ for fixed ϵ as $N \rightarrow \infty$ (which is consistent with the law of large numbers), the error in an estimate decreases essentially as $N^{-1/2}$. That is, to reduce the error by a factor of 10, we must increase the sample size by a factor of 100. This represents a major drawback of the Monte Carlo method.

Let us make this more precise by identifying the limiting probability in the central limit theorem as the *confidence level*^{3,5} of an error estimate

$$\text{confidence level} \equiv \left(\frac{2}{\pi}\right)^{1/2} \int_0^{\epsilon\sqrt{N}/\sigma} dt \exp\left(-\frac{t^2}{2}\right)$$

That is, a sample average $\bar{\psi}_N$ produces an estimate of $E[\psi]$ with a confidence of this amount that the error is less than $\pm \epsilon$.

One can actually estimate^{1,6} the fractional square error associated with a given estimate $\bar{\psi}_N$ as

$$\epsilon^2 \equiv \frac{\text{var}[\psi]}{E^2[\psi]} = \frac{1}{N} \left\{ \frac{E[\psi^2]}{E^2[\psi]} - 1 \right\} \cong \frac{1}{N-1} \left\{ \frac{\overline{\psi_N^2}}{\bar{\psi}_N^2} - 1 \right\}$$

It is therefore not surprising that reducing the statistical error in a Monte Carlo estimate by increasing sample size can be very expensive because of this $N^{-1/2}$ dependence.

But notice that the error also depends on the variance of the quantity of interest. If we could somehow reduce this variance, we could reduce the statistical error characterizing a Monte Carlo estimate without increasing the sample size.

Of course in a direct simulation of a physical process such as particle transport, the variance is determined by the physical laws governing the process. But if we could manage to replace this physical analogue with an artificial problem that yields the same expectation $E[\psi]$, but with a smaller

variance $\text{var}[\psi]$, we could dramatically increase the efficiency of a Monte Carlo calculation.

This *variance reduction* concept plays a very central role in the solution of transport problems using Monte Carlo methods. Without such techniques, the sample size required by a direct physical analogue Monte Carlo simulation would frequently be prohibitive. We discuss the more popular variance reduction methods in the next section in connection with the specific application of Monte Carlo methods to particle transport problems.

9.1.2 □ Application of Monte Carlo Methods to Particle Transport □

One usually thinks of a Monte Carlo calculation as a statistical simulation of a number of particle histories. However we have noted that this direct physical analogue approach can entail severe difficulties. It may require an excessive number of samples (hence computation time) to achieve the desired accuracy. It is frequently awkward to modify a physical analogue simulation to permit variance reduction methods without introducing unwanted bias into the results of interest.

For that reason, many modern Monte Carlo transport computer codes develop sampling procedures from the particle transport equation (usually in integral form) rather than as direct analogues to the physical transport process.

Physical Analogue Approach □ Since particle transport is a stochastic process, it is directly amenable to simulation by random sampling methods. As we noted in our introductory example, certainly the simplest and most direct manner in which to develop Monte Carlo sampling schemes to describe particle transport is to simulate the detailed physics at each point in the history of a particle. No reference to the transport equation ever need be made.

Therefore we simply require a probabilistic description of what can happen to a particle at each point in its history. This would entail not only a detailed library of microscopic cross section information, but as well the specification of geometric boundaries and material compositions. We return later in this section to discuss how such data are utilized in Monte Carlo calculations.

Monte Carlo Calculations Based on the Integral Transport Equation □ The most common procedure for developing a Monte Carlo transport calculation begins with one of the various forms of the integral transport equation

(cf. Section 2.2.5). For convenience, we utilize the time-independent integral transport equation for the collision rate density¹ (although we could just as easily begin with the integral equation for emission densities¹² or include time dependence or a multigroup format)

$$f(\mathbf{r}, E, \hat{\Omega}) = \int_0^\infty dR \Sigma_t(\mathbf{r}, E) e^{-\alpha(\mathbf{r}, R, \hat{\Omega}, E)} \\ \times \left[\int dE' \int d\hat{\Omega}' \frac{\Sigma_s(\mathbf{r}', E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega})}{\Sigma_t(\mathbf{r}', E')} f(\mathbf{r}', E', \hat{\Omega}') + s(\mathbf{r}', E, \hat{\Omega}) \right]$$

We can rewrite this equation in a form similar to Eq. 9.5

$$f(x) = \int dx' k(x', x) f(x') + s(x) \quad (9.7)$$

by identifying:

$x = (\mathbf{r}, E, \hat{\Omega})$ as the particle phase space coordinates
 $s(x)$ = first-flight collision rate density due to sources
 $k(x', x)$ = next flight collision rate density at x due to collision at x'
 $f(x)$ = particle collision rate density

We further suppose that we wish to calculate some function of $f(\mathbf{r}, E, \hat{\Omega})$ (e.g., a detector response), which can be written as

$$J = \int d^3r \int dE \int d\hat{\Omega} \frac{\Sigma_d(\mathbf{r}, E)}{\Sigma_t(\mathbf{r}, E)} f(\mathbf{r}, E, \hat{\Omega}) = \int dx g(x) f(x)$$

Let us begin by factoring $k(x', x)$ as

$$k(x', x) \equiv [1 - \gamma(x')] \eta(x') \beta(x', x)$$

where $\gamma(x') \equiv$ capture probability at x' and $\eta(x')$ and $\beta(x', x)$ are a normalization factor and a normalized collision kernel defined by

$$\eta(x') \equiv \frac{\int dx k(x', x)}{[1 - \gamma(x')]} \\ \beta(x', x) \equiv \frac{k(x', x)}{\int dx'' k(x', x'')}$$

Next we formally solve the integral equation (9.7) using a Neumann expansion to find

$$f(x) = \sum_{n=0}^{\infty} \int dx_0 \int dx_1 \cdots \int dx_{n-1} s(x_0) k(x_0, x_1) k(x_1, x_2) \cdots k(x_{n-1}, x)$$

so that J can be expressed as

$$J = \sum_{n=0}^{\infty} \int dx_0 \cdots \int dx_n s(x_n) [1 - \gamma(x_0)] \beta(x_0, x_1) \cdots [1 - \gamma(x_{n-1})] \beta(x_{n-1}, x_n) \gamma(x_n) w(x_0 \cdots x_n)$$

where we define

$$w(x_0 \cdots x_n) \equiv \frac{g(x_n)}{\gamma(x_n)} \eta(x_0) \cdots \eta(x_{n-1})$$

In this way, we have written J in a form that suggests a random walk sampling scheme for its evaluation:

- i Sample $s(x_0)$ for the initial coordinates x_0 of a particle history.
- ii Sample $\gamma(x_{n-1})$ for termination at the n th collision.
- iii Sample $\beta(x_{n-1}, x_n)$ for the next collision point, given that the chain continues.

Then we can identify

$$\{s(x_0)[1 - \gamma(x_0)] \beta(x_0, x_1) \cdots [1 - \gamma(x_{n-1})] \beta(x_{n-1}, x_n) \gamma(x_n)\} dx_0 \cdots dx_n$$

as the probability that the initial coordinates for the first collision are in dx_0 , second collision in $dx_1, \dots$, and so on, until the chain terminates at the $(n+1)$ st collision. We also note that $w(x_0, \dots, x_n)$ is the “score” for such a history in the Monte Carlo calculation of J .

But we now see that

$$J = \sum_n \int dx_0 \cdots \int dx_n \{ \cdots \} w(x_0, \dots, x_n) = E[w]$$

is just the expectation value of the score. Therefore we can estimate J by just sampling a number of histories, computing w for each history, and averaging these scores as

$$J \cong \frac{1}{N} \sum_i w(x_0^i, \dots, x_n^i)$$

where $x_0^i, x_1^i, \dots, x_n^i$ are sampled from distributions given by $s(x_0)$, $\beta(x_{n-1}, x_n)$, and n is determined by $\gamma(x_n)$.

We can reinterpret this sampling scheme in more physical terms by first selecting the initial particle coordinates $\mathbf{r}_0, E_0, \hat{\Omega}_0$ by means of sampling the first collision source $s(\mathbf{r}, E, \hat{\Omega})$. Then we determine the flight distance to first collision R by sampling

$$\Sigma_t(\mathbf{r}_0, E_0) \exp[-\alpha(\mathbf{r}_0, R, E_0, \hat{\Omega}_0)]$$

and use R and $(\mathbf{r}_0, \hat{\Omega}_0)$ to determine the location of this collision as $\mathbf{r}_1 = \mathbf{r}_0 + R \hat{\Omega}_0$.

At this point we could sample from the capture probability $\gamma(\mathbf{r}_0, E_1) = \Sigma_a(\mathbf{r}_0, E_1) / \Sigma_t(\mathbf{r}_0, E_1)$ to see whether the particle is captured in the collision so that the history should be terminated. In practice, however, it is extremely inefficient to terminate particle histories because of capture events. Instead it is common to continue the particle history, but to reduce the particle "weight" or score by the noncapture probability $[1 - \gamma(x_1)] = \Sigma_s(\mathbf{r}_1, E_0) / \Sigma_t(\mathbf{r}_1, E_0)$. That is, *all* particles are forced to scatter at $\mathbf{r}_1$, and their weight is reduced accordingly.

Next a new particle energy E_1 and flight direction $\hat{\Omega}_1$ are selected by sampling from the scattering distributions. The energy E_1 is sampled from

$$\frac{1}{4\pi \Sigma_s(\mathbf{r}_1, E_0)} \int d\hat{\Omega} \Sigma_s(E_0 \rightarrow E, \hat{\Omega}_0 \rightarrow \hat{\Omega})$$

while the flight direction $\hat{\Omega}_1$ is sampled from

$$\Sigma_s(E_0 \rightarrow E_1, \hat{\Omega}_0 \rightarrow \hat{\Omega}) \left[\int d\hat{\Omega} \Sigma_s(E_0 \rightarrow E_1, \hat{\Omega}_0 \rightarrow \hat{\Omega}) \right]^{-1}$$

This sampling procedure is applied to successive collision events until the random walk is terminated because the particle's weight has been reduced below some cutoff value, or because the particle has escaped from that portion of phase space associated with a particular problem. All the particle history's contribution to J is then summed and recorded, and the next history is initiated.

Variance Reduction Methods □ The application of Monte Carlo methods to the direct simulation of transport processes in which rare events are important (e.g., radiation shielding) is very inefficient because most computation time is spent on more probable particle histories that do not contribute significantly to the desired result. Such physical analogue

calculations not only require enormous sample sizes to yield results of sufficient accuracy, but they can also push the problem computation requirements beyond the capability of random number generators, possibly giving rise to correlated samples. That is, one is bounded by a maximum sample size that is dictated not only by computational (or economic) feasibility, but as well by the finite period of random number generators.

Therefore it is of great interest to determine whether the error associated with a Monte Carlo calculation can be reduced without necessarily increasing the sample size. Such errors arise from two primary sources:

- i *Numerical errors.* Examples occur in programming strategy; another case is roundoff error.
- ii *Statistical uncertainty.* This is associated with sample size and variance.

We can quantify the efficiency of a Monte Carlo calculation by defining its “ Q -value”¹⁹

$$Q = \left(\frac{\text{var}[\psi]}{E^2[\psi]} \right) T$$

where T is the average computation time required per sample. This quantity gives the time needed on the average to achieve a relative error of 100%. It is evident from this expression that we can increase the efficiency of a Monte Carlo calculation either by improving the programming strategy (decreasing the computation time T required per sample) or by reducing the variance σ^2 of the calculation.

We focus our attention on variance reduction methods. In essence these methods attempt to bias the original problem so that the regions of phase space that contribute most to the desired answer are sampled most frequently.

- i *Importance sampling.* To illustrate the general idea, suppose we wish to evaluate the expectation value of a random function

$$E[\psi] = \int_a^b dx \psi(x) p(x)$$

The essential goal will be to attempt to reduce the error by reducing the variance

$$\sigma^2 \equiv E[\psi^2] - E^2[\psi]$$

To this end, let us sample x from a different probability distribution function $\tilde{p}(x)$. To correct for this, we assign a weight for each point x_i

$$w(x_i) \equiv \frac{p(x_i)}{\tilde{p}(x_i)}$$

and score our samples as $\tilde{\psi}(x_i) = w(x_i)\psi(x_i)$ rather than just as $\psi(x_i)$. In this way we preserve the expectation value

$$E[\tilde{\psi}] = \int_a^b dx \tilde{\psi}(x) \tilde{p}(x) = \int_a^b dx \psi(x) p(x) = E[\psi]$$

However the *variance* will be different:

$$E[\tilde{\psi}^2] = \int_a^b dx \tilde{\psi}^2(x) \tilde{p}(x) = \int_a^b dx \left[\frac{p(x)}{\tilde{p}(x)} \right] \tilde{\psi}^2(x) p(x) \neq E[\psi^2]$$

so that

$$\tilde{\sigma}^2 = E[\tilde{\psi}^2] - E^2[\tilde{\psi}] = E[\tilde{\psi}^2] - E^2[\psi]$$

Since $\sigma^2 > 0$, it is apparent that if we can choose $p(x)$ such that $p(x)/\tilde{p}(x) < 1$ over an important region of phase space for $E[\psi^2]$, we can reduce σ^2 .

Actually, if we could choose¹

$$\tilde{p}(x) = \frac{p(x)\psi(x)}{E[\psi]}$$

we would find that

$$\tilde{\sigma}^2 = E[\tilde{\psi}^2] - E^2[\tilde{\psi}] = 0$$

But of course we do not know $E[\psi]$. Rather, since we will calculate

$$E[\tilde{\psi}] \approx \tilde{\psi}_N = \frac{1}{N} \sum_{i=1}^N \tilde{\psi}(x_i)$$

we can try to choose $p(x)$ such that

$$\frac{\psi(x)\tilde{p}(x)}{p(x)} \sim \text{constant}$$

Example. Consider again our inhomogeneous integral equation (9.7)

$$f(x) = \int dx' k(x', x) f(x') + s(x)$$

with the goal of calculating

$$J = \int dx g(x) f(x)$$

We can bias this problem by defining new weighting functions

$$\tilde{s}(x) = s(x) I(x) \left[\int dx' s(x') I(x') \right]^{-1}$$

and

$$\tilde{k}(x', x) = \frac{k(x', x) I(x)}{I(x')}$$

where $I(x)$ is an “importance function” that places most emphasis on the regions of phase space that contribute most to J . We then sample from $S(x)$ and $k(x', x)$ to construct the collision expansion solution for J .

One can demonstrate¹ that the optimum choice of weighting function is the solution $f^\dagger(x)$ to the adjoint problem

$$f^\dagger(x) = \int dx' k(x, x') f^\dagger(x') + g(x)$$

Then, in fact, $\tilde{\sigma}^2$ is zero—a zero-variance sampling scheme. But of course we usually do not know $f^\dagger(x)$. Rather, we must attempt to construct estimates of $f^\dagger(x)$ to develop a suitable importance sampling scheme. Frequently a deterministic solution of the adjoint transport equation is used to provide a suitable importance weighting function $I(x)$ (e.g., a low order discrete ordinates calculation).

ii *Splitting and Russian roulette.* We can artificially bias a Monte Carlo calculation to emphasize those particles moving toward more important phase space regions by replacing each such particle with n particles, each with a new weight reduced by $1/n$. In a similar fashion we can randomly terminate particle histories moving toward less important phase space regions using a Russian roulette procedure.^{1, 16}

To be more precise, consider a deep penetration shielding problem in which we are most interested in the very few particles that penetrate deeply into the medium. To implement a splitting procedure, we assume that any particle that manages to penetrate to a depth x_1 is split into n particles (see Figure 9.9), and each of these particles is followed with a weighting reduced by $1/n$ (to avoid biasing the score estimate). We continue in this fashion, implementing a splitting procedure at various penetration depths x_i . This enables us to process more deep penetration histories while

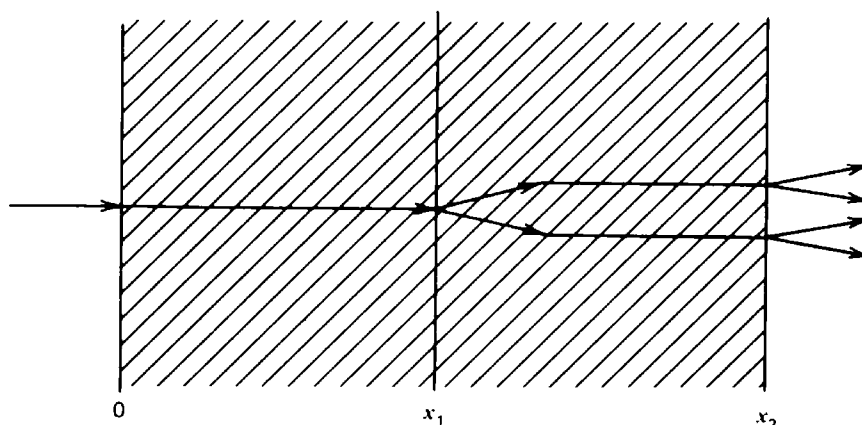


Fig. 9.9 □ Particle splitting.

preserving the total particle weight. It is common to split particles two for one at boundaries one mfp apart.

One can similarly decrease the number of particle histories moving toward phase space regions of lesser importance using a Russian roulette procedure. That is, if a particle in our shielding problem crosses a splitting plane x_i in the opposite direction, it is allowed to survive with a probability $1/n$ and a weight scaled by n . One can actually assign each region of a problem an importance parameter to determine whether splitting or Russian roulette should be used.

Splitting and Russian roulette are the most common variance reduction methods. Most Monte Carlo codes have built-in options to implement these methods if desired. Since these are the only biasing methods that leave the probability distributions of the physical analogue model unchanged, they are the safest variance reduction methods to use.

iii *Choice of estimators.* In a physical analogue simulation, scoring occurs whenever events happen in the phase space region of interest. But we have noted that this can be quite inefficient if our interest is in very low probability events. Therefore it is common to choose nonanalogue “estimators” that allow a particle to score (contribute to the desired answer) without actually entering the phase space region of interest.^{1,3}

Suppose we are interested in the response of a detector characterized by a cross section Σ_d distributed over a phase space volume V_c . Several of the more popular estimators are listed below:

Collision estimators:	score $w(\Sigma_d/\Sigma_t)$ for each collision event in V_c
Last-event estimator:	score $w(\Sigma_d/\Sigma_c)$ only when the particle history is terminated by a capture in V_c
Flux or track-length estimator:	score $w \int_0^s ds' \Sigma_d(\mathbf{r})$ for each track length s in V_c

iv *Some final remarks on variance reduction methods.* In all these variance reduction schemes we have altered the sampling scheme suggested by a direct analogue model by multiplying the particle weight of the analogue scheme by a correction factor at each stage of the sampling. That is, all these schemes are essentially variations of importance sampling.

One should be extremely cautious in implementing such altered sampling schemes. Frequently they increase rather than reduce the variance, thus leading to an increase in statistical error. Furthermore, even when a scheme can lead to a variance reduction, it may be so complicated that the computation time required for its implementation may exceed the time required to achieve a comparable error reduction by simply following more particle case histories.

Monte Carlo Computer Codes □ Monte Carlo transport calculations are implemented via complex and versatile computer programs or codes. For example, the MORSE transport code¹² (for multigroup Oak Ridge stochastic experiment) is a state-of-the-art Monte Carlo code that is capable of describing either neutron or gamma transport in three-dimensional geometries. The code accepts a variety of cross section input data and provides extensive statistical analysis of the results. It can be used to solve either the forward or adjoint transport equation in time-dependent or time-independent form (including criticality problems). It contains a number of variance reduction options.

The structure of such a Monte Carlo computer code is diagrammed in Figure 9.10.¹² One begins by reading into the program necessary problem definition data (geometry, source characteristics, cross section data). The code then generates and stores a batch of source particles using the SOURCE module. It next selects one particle from this batch and begins the random walk simulation, transporting the particle from collision to collision, splitting or killing the particle by Russian roulette or emitting secondary particles when necessary (and storing them in the SOURCE memory for further processing). Termination of random walk histories occurs when the particle leaks from the system, reaches an energy or time cutoff, or is killed by Russian roulette. During the random walk calculation, the GEOMETRY module tracks the particles from collision to collision, and the COLLISION module determines the type and consequences of collision events. The ANALYSIS module continually monitors the random walk histories, computing contributions to the desired answer during the tracking process (i.e., keeping “score”).

It is appropriate to review several of the more mechanical aspects of such Monte Carlo transport codes.

i *Geometry.* Unlike deterministic methods such as discrete ordinates or collision probability methods, the computational requirements of Monte

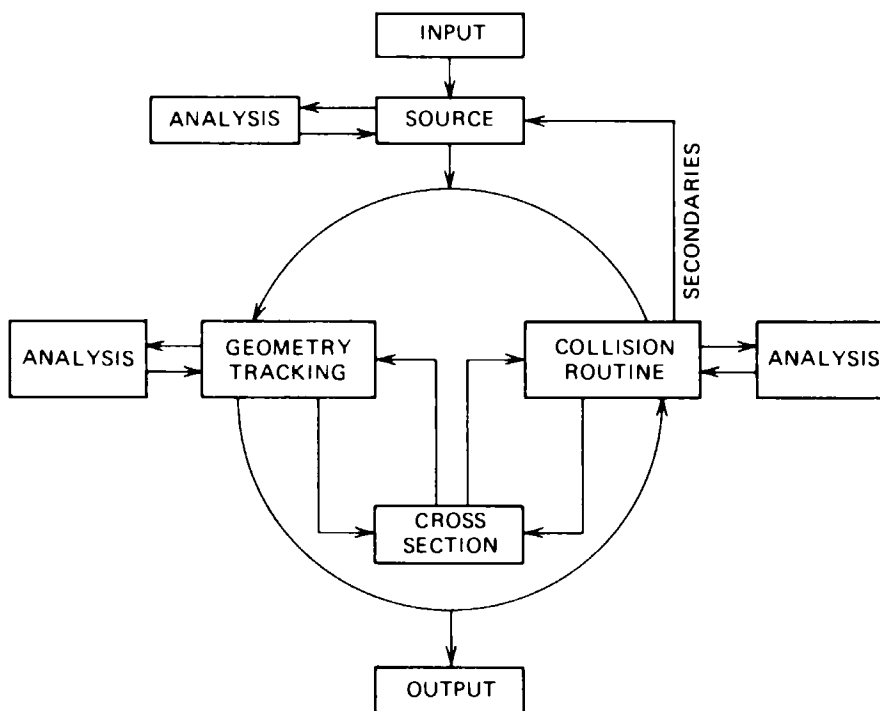


Fig. 9.10 □ General organization of a Monte Carlo transport code.

Carlo calculations do not increase dramatically in passing from one- to two- or even three-dimensional geometries. In fact, perhaps the primary motivation for the extensive use of Monte Carlo methods in analyzing transport problems is that they are presently the only methods capable of treating complicated three-dimensional geometries.

One of the critical features of any Monte Carlo code is the manner in which it handles geometric information. Region boundaries are conventionally specified as quadratic surfaces of the form^{1,12}

$$Ax^2 + By^2 + Cz^2 + Dxy + Eyz + Fzx + Gx + Hy + Jz + K = 0$$

Typically this information is handled and applied to the particle transport simulation by a separate module in the computer code.

It is customary to utilize Cartesian coordinate systems (even to describe curvilinear geometries), since this greatly simplifies the calculation of particle trajectories. To illustrate, consider a particle that streams freely a distance s between collisions. Then if (x, y, z) are the coordinates of the first collision and $\hat{\Omega}$ is the flight direction following this collision, we can easily calculate the location of the next collision as

$$x' = x + \Omega_x s, \quad y' = y + \Omega_y s, \quad z' = z + \Omega_z s$$

since the direction cosines do not change along the flight path (an advantage of Cartesian coordinates).

ii *Time dependence.* It is a trivial task to include time dependence in a Monte Carlo calculation, in sharp contrast to deterministic numerical methods for solving the transport equation. One merely advances the time of the particle after each flight and scores in the appropriate time bins for the quantities of interest.

iii *Source sampling.* One can easily bias an external source distribution using an importance function $I(x)$:

$$\tilde{S}(x) = \frac{s(x)I(x)}{\int dx s(x)I(x)}, \quad x \equiv (\mathbf{r}, E, \hat{\Omega}, t)$$

One then samples $\tilde{S}(x)$ for the coordinates of a source particle, and assigns a weight $w(x) = S(x)/\tilde{S}(x)$ to this particle.

iv *Attenuation and leakage.* Recall that since the probability distribution for a collision in path length ds about s is

$$p(s) ds = \Sigma_t(s) \exp\left[-\int_0^s ds' \Sigma_t(s')\right]$$

we can determine the cumulative distribution function as

$$P(s) = 1 - \exp\left[-\int_0^s ds' \Sigma_t(s')\right]$$

and invert to find our sampling prescription

$$\int_0^s ds' \Sigma_t(s') = -\ln[1 - P(s)] = -\ln \xi$$

since both $P(s)$ and $1 - P(s)$ are uniformly distributed on the interval $[0, 1]$.

Since most systems under consideration are sectionally homogeneous, one can develop a somewhat more systematic sampling procedure¹ as follows. First choose a random number $\xi_i \in [0, 1]$. Then if $\xi_i > \exp(-\Sigma_{t_1}s_1)$, where s_1 is the path length to the first boundary of region 1, we choose collision point

$$s_i = -\Sigma_{t_1}^{-1} \ln \xi_i$$

However if $\xi_i < \exp(-\Sigma_{t_1}s_1)$, the particle will reach the next region without suffering a collision. Therefore we advance the particle coordinate to this next region and repeat the procedure (see Figure 9.11).

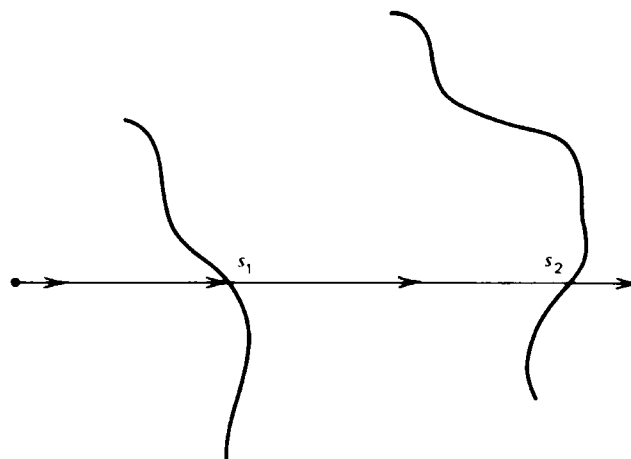


Fig. 9.11 □ Particle tracking in sectionally homogeneous media.

v Collision events. One typically breaks up the sampling procedure to determine the consequences of a collision event. We illustrate this for neutron transport.

One begins by determining the type of nucleus involved in the collision by sampling according to the isotopic probabilities given by $p_i = \Sigma_i^{(i)} / \Sigma_t$, where the index i refers to the nuclide type. Next one samples for the type of event using the probabilities $p_i^k = \sigma_k^i / \sigma_t^i$, where k is the index for event type. Further sampling will depend on the type of event selected.

If one selects a capture event, the particle history could be terminated at the collision. However, as noted earlier, it is more efficient to simply reduce the particle weight by the noncapture probability and sample for the type of collision only from noncapture events. For example, if a scattering event is selected, one would sample the differential scattering cross sections to determine the energy and flight direction of the scattered neutron. If the sampling yields a fission event, one samples for the number, energy, and direction of fission neutrons emitted in the fission process.

Monte Carlo Code Systems □ A wide variety of flexible and powerful Monte Carlo transport codes have been developed for the analysis of neutron and gamma transport.¹²⁻¹⁵ Although these codes—more specifically, *code systems*, since they contain a number of modules to facilitate geometry specification, cross section preparation, and statistical analysis—are under continuous development, we mention several of the more popular Monte Carlo transport codes here.

MORSE (ORNL-RSIC)¹² The MORSE code is an extremely general and flexible code capable of describing neutron, gamma, or coupled neutron-gamma transport in arbitrary geometries. It is written in multi-

group form to facilitate its compatibility with evaluated nuclear data libraries (e.g., ENDF/B or ENDL) and can use cross section libraries prepared for discrete ordinates codes such as ANISN or DOT. It is capable of analyzing the forward or adjoint transport equation in either time-dependent or steady-state form (including criticality calculations), and it contains a variety of options for variance reduction.

MCN, MGN, MCNG (LASL)^{13,14} These Monte Carlo codes are designed for neutron, gamma, and coupled neutron–gamma transport, respectively. They contain most of the features of MORSE, except that they use a continuous rather than a multigroup energy format. They also contain special provisions for handling thermal neutron scattering (as described by the free gas kernel).

TART (LLL)¹⁵ A general purpose Monte Carlo transport code based on a multigroup format (although a continuous energy treatment of secondary neutron emission is included).

A variety of modified Monte Carlo methods have been developed for specialized problems.² For example, when comparing the results of two similar problems whose differences would ordinarily be less than the statistical error of independent Monte Carlo estimates (e.g., temperature effects on neutron absorption), it is common to employ correlated Monte Carlo methods in which the same case histories are used to analyze both problems. One can also decompose the original problem into two problems—one of which is easy to solve by deterministic methods and a perturbation that can be handled as a correlated Monte Carlo calculation. The use of hybrid methods, which combine both deterministic and Monte Carlo methods by using the former to develop biasing schemes for the latter, is also increasing. For example, a two-dimensional discrete ordinates calculation of the adjoint flux might be performed to determine the importance weighting for a three-dimensional Monte Carlo calculation.²⁰

9.1.3 □ Application of Monte Carlo Methods to Collective Transport Processes □ It should be apparent that Monte Carlo transport methods are most ideally suited to linear (test particle) transport problems in which individual particle histories can be simulated one at a time. They are rather cumbersome to apply to the description of collective phenomena in which large numbers of particles interact simultaneously. Nevertheless, Monte Carlo methods have been used extensively in the field of gas dynamics.

The simplest such applications have been to free molecular flow problems in which particle interactions are ignored. One can either simulate

these processes directly, as one would do in test particle problems, or develop sampling schemes from the integral equation formulation of free molecular flow problems.²¹

For smaller Knudsen number ($Kn = mfp/L$) one must take into account particle interactions. One approach involves an iterative treatment in which each particle is regarded as a test particle interacting with a background characterized by an assumed distribution function. This distribution function is then recalculated from the test particle information, and the test particle calculation is repeated until convergence is achieved.²²

Yet another approach divides the gas into cells, then samples for the probability of a collision event among each pair of particles in the cells.²³ When collisions are selected, new particle velocities are sampled from the corresponding collision cross sections. Each collision event advances a time counter by the average collision time. After a certain total accumulated time, the particles are allowed to advance to new positions by streaming, and the sampling process is repeated. At each time step various statistical averages are performed to calculate macroscopic quantities of interest (e.g., densities, local flow velocities, temperatures).

Such Monte Carlo methods have become quite popular for a variety of complicated flow problems including shock wave propagation and high speed flows past complex geometrical shapes.

9.1.4 □ Some Final Remarks □ Monte Carlo methods have gained a reputation as the “last resort” in analyzing transport problems. Since the degree of detail in the description of the transport process (e.g., geometric dimension, cross section detail, time dependence) does not significantly affect the computer time necessary to perform a Monte Carlo calculation, it is frequently the only way in which one can analyze complex problems that have exceeded the capability of deterministic methods (e.g., discrete ordinates).

However Monte Carlo methods do suffer from serious drawbacks. The major limitation is that of statistical error. We have noted that this error decreases as only the square root of sample size. Therefore Monte Carlo calculations can be extremely expensive if accurate results are required. This feature is compounded by the relative speed of a Monte Carlo calculation, which is generally quite slow because of the large amount of data handling necessary in tracking a particle case history. The coding logic of a Monte Carlo program is also formidable.^{1,2}

Furthermore it should be noted that Monte Carlo methods are most suited for determining integral quantities (e.g., weighted averages of the flux or leakage rates through specified surfaces). They are quite inefficient

at determining local or distributed quantities such as density or reaction rate distributions.

Finally, it should be stressed that the use of a large Monte Carlo code calls for a significant amount of effort, including input preparation to specify the problem of interest, sufficient experience to determine the degree and type of variance reduction required, and an adequate understanding of the limitations of Monte Carlo calculations to assess the significance of the results. In many cases, the application of Monte Carlo codes to analyze transport problems is more an art than a science. For this reason, Monte Carlo methods are generally employed only when there is no other suitable method available.

9.2 □ DETERMINISTIC TRANSPORT SIMULATION METHODS □

Monte Carlo methods are most ideally suited for simulating a linear transport process in which case histories of particles can be traced one at a time. It would be quite awkward to use such random sampling methods to simulate the dynamics of collective transport processes such as gas or plasma dynamics in which large numbers of particles interact simultaneously (although Monte Carlo methods can be used to simulate the equilibrium properties of such systems, as shown below).

A more direct approach to simulating the dynamics of such collective phenomena is simply to solve the microscopic equations of motion characterizing the particles using finite difference techniques. That is, by taking advantage of the computational power of modern high speed computers, one can investigate the macroscopic behavior of a fluid by solving the microscopic *many body problem*. In essence, the only input necessary is the detailed interaction potential between particles.

The first such microscopic dynamics simulations were performed at the Lawrence Livermore Laboratory by Alder and Wainwright²⁴ in the late 1950s to simulate the behavior of dense gases and liquids by solving the equations of motion characterizing systems of rigid sphere particles. These studies were subsequently extended to systems interacting by way of more general potentials by Rahman²⁵ and Verlet²⁶ during the mid-1960s. Since most of the initial attention was directed toward simulating the behavior of dense gases and liquids, the microscopic dynamics simulation came to be known as the *molecular dynamics* method. Closely related methods have been developed in a wide variety of other fields including the simulation of plasma dynamics, lattice vibrations in solids, and polymer structure and dynamics.

In fact, molecular dynamics simulation today is competing rather directly with more conventional experimental measurements in providing

information about the behavior of many body systems. In many ways, such computer simulation models are superior to laboratory experiments because they can give essentially exact data on the macroscopic behavior of well-defined models, as well as additional information of theoretical interest that may not be accessible to experimental measurement. There is little doubt that molecular dynamics simulation has been the major impetus for the upsurge in activity that has been experienced in the field of nonequilibrium statistical mechanics during the past decade. It is also becoming more apparent that certain types of transport problem—notably those arising in plasma physics—are so complicated that computer simulation has become the necessary bridge between experimental measurements and theoretical interpretation.

9.2.1 □ Microscopic Dynamics Methods (Molecular Dynamics) □ To simulate the dynamics of a fluid of particles, we can consider the dynamics of a system of N particles as they interact within a cell of fixed volume.²⁷ The essential idea is to integrate the equations of motion characterizing the particles as they interact, moving about the cell. Typically one employs periodic boundary conditions on the cell (see Figure 9.12) so that as one particle leaves the cell, its mirror image enters from the opposing boundary.

Since a significant amount of effort is required to compute the forces acting on each of the particles during the integration of the equations of motion, one is restricted to rather small sample sizes (typically less than 1000 particles). Generally one chooses cubic cells with $N = 4n^3$ particles, where n is an integer (corresponding to systems of 256, 500, 864, etc., particles).

A number of investigators have studied the dynamics of particles interacting through hard sphere (short range) potentials.²⁴ Such systems are particularly simple to analyze because the particles stream freely between collisions. One can treat the time evolution of such a system as a sequence of binary, elastic collision events.

The study of systems characterized by continuous (although short range) potentials is only slightly more difficult.^{25,26} In this instance, one must explicitly calculate the particle trajectories rather than merely follow a sequence of collision events. One can integrate the $3N$ coupled second order differential equations of motion characterizing the system using an algorithm giving the particle coordinates at the advanced time step by

$$r_i(t + \Delta t) \cong -r_i(t - \Delta t) + 2r_i(t) + \frac{(\Delta t)^2}{m} \sum_{j \neq i} \mathbf{F}_{ij}(t) \quad (9.8)$$

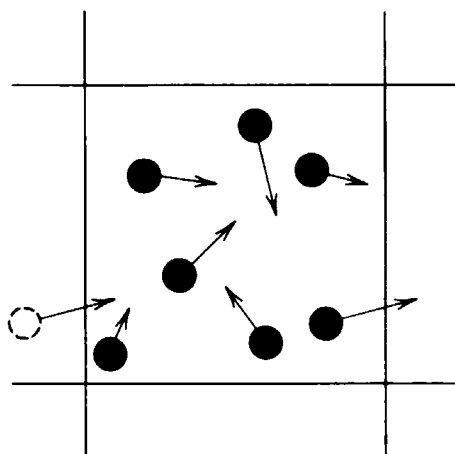


Fig. 9.12 □ Use of periodic boundary conditions in molecular dynamics calculations.

where $\mathbf{F}_{ij}(t)$ is the force exerted by particle j on particle i at time t . The time step size is kept smaller than a characteristic collision time. Typical simulation runs involve roughly 10^3 time steps. The force term is usually limited to include only particles within an interaction sphere of radius $L/2$, where L is the cell width (interactions with particle images in the adjacent cells created by the periodic boundary conditions are included, of course).

Such simulations have been performed for systems characterized by a variety of short range interaction potentials, including the Lennard-Jones potential and exponential repulsive potentials. The simulation of systems interacting by way of long range forces—particularly Coulomb forces—is a bit more difficult, since a very large number of particles may interact (10^5 to 10^6) to produce “self-consistent” fields that act on the particles.²⁸ In these problems, one must treat the interactions in an average fashion by calculating an effective force field that acts on each of the particles. For this reason, the field of microscopic plasma simulation has become highly specialized, and we make no attempt to review these methods here.^{28,29}

Since any such computer simulation is capable of analyzing the detailed dynamics of only a relatively small number of particles, there is always some question about how accurately these simulations predict the behavior of macroscopic sized systems. It has been demonstrated that many of the bulk properties of matter can be adequately described by such simulations, although there are notable exceptions, such as the study of fluctuations whose wavelengths are longer than the cell dimensions of the simulation

system (these arise, e.g., in the study of critical phenomena). Molecular dynamics simulation has proved to be extremely effective in predicting the physical properties of systems ranging from simple liquids and plasmas to systems governed by more complex potentials such as liquid metals, diatomic liquids, and gases. In fact, such computer simulations have even experienced some success in predicting the properties of more peculiar substances such as water.³⁰

9.2.2 □ Monte Carlo Simulation of Many Body Systems □ Monte Carlo methods have been used to simulate the equilibrium behavior of many body systems by using random sampling methods to estimate the ensemble averages characterizing such systems.^{27,31,32} Recall that the average of a dynamic variable with respect to a canonical ensemble can be written as

$$\langle \psi(\Gamma_N) \rangle = \frac{\int d\Gamma_N e^{-\beta V_N(\Gamma_N)} \psi(\Gamma_N)}{\int d\Gamma_N e^{-\beta V_N(\Gamma_N)}}$$

One can replace this integration over phase space by a statistical average over a finite set of discrete particle configurations indexed by “ i ”:

$$\langle \psi \rangle \cong \frac{\sum_i e^{-\beta V_N(i)} \psi(i)}{\sum_i e^{-\beta V_N(i)}}$$

Then we use Monte Carlo methods to generate and sample from an ensemble of particle configurations generated by a sequence of successive random displacements. It is necessary to employ importance sampling by selecting the configurations according to a prescribed probability distribution $P(i)$. The most common sampling scheme utilizes a distribution³¹

$$P(i) = \frac{e^{-\beta V_N(i)}}{\sum_{j=1}^M e^{-\beta V_N(j)}}$$

then calculates the estimate of the ensemble average as

$$\langle \psi \rangle \cong \frac{1}{M} \sum_{i=1}^M \psi(i)$$

Typically between 10^5 and 10^6 configurations are generated in the simulation.

It should be stressed that although such Monte Carlo methods are quite useful for calculating equilibrium properties, they are not well suited for simulating the dynamic behavior of collective processes.

9.2.3 □ Phase Space Simulation Methods □ An interesting variation on both statistical and deterministic simulation methods proceeds by directly tracking a collection of particles as they move about in the six-dimensional phase space $(\mathbf{r}, \mathbf{v})$.³³ To accomplish this, one assigns a portion of computer memory to represent this phase space and keeps track of the particles as

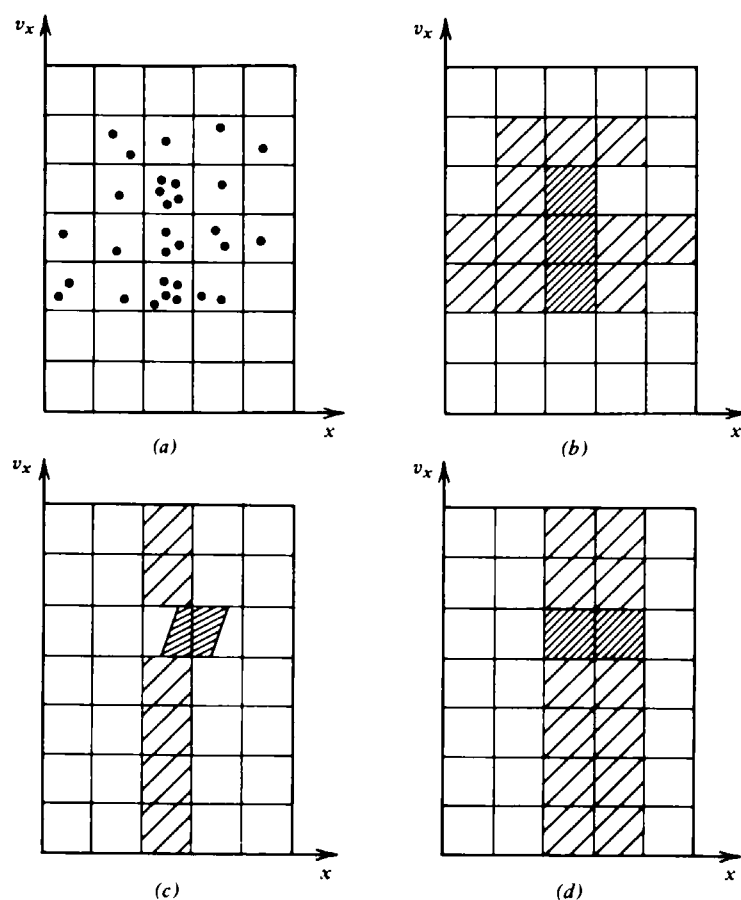


Fig. 9.13 □ Phase space simulation method. (a) Assignment of particles to phase space cells. (b) Distribution of phase space cells. (c) Redistribution and deformation of cell due to particle collisions and streaming during time step. (d) Reassignment of particles to cell for next time step.

they move from one part of phase space to another as determined by streaming motion or collision interactions.

To make this more transparent, consider a simple two-dimensional phase space (x, v_x) as shown in Figure 9.13. One first imposes a grid structure on this phase space, then assigns each of the particles of interest to one of the rectangular grid elements. Now the time evolution of the system can be described by noting how the grid elements deform horizontally because of particle motion, and how particles are transferred vertically out of one element to another because of collision events. At the end of each time step, one returns to a rectangular phase space grid by reassigning portions of the phase space volumes that have been deformed as a result of streaming motion. To accelerate this calculation, one can develop Green's function matrices, which give the particle density at a time $t + \Delta t$ in the phase space element (i', j') due to a unit density at time t in the phase space element (i, j) . Then the time evolution of the system can be easily obtained by repeated matrix multiplication.

Since this phase space simulation method is in essence just a bookkeeping scheme to keep track of conservation of particles in phase space, one can easily see how to generalize it to apply to higher dimension phase spaces (e.g., including energy dependence). In practice, however, the method has been applied to date only to analyze one-dimensional, time-dependent transport problems in which relatively short time information is desired.

□ PROBLEMS □

9.1 Determine a rejection technique to sample from the probability distribution $p(x) = e^{-x}$ and determine the efficiency of this technique.

9.2 Estimate the variance in the distance traveled to collision in a uniform medium.

9.3 How many samples are required to yield a confidence level of 99% that the estimate of the average distance to collision is within 0.1% of the true mean?

9.4 Verify the expression on page 552 for the fractional square error associated with a given estimate $\bar{\psi}_N$.

9.5 Describe the Monte Carlo algorithm for determining the leakage rate from the surface of a nonmultiplying sphere with an isotropic and monoenergetic point source at its origin.

9.6 Describe the Monte Carlo algorithm for determining the criticality eigenvalue k_{eff} for a uniform sphere of multiplying material.

- 9.7 How could you estimate the total flux in a region using Monte Carlo methods?
- 9.8 Demonstrate that the use of the true adjoint solution to an integral equation as the weighting function in a biased Monte Carlo sampling scheme will lead to zero variance.
- 9.9 Devise a boundary crossing routine for zones consisting of concentric spheres.

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The Wiener-Hopf Method

Consider an integral equation of the form

$$\varphi(x) = \int_0^{\infty} dx' K(x-x')\varphi(x') + g(x), \quad 0 \leq x < \infty \quad (\text{A.1})$$

Define the Fourier transform

$$\begin{aligned} \tilde{\Phi}(k) &= \int_{-\infty}^{\infty} dx e^{ikx} \varphi(x) = \int_{-\infty}^0 dx e^{ikx} \varphi(x) + \int_0^{\infty} dx e^{ikx} \varphi(x) \\ &\equiv \tilde{\Phi}_-(k) + \tilde{\Phi}_+(k) \end{aligned}$$

We use the integral equation itself to define $\varphi(x)$ for $x < 0$. We can now use the convolution theorem to Fourier transform the integral equation (A.1) to find

$$\tilde{\Phi}_+(k) + \tilde{\Phi}_-(k) = \tilde{K}(k)\tilde{\Phi}_+(k) + \tilde{g}(k)$$

where

$$\tilde{K}(k) \equiv \int_{-\infty}^{\infty} dx e^{ikx} K(x)$$

If we rearrange, we can write

$$\tilde{h}(k)\tilde{\Phi}_+(k) + \tilde{\Phi}_-(k) = \tilde{g}(k) \quad (\text{A.2})$$

where we define $\tilde{h}(k) = 1 - \tilde{K}(k)$.

If we assume that $\varphi(x) = O(e^{ax})$ as $x \rightarrow \infty$, then since $e^{(ik+a)x}$ is bounded if $\text{Im} k > a$, we find that $\tilde{\Phi}_+(k)$ is analytic for $\text{Im} k > a$, that is, in the upper half-plane as indicated in Figure A.1a.¹ In a similar manner, if we assume that $\varphi(x) = O(e^{bx})$ as $x \rightarrow -\infty$, we note that $\tilde{\Phi}_-(k)$ is analytic in k for $\text{Im} k < b$, that is, in the lower half-plane indicated in Figure A.1b. The asymptotic behavior of $\varphi(x)$ necessary to determine the domains of analyticity of $\tilde{\Phi}_+(k)$ and $\tilde{\Phi}_-(k)$ usually is specified in the problem [although frequently one must first assume this behavior, then verify it after solving for $\varphi(x)$].

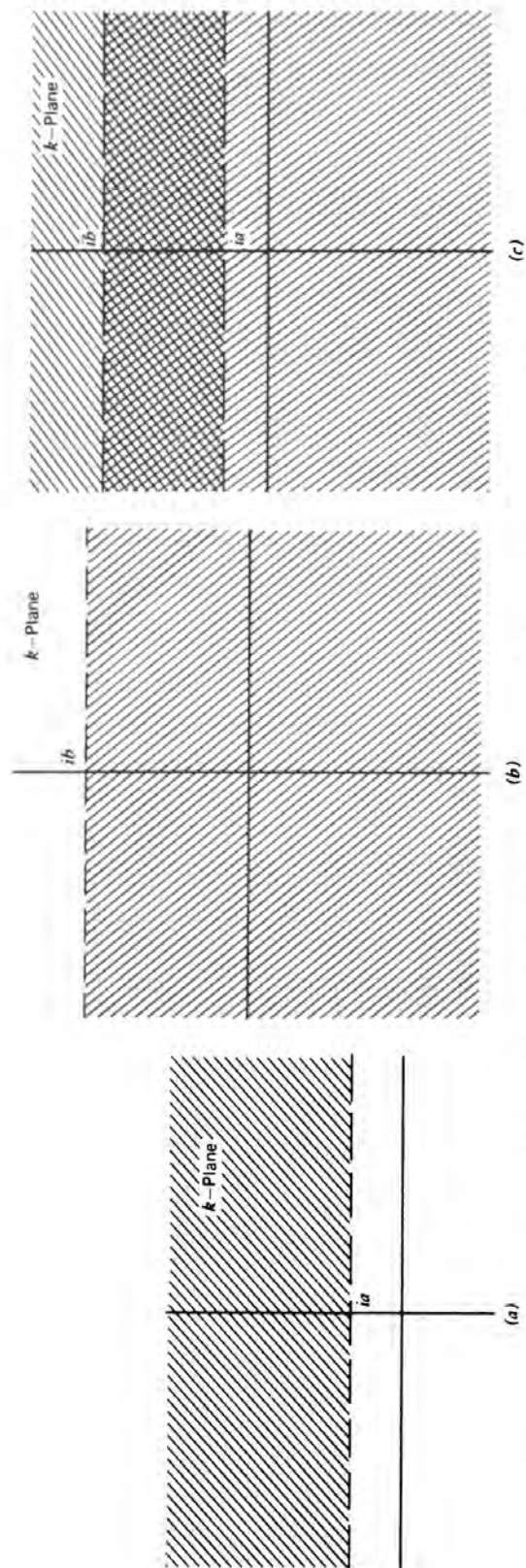


Fig. A.1 $\square$ Analytic structure for Wiener-Hopf decomposition. (a) $\tilde{\Phi}_+(k)$. (b) $\tilde{\Phi}_-(k)$. (c) $\tilde{H}(k)\tilde{\Phi}_+(k) + \tilde{\Phi}_-(k) = \tilde{g}(k)$.

Notice now that if $b > a$, there will be an overlapping strip of analyticity. Such an overlapping strip is essential for the successful application of the Wiener-Hopf technique. Let us furthermore suppose that we can find a strip within this overlap region in which $\tilde{h}(k)$ is analytic.

Now suppose we could decompose $\tilde{h}(k)$ into a quotient of two functions $\tilde{h}(k) = h_+(k)/h_-(k)$, where $h_+(k)$ is analytic in some upper half-plane and $h_-(k)$ is analytic in some lower half-plane with a common strip of analyticity within the previous strip. Then we can rewrite Eq. A.2 as follows:

$$h_+(k)\tilde{\Phi}_+(k) + h_-(k)\tilde{\Phi}_-(k) = \tilde{g}(k)h_-(k) \quad (\text{A.3})$$

(see Figure A.1c). Next, suppose we can perform a second decomposition, this time of $\tilde{g}(k)h_-(k)$ into a difference, $\tilde{g}(k)h_-(k) = \gamma_+(k) - \gamma_-(k)$, where $\gamma_+(k)$ is analytic in some upper half-plane and $\gamma_-(k)$ is analytic in some lower half-plane with a common strip of analyticity within the previous strip. Then we can rewrite Eq. A.3 as follows:

$$h_+(k)\tilde{\Phi}_+(k) - \gamma_+(k) = -h_-(k)\tilde{\Phi}_-(k) - \gamma_-(k) \quad (\text{A.4})$$

in some nondegenerate horizontal strip.

Now define a function

$$J(k) \equiv \begin{cases} h_+(k)\tilde{\Phi}_+(k) - \gamma_+(k) & \text{for } k \text{ in the upper half-plane} \\ -h_-(k)\tilde{\Phi}_-(k) - \gamma_-(k) & \text{for } k \text{ in the lower half-plane} \end{cases}$$

We notice that $J(k)$ is an entire function, since it coincides with analytic functions in both half-planes with a common region (strip). (You can show this using the identity theorem for analytic functions or by analytic continuation.) Hence we can determine $J(k)$ completely by using its behavior at infinity and applying Liouville's theorem.² Then once we know $J(k)$, we can solve algebraically for $\tilde{\Phi}_+(k)$ and $\tilde{\Phi}_-(k)$

$$\tilde{\Phi}_+(k) = \frac{J(k) + \gamma_+(k)}{h_+(k)}, \quad \tilde{\Phi}_-(k) = \frac{-J(k) - \gamma_-(k)}{h_-(k)}$$

and find

$$\varphi(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{-ikx} [\tilde{\Phi}_+(k) + \tilde{\Phi}_-(k)]$$

$k \in \text{strip}$

To get the final form of the solution, we complete the remainder of the steps in the usual integral transform approach by finding the singularities of $\tilde{\Phi}_+(k)$ and $\tilde{\Phi}_-(k)$ and making an appropriate contour deformation of the original inversion path about these singularities.

Of course the key to the Wiener-Hopf technique is the ability to decompose functions into quotients and differences of functions analytic in various half-planes so that we can manipulate Eq. A.2 into the form of Eq. A.4. To facilitate this, we state and prove two key theorems.³

Theorem I. Decomposition into a Difference. Let $\alpha(k)$ be analytic in the strip $a < \text{Im } k < b$ (see Figure A.2) and suppose furthermore that

- i $\int_{-\infty}^{\infty} du |\alpha(u + iv)|$ exists for every $v \in (a, b)$.
- ii $\alpha(k)/k \rightarrow 0$ as $k \rightarrow \infty$ in the strip uniformly in k for $a + \delta < \text{Im } k < b - \delta$, $\delta > 0$ (every closed substrip).

Let $a < a_1 < \text{Im } k < b_1 < b$ be a substrip. Then

$$\alpha(k) = \alpha_+(k) - \alpha_-(k), \quad a_1 < \text{Im } k < b_1$$

where

$$\alpha_+(k) = \frac{1}{2\pi i} \int_{-\infty + ia_1}^{+\infty + ia_1} dz \frac{\alpha(z)}{z - k}, \quad \text{Im } k > a_1$$

$$\alpha_-(k) = \frac{1}{2\pi i} \int_{-\infty + ib_1}^{+\infty + ib_1} dz \frac{\alpha(z)}{z - k}, \quad \text{Im } k < b_1$$

Here $\alpha_+(k)$ is analytic for $\text{Im } k > a_1$, and $\alpha_-(k)$ is analytic for $\text{Im } k < b_1$. [Comment. Notice that condition i ensures that the integrals defining $\alpha_+(k)$ and $\alpha_-(k)$ converge, whereas condition ii kills off the contributions from the ends of the rectangular integration path described below.]

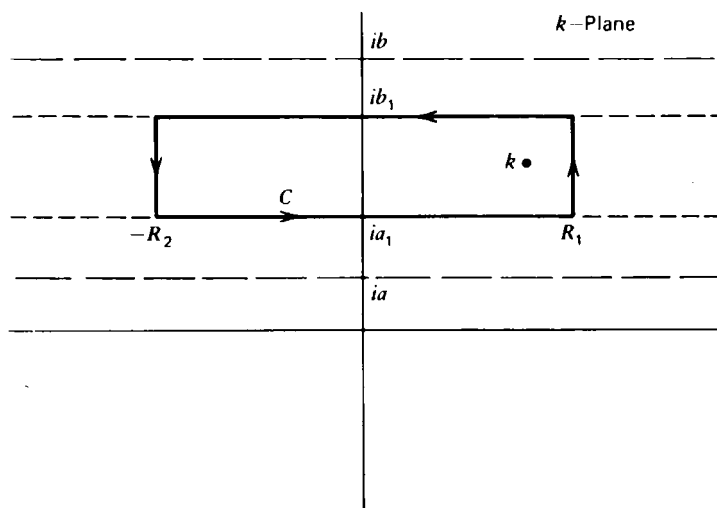


Fig. A.2 □ Integration contour for Wiener-Hopf decomposition into a difference.

Proof. We first establish that $\alpha_+(k)$ is analytic for $\text{Im } k > a_1$. Notice that the integrand $\alpha(z)/(z-k)$ is analytic for all $z \neq k$ and is jointly continuous in (z, k) . Let G be a closed, bounded subset of $\text{Im } k > a_1$. For any $k \in G$, there exists a $\delta > 0$ such that $|z - k| \geq \delta$ for all z along the integration path. Thus $|\alpha(z)/(z - k)| \leq |\alpha(z)/\delta|$. By condition i, we therefore have $\int_{-\infty}^{\infty} du |\alpha(u + ia_1)/(z - k)| < \infty$ for all $k \in G$. Thus the integral defining $\alpha_+(k)$ converges uniformly on every closed, bounded subset of $\text{Im } k > a_1$, and we therefore have shown that $\alpha_+(k)$ is analytic for $\text{Im } k > a_1$. A similar argument demonstrates that $\alpha_-(k)$ is analytic for $\text{Im } k < b_1$.

To verify the decomposition, let k be any point in the substrip $a_1 < \text{Im } k < b_1$. Now apply Cauchy's formula to the rectangular contour C as shown in Figure A.2:

$$\alpha(k) = \frac{1}{2\pi i} \left[\int_{-R_2 + ia_1}^{R_1 + ia_1} + \int_{R_1 + ia_1}^{R_1 + ib_1} + \int_{R_1 + ib_1}^{-R_2 + ib_1} + \int_{-R_2 + ib_1}^{-R_2 + ia_1} \right] \frac{\alpha(z) dz}{z - k} \quad (\text{A.5})$$

Now as $R_1 \rightarrow \infty$, we can use condition ii (particularly the uniform convergence of the limit) to show

$$\left| \int_{R_1 + ia_1}^{R_1 + ib_1} dz \frac{\alpha(z)}{z - k} \right| \rightarrow 0, \quad R_1 \rightarrow \infty$$

Similarly we can show

$$\left| \int_{-R_2 + ia_1}^{-R_2 + ib_1} dz \frac{\alpha(z)}{z - k} \right| \rightarrow 0, \quad -R_2 \rightarrow -\infty$$

thus from Eq. A.5 we find

$$\alpha(k) = \alpha_+(k) - \alpha_-(k) \quad \text{for } a_1 < \text{Im } k < b_1$$

Theorem II. Decomposition into a Quotient. Let $\alpha(k)$ be analytic for $a < \text{Im } k < b$ and suppose that conditions i and ii of Theorem I hold. Let $k_1, k_2, \dots, k_n$ be the zeros (if any) of $\alpha(k)$ that lie in the strip $a < \text{Im } k < b$. Then there exist functions $\alpha_+(k)$ and $\alpha_-(k)$ with the following properties:

- i $\alpha_+(k)$ [$\alpha_-(k)$] is analytic for $\text{Im } k > a_1$ [$\text{Im } k < b_1$], where a_1, b_1 are the same as in Theorem I.
- ii $\alpha_+(k)$ [$\alpha_-(k)$] is free of zeros in $\text{Im } k > a_1$ [$\text{Im } k < b_1$].
- iii $\alpha(k) = [\alpha_+(k)/\alpha_-(k)]P(k)$, where

$P(k) = 1$ if $\alpha(k)$ has no zeros in strip

$= (k - k_1)(k - k_2) \cdots (k - k_n)$ if $\alpha(k)$ has n zeros in strip

The actual forms of $\alpha_+(k)$ and $\alpha_-(k)$ are given in the proof.

Proof. Roughly, the proof is as follows. Suppose we could take the log of $\alpha(k)$ and apply the result of Theorem I to decompose $\ln \alpha(k) = \gamma_+(k) - \gamma_-(k)$. Then we could find $\alpha(k) = \exp[\ln \alpha(k)] = \exp[\gamma_+(k)] / \exp[\gamma_-(k)] \equiv \alpha_+(k) / \alpha_-(k)$. The essential procedure in the proof is to demonstrate that we can do just this.

More precisely, by the definition of $P(k)$, the function $\alpha(k)/P(k)$ is analytic and free of zeros in the strip $a < \text{Im} k < b$. However it vanishes as $1/k^n$ as $k \rightarrow \infty$, hence we cannot take its log because we would run into difficulties as $u = \text{Re} k \rightarrow \pm \infty$. To patch this up, multiply $\alpha(k)/P(k)$ by $(k - ia)^{n/2} (k - ib)^{n/2}$. If n is even, these are well defined. However if n is odd, this function has branch points, and we must make sure to define the corresponding branch cuts so that they do not appear in the strip. That is, we define $(k - ia)^{n/2}$ to be analytic in the plane cut along the imaginary axis from ai to $-i\infty$. Furthermore $(k - ib)^{n/2}$ is analytic in the plane cut along the imaginary axis from ib to $+i\infty$. These branches have been chosen such that

$$(k - ib)^{n/2} (k - ia)^{n/2} \sim k^n \text{ as } k \rightarrow \infty \text{ in the strip}$$

Now define

$$R(k) \equiv \left[\frac{\alpha(k)}{P(k)} \right] (k - ib)^{n/2} (k - ia)^{n/2}$$

It is evident by construction that $R(k) \sim 1$ as $k \rightarrow \infty$ in the strip, hence $\ln R(k)$ exists and approaches zero as $k \rightarrow \infty$. However as we travel along some horizontal path in the strip, $\arg[R(k)]$ may change by some multiple of 2π (i.e., we get a circling of the origin in the R -plane). We want to ensure that this does not happen. Suppose as k goes from $-\infty + iv$ to $+\infty + iv$ along a line $v = \text{constant}$ in the strip (see Figure A.3), the $\arg[R(k)]$ changes by $2\pi N$ for some integer N [N must be an integer because $R(-\infty + iv) = 1 = R(+\infty + iv)$ by construction]. If $N \neq 0$, we have $R(k)$ wrapping itself around the origin. Now define

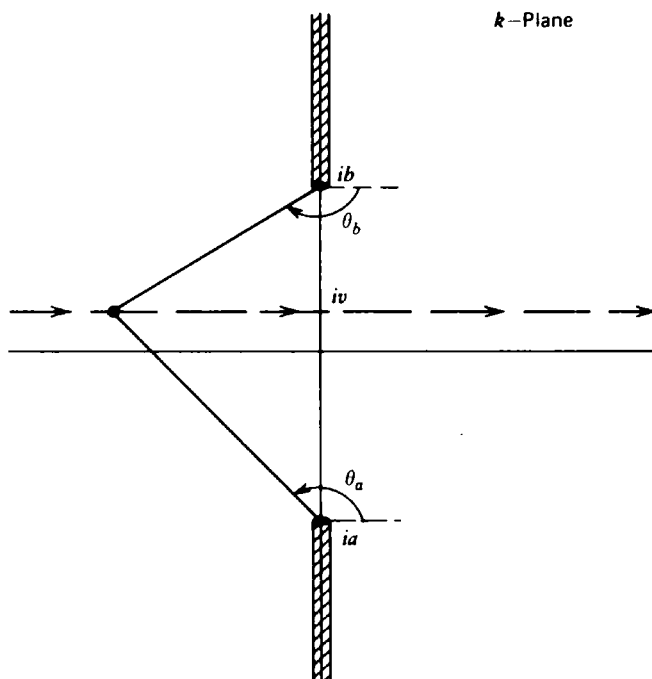
$$\psi(k) \equiv R(k) (k - ib)^l (k - ia)^{-l}$$

Evidently

$$\arg \psi(k) = \arg[R(k)] + l \arg[k - ib] - l \arg[k - ia]$$

Hence the change in $\arg[\psi(k)]$ is just

$$\Delta \arg[\psi(k)]_{-\infty + iv}^{+\infty + iv} = 2\pi N + l\pi - l(-\pi) = 2\pi(N + l)$$

Fig. A.3 □ Change in the argument of $\psi(k)$.

Therefore we choose $l = -N$ so that

$$\psi(k) = R(k)(k - ib)^{-N}(k - ia)^N$$

or

$$\psi(k) = \left[\frac{\alpha(k)}{P(k)} \right] (k - ia)^{(n/2) + N} (k - ib)^{(n/2) - N} \quad (\text{A.6})$$

Now we can see by construction that $\psi(k)$ is (i) regular in the strip $a < \text{Im } k < b$, (ii) free of zeros in the strip, and (iii) $\Delta \arg[\psi(u + iv)] \Big|_{u = -\infty}^{u = +\infty} = 0$. Hence we conclude that

- i $\int_{-\infty}^{\infty} du |\ln \psi(u + iv)|$ exists.
- ii $k^{-1} \ln \psi(k) \rightarrow 0$ as $k \rightarrow \infty$.

We can therefore apply Theorem I to find

$$\ln \psi(k) = \psi_+(k) - \psi_-(k), \quad a < a_1 < \text{Im } k < b_1 < b \quad (\text{A.7})$$

where $\psi_+(k)$ is analytic for $\text{Im } k > a_1$, and $\psi_-(k)$ is analytic for $\text{Im } k < b_1$.

We can then write

$$\psi(k) = \exp[\psi_+(k) - \psi_-(k)] = \frac{e^{\psi_+(k)}}{e^{\psi_-(k)}}$$

But

$$\psi(k) = \left[\frac{\alpha(k)}{P(k)} \right] (k - ia)^{(n/2) + N} (k - ib)^{(n/2) - N}$$

or

$$\alpha(k) = \left[\frac{e^{\psi_+(k)} (k - ia)^{-(n/2) - N}}{e^{\psi_-(k)} (k - ib)^{(n/2) - N}} \right] (k - k_1) \cdots (k - k_n)$$

Therefore our final expressions become

$$\begin{aligned} \alpha_+(k) &= e^{\psi_+(k)} (k - ia)^{-(n/2) - N} \\ \alpha_-(k) &= e^{\psi_-(k)} (k - ib)^{(n/2) - N} \end{aligned} \quad (\text{A.8})$$

and our theorem is proved.

Although Theorem II might appear awkward to use in a practical calculation, it can actually be applied rather easily by (i) determining the number of zeros n of $\alpha(k)$ in the strip, (ii) determining the change in the argument of $R(k)$ along an infinite horizontal path in this strip (call this change $2\pi N$), and (iii) using Eqs. A.6 to A.8 to find

$$\alpha(k) = \frac{\alpha_+(k)}{\alpha_-(k)} P(k)$$

Example.⁴ Consider the decomposition of the dispersion function $\Lambda(k)$ that arises in the Milne problem:

$$\Lambda(k) = \frac{\lambda_+(k)}{\lambda_-(k)}, \quad \kappa_0 < \text{Im } k < \Sigma,$$

The quotient decomposition theorem suggests that we take $\ln \Lambda(k)$, then use a difference decomposition. But any zeros of $\Lambda(k)$ will give rise to singularities of $\ln \Lambda(k)$. And we know that $\Lambda(k)$ has two zeros, $\pm i\kappa_0$. Hence it is apparent that $(k^2 + \kappa_0^2)^{-1} \Lambda(k)$ has no zeros in the finite cut-plane. But we now have a $1/k^2$ behavior at $k \rightarrow \infty$ (i.e., two more

zeros), which we must patch up. Therefore we multiply by $(k^2 + \Sigma_t^2)$ and define

$$\psi(k) \equiv \ln \left[\left(\frac{k^2 + \Sigma_t^2}{k^2 + \kappa_0^2} \right) \Lambda(k) \right]$$

By construction, $\psi(k)$ is well behaved in the cut-plane *and* as $k \rightarrow \infty$.

We can now apply the difference decomposition Theorem I to write

$$\psi(k) = \psi_+(k) - \psi_-(k)$$

where

$$\psi_+(k) = \frac{1}{2\pi i} \int_{-\infty + ia_1}^{\infty + ia_1} dz \frac{\psi(z)}{z - k}, \quad \text{Im } k > a_1$$

$$\psi_-(k) = \frac{1}{2\pi i} \int_{-\infty + ib_1}^{\infty + ib_1} dz \frac{\psi(z)}{z - k}, \quad \text{Im } k < b_1$$

Hence we find

$$\left(\frac{k^2 + \Sigma_t^2}{k^2 + \kappa_0^2} \right) \Lambda(k) = \frac{e^{\psi_+(k)}}{e^{\psi_-(k)}}$$

or

$$\Lambda(k) = \frac{\lambda_+(k)}{\lambda_-(k)} = \frac{\left(\frac{k^2 + \kappa_0^2}{k + i\Sigma_t} \right) e^{\psi_+(k)}}{(k - i\Sigma_t) e^{\psi_-(k)}} \quad (\text{A.9})$$

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□ B □

Principal Value Integration
and Cauchy Integrals

Consider an integral of the form

$$\int_a^b d\mu \frac{\varphi(\mu)}{\mu - \nu}$$

Ordinarily this integral would not be defined for $\nu \in [a, b]$. But suppose we were to perform the integration “symmetrically” in such a way that the two infinite areas cancel (see Figure B.1). In this sense, we define the *principal value*^{1,2} of such an integral as

$$P \int_a^b d\mu \frac{\varphi(\mu)}{\mu - \nu} = \lim_{\epsilon \rightarrow 0} \left[\int_a^{\nu - \epsilon} d\mu \frac{\varphi(\mu)}{\mu - \nu} + \int_{\nu + \epsilon}^b d\mu \frac{\varphi(\mu)}{\mu - \nu} \right] \equiv \oint_a^b d\mu \frac{\varphi(\mu)}{\mu - \nu}$$

Example. To illustrate this, let us compute

$$\begin{aligned} P \int_{-1}^{+1} \frac{d\mu}{\mu - \nu} &= \lim_{\epsilon \rightarrow 0} \left\{ \ln(\mu - \nu) \Big|_{-1}^{\nu - \epsilon} + \ln(\mu - \nu) \Big|_{\nu + \epsilon}^1 \right\} \\ &= \lim_{\epsilon \rightarrow 0} [\ln(-\epsilon) - \ln(-1 - \nu) + \ln(1 - \nu) - \ln(\epsilon)] = \ln \frac{1 - \nu}{1 + \nu} \end{aligned}$$

Integrals of the form

$$\Phi(z) = \frac{1}{2\pi i} \int_L dt \frac{\varphi(t)}{t - z}$$

where L is some arc in the complex t -plane are referred to as *Cauchy integrals*.³ These integrals possess a number of interesting properties provided $\varphi(t)$ is “sufficiently well-behaved.” To be more precise, consider the following definition.

Definition. The function $\varphi(t)$ is said to satisfy a *Hölder condition* (denoted by $\varphi \in H$) if for any two points t_1 and t_2 on L ,

$$|\varphi(t_2) - \varphi(t_1)| \leq A |t_2 - t_1|^\mu$$

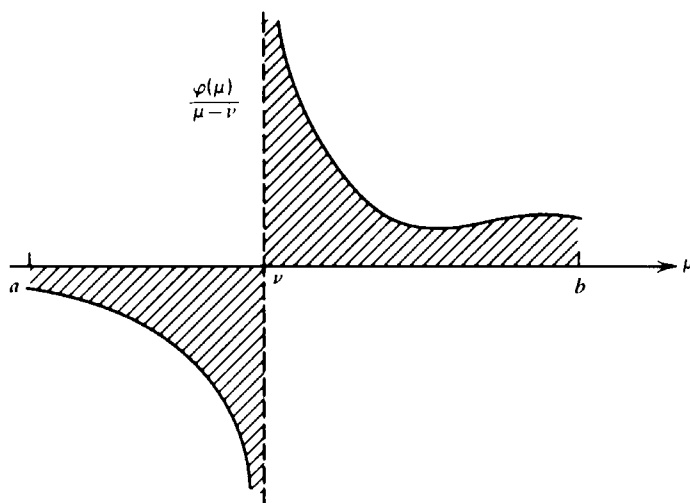


Fig. B.1 □ Divergence of the integrand of a Cauchy integral.

where A and μ are positive constants. If, furthermore, near the endpoints of L

$$\varphi(t) = \frac{\varphi^*(t)}{(t-c)^\alpha}, \quad 0 \leq \alpha < 1$$

where $\varphi^* \in H$, we say that $\varphi(t)$ satisfies an H^* condition on L (denoted by $\varphi \in H^*$).

This definition allows us to state a very important theorem concerning Cauchy integrals.

Theorem. Let $\varphi(t) \in H^*$ on L . Then

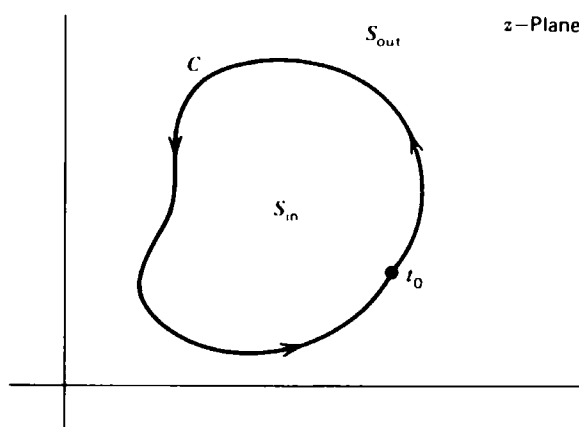
$$\Phi(z) = \frac{1}{2\pi i} \int_L dt \frac{\varphi(t)}{(t-z)}$$

is analytic in the z -plane cut by L . (Sometimes functions that are analytic in a cut-plane are referred to as sectionally holomorphic functions.)

Proof. See Muskhelishvili, Chapter 2.⁴

Furthermore, the condition $\varphi \in H^*$ allows us to define the limiting values of a Cauchy integral $\Phi(z)$ as z approaches the cut L . Consider the Cauchy integral

$$\Phi(z) = \frac{1}{2\pi i} \int_C dt \frac{\varphi(t)}{t-z} \quad (\text{B.1})$$

Fig. B.2 □ Contour for the Cauchy integral $\Phi(z)$.

where C is a closed contour (see Figure B.2). Now write

$$\Phi(z) = \frac{1}{2\pi i} \int_C dt \frac{\varphi(t) - \varphi(t_0)}{t - z} + \frac{\varphi(t_0)}{2\pi i} \int_C \frac{dt}{t - z} \equiv \Psi(z) + \frac{\varphi(t_0)}{2\pi i} \int_C \frac{dt}{t - z}$$

For $z \in S_{\text{in}}$, we have a pole at z so that applying the residue theorem yields

$$\Phi(z) = \Psi(z) + \varphi(t_0)$$

But if $z \in S_{\text{out}}$, there is no pole in C so that

$$\Phi(z) = \Psi(z)$$

Now consider $z \in S_{\text{in}}$ as $z \rightarrow t_0$

$$\Phi^+(t_0) \equiv \lim_{z \rightarrow t_0} \Phi(z) = \frac{1}{2\pi i} \int_C dt \frac{\varphi(t) - \varphi(t_0)}{t - t_0} + \varphi(t_0)$$

and $z \in S_{\text{out}}$ as $z \rightarrow t_0$

$$\Phi^-(t_0) \equiv \lim_{z \rightarrow t_0} \Phi(z) = \frac{1}{2\pi i} \int_C dt \frac{\varphi(t) - \varphi(t_0)}{t - t_0}$$

But if we recall that $P \int_C dt (t - t_0)^{-1} = \pi i$, we can extract the factor $\varphi(t_0) \int_C dt (t - t_0)^{-1}$ to find

$$\Phi^\pm(t_0) = \frac{P}{2\pi i} \int_C dt \frac{\varphi(t)}{t - t_0} \pm \frac{1}{2} \varphi(t_0) \quad (\text{B.2})$$

For a more general statement, we can let $\varphi(t) = 0$ along part of the contour

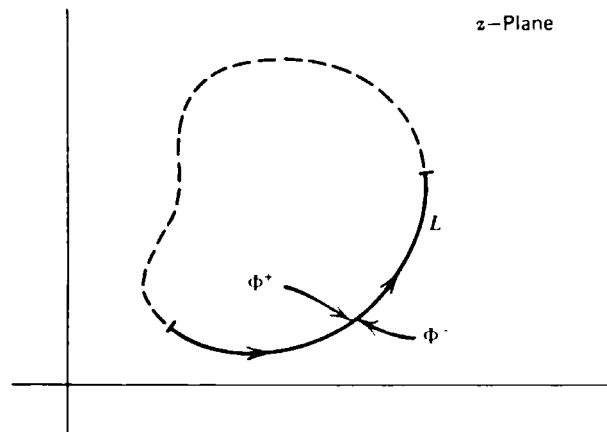


Fig. B.3 □ Limiting values of a Cauchy integral on an arc L .

(see Figure B.3) to apply Eq. B.2 to any smooth arc L .

In summary then, if

$$\Phi(z) = \frac{1}{2\pi i} \int_L dt \frac{\varphi(t)}{t-z}$$

the limits of the Cauchy integral on the cut become

$$\Phi^\pm(t_0) = \frac{P}{2\pi i} \int_L dt \frac{\varphi(t)}{t-t_0} \pm \frac{1}{2} \varphi(t_0) \quad (\text{B.3})$$

This relation is known as the *Plemelj formula*.^{5,6} Alternative forms of this result are

$$\Phi^+(t_0) - \Phi^-(t_0) = \varphi(t_0)$$

$$\Phi^+(t_0) + \Phi^-(t_0) = \frac{P}{\pi i} \int_L dt \frac{\varphi(t)}{t-t_0}$$

A more heuristic “proof” can be given for the Plemelj formula as follows. Consider an arc and try to approach it from above (see Figure B.4). Bend out a little semicircle about t_0 . This leaves a principal value integral from a to b plus half the residue from the semicircle about the “pole.” But this is just what the Plemelj formula (B.3) tells us.

Example. Suppose we want to find some function $\Phi(z)$ that is analytic in a cut-plane but with a given discontinuity across the cut L :

$$\Phi^+(t_0) - \Phi^-(t_0) = \varphi(t_0), \quad t_0 \in L \quad (\text{B.4})$$

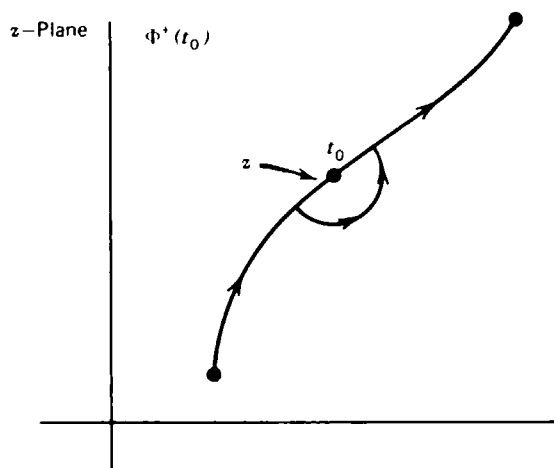


Fig. B.4 □ Heuristic “proof” of the Plemelj formula.

Claim. If we assume $\varphi \in H^*(L)$, and at infinity $\Phi(z)$ is of degree not greater than k , then by the Plemelj formula

$$\Phi(z) = \frac{1}{2\pi i} \int_L dt \frac{\varphi(t)}{t-z} + P_k(z)$$

where $P_k(z)$ is a polynomial of degree k .

Proof. The only puzzle might be where the polynomial $P_k(z)$ arises. The boundary condition on $\Phi(z)$ determines Φ only to within a polynomial—not uniquely. For if we consider two solutions, each analytic in the cut-plane and satisfying

$$\Phi_1^+ - \Phi_1^- = \varphi, \quad \Phi_2^+ - \Phi_2^- = \varphi$$

then on the cut, $Q(z) \equiv \Phi_1(z) - \Phi_2(z)$ is continuous and analytic. Furthermore $Q(z)$ is analytic in the cut-plane. Thus $Q(z)$ is an entire function of z . But that is all we can say. Hence if $Q(z) \rightarrow z^k$ as $|z| \rightarrow \infty$, Liouville's theorem tells us that $Q(z) = P_k(z)$, where $P_k(z)$ is a polynomial in z of degree k . Therefore we have determined $\Phi(z)$ only to within a polynomial $P_k(z)$.

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Singular Integral Equations of the Cauchy Type

Consider an integral equation of the form

$$a(x)\varphi(x) + \frac{1}{\pi} \int_L dy \left[\frac{K(x,y)}{y-x} \right] \varphi(y) = f(x) \quad (\text{C.1})$$

We would first like to separate out the singular part of this integral equation and “solve” it, thereby converting Eq. C.1 into a nonsingular Fredholm equation. We can add and subtract a term $K(x,x)/(y-x)$ to the integral to write

$$a(x)\varphi(x) + \frac{K(x,x)}{\pi} \int dy \frac{\varphi(y)}{y-x} + \frac{1}{\pi} \int_L dy \left[\frac{K(x,y) - K(x,x)}{y-x} \right] \varphi(y) = f(x)$$

or

$$a(x)\varphi(x) + \frac{b(x)}{\pi} \int_L dy \frac{\varphi(y)}{y-x} = f(x) - \frac{1}{\pi} \int_L dy k(x,y)\varphi(y) \equiv f'(x)$$

where the integral on the left-hand side is known as the “dominant” (or singular) part and the integral on the right is known as the “Fredholm” (or nonsingular) part. Our primary interest is in solving integral equations of the form

$$a(\mu)\varphi(\mu) + \frac{b(\mu)}{\pi} \int_L dv \frac{\varphi(v)}{v-\mu} = f(\mu), \quad \mu \in L \quad (\text{C.2})$$

which are referred to as *singular integral equations of the Cauchy type*.¹

We solve Eq. C.2 by converting it into a boundary value problem in complex variables. To this end, define the Cauchy integral

$$\Phi(z) \equiv \frac{1}{2\pi i} \int_L dv \frac{\varphi(v)}{v-z} \quad (\text{C.3})$$

If we now use the Plemelj formula, we can rewrite Eq. C.2 in the form

$$[a(\mu) + ib(\mu)]\Phi^+(\mu) - [a(\mu) - ib(\mu)]\Phi^-(\mu) = f(\mu) \quad (\text{C.4})$$

Let us now restrict ourselves to the case in which a and b are real, and $a^2 + b^2 \neq 0$, so that we can divide through to find our boundary value problem

$$G(\mu)\Phi^+(\mu) - \Phi^-(\mu) = [a(\mu) - ib(\mu)]^{-1}f(\mu) \equiv f'(\mu) \quad (\text{C.5})$$

where we have defined

$$G(\mu) = \frac{a + ib}{a - ib} \equiv \exp[2i\Theta(\mu)], \quad \Theta(\mu) \equiv \tan^{-1} \left[\frac{b(\mu)}{a(\mu)} \right]$$

Here, $G(\mu)$, $f'(\mu)$, $a(\mu)$, and $b(\mu)$ are known, and we must solve for $\Phi^+(\mu)$ and $\Phi^-(\mu)$, the limits of a function $\Phi(z)$ on the cut. Such problems as Eq. C.5 are known as the *inhomogeneous Hilbert problem*.²

To solve this problem, we must first consider a related problem, the homogeneous Hilbert or *Riemann-Hilbert problem*.³ Find a function $X(z)$ analytic on the cut-plane that is nonzero and such that

$$\frac{X^+(\mu)}{X^-(\mu)} = G(\mu) \quad (\text{C.6})$$

We first solve this problem, then use the solution to solve the inhomogeneous Hilbert problem, Eq. C.5. Finally we determine the solution to the singular integral equation (C.2) as the difference of boundary values on the cut, $\varphi(\mu) = \Phi^+(\mu) - \Phi^-(\mu)$.

The Riemann-Hilbert Problem □ Find a function $X(z)$ that is

- i Analytic in the cut-plane.
- ii Nonzero.
- iii Such that $X^+(\mu)/X^-(\mu) = G(\mu) = \exp[2i\Theta(\mu)]$.

For convenience we first fix the argument of $G(\mu)$ so that $\Theta(a) = 0$. By tracing along the cut we can then find that $\Theta(b) = \alpha\pi$.

Now consider a function

$$\Gamma(z) = \frac{1}{\pi} \int_a^b dv \frac{\Theta(v)}{v - z}$$

Using the Plemelj formula, we find

$$\exp[\Gamma^\pm(\mu)] = \exp\left[\frac{1}{\pi} P \int_a^b d\nu \frac{\Theta(\nu)}{\nu - \mu} \pm i\Theta(\mu)\right], \quad \mu \in [a, b]$$

Therefore $\exp[\Gamma(z)]$ looks like a good candidate for our solution, since

$$\frac{\exp[\Gamma^+(\mu)]}{\exp[\Gamma^-(\mu)]} = \exp[\Gamma^+(\mu) - \Gamma^-(\mu)] = \exp[2i\Theta(\mu)]$$

and therefore condition iii is satisfied. But what about conditions i and ii? Away from the endpoints, $\Gamma(z)$ is well behaved. But we should remember that a principal value integral can blow up like a log near the endpoints. Thus we must study the endpoint behavior more carefully.

Near $z = a$ we can write

$$\Gamma(z) \sim \frac{\Theta(a)}{\pi} \int_a^{a+\delta} \frac{d\nu}{\nu - z} + \frac{1}{\pi} \int_{a+\delta}^b d\nu \frac{\Theta(\nu)}{\nu - z} \sim -\frac{\Theta(a)}{\pi} \ln(a - z) + \Gamma_1(z)$$

and therefore

$$\exp[\Gamma(z)] \sim (a - z)^{-\Theta(a)/\pi} \exp[\Gamma_1(z)]$$

But since we have set $\Theta(a) = 0$, there is no trouble.

Near $z = b$,

$$\Gamma(z) \sim \frac{\Theta(b)}{\pi} \ln(b - z) + \Gamma_2(z)$$

or

$$\exp[\Gamma(z)] \sim (b - z)^{\Theta(b)/\pi} \exp[\Gamma_2(z)] = (b - z)^\alpha \exp[\Gamma_2(z)]$$

Thus if α is a positive integer, $\exp[\Gamma(z)]$ has a *zero* at b of order α . If α is a negative integer, $\exp[\Gamma(z)]$ has a *pole* at b of order α . Therefore to make $X(z)$ nonzero, we divide out $(b - z)^\alpha$ to find

$$X(z) = (b - z)^{-\alpha} \exp\left[\frac{1}{\pi} \int_a^b d\nu \frac{\Theta(\nu)}{\nu - z}\right] \quad (\text{C.7})$$

This, then, is the solution to the Riemann-Hilbert problem. Now on to the next phase.

The Inhomogeneous Hilbert Problem □ Recall that we wanted to solve Eq. C.5. But using $G(\mu) = X^+(\mu)/X^-(\mu)$, we find

$$\left[\frac{X^+(\mu)}{X^-(\mu)} \right] \Phi^+(\mu) - \Phi^-(\mu) = [a(\mu) - ib(\mu)]^{-1} f(\mu)$$

or

$$X^+(\mu)\Phi^+(\mu) - X^-(\mu)\Phi^-(\mu) = [a(\mu) - ib(\mu)]^{-1} X^-(\mu) f(\mu)$$

If we regard $X(z)\Phi(z)$ as analytic in the cut-plane, we can use the Plemelj formula to find

$$X(z)\Phi(z) = \frac{1}{2\pi i} \int_L dv \frac{X^-(v)f(v)}{[a(v) - ib(v)](v-z)} + P_k(z)$$

or since we have constructed $X(z)$ to be nonzero,

$$\Phi(z) = \frac{1}{X(z)} \left[\frac{1}{2\pi i} \int_L dv \frac{X^-(v)f(v)}{(a-ib)(v-z)} + P_k(z) \right] \quad (\text{C.8})$$

How do we determine $P_k(z)$? Well, we know that $\Phi(z)$ is an analytic function in the cut-plane that vanishes as $O(1/z)$ as $z \rightarrow \infty$. Hence the expression above must also do this.

From Eq. C.7 we can see that $X(z) \sim O(1/z^\alpha)$ as $z \rightarrow \infty$. Therefore we can distinguish three possible cases:

- i $\alpha = 0 \Rightarrow X(z) \rightarrow \text{constant}$. Then $\Phi(z) \sim \text{constant}$ [$O(1/z) + P(z)$], which implies that $P_k(z) = 0$ [since $P_k(z) \rightarrow \infty$ otherwise].
- ii $\alpha > 0 \Rightarrow X(z) \rightarrow z^\alpha$. We now find

$$P_{\alpha-1}(z) = az^{\alpha-1} + bz^{\alpha-2} + \dots$$

- iii $\alpha < 0 \Rightarrow X(z) \rightarrow 1/z^{|\alpha|}$. Now not only is $P_k(z) = 0$, but we must add more restrictions, since we want $\Phi(z) \sim O(1/z)$. This typically involves requiring that certain integrals of the $X^\pm(\mu)$ functions vanish:

$$\frac{1}{2\pi i} \int_L dv \frac{X^-f}{(a-ib)(v-z)} = -\frac{1}{2\pi iz} \sum_{n=0}^{\infty} \frac{1}{z^n} \left[\int_L dv \frac{X^-f v^n}{(a-ib)} \right]$$

to conclude that the integral must vanish as $z^{-(|\alpha|+1)}$ to kill off the $1/z^{|\alpha|}$ behavior. Therefore the $n=0, 1, \dots, \alpha-1$ terms must be zero.

Hence we require

$$P_k(z)=0, \quad \int_L dv \frac{X^-(v)f(v)v^n}{a(v)-ib(v)} \equiv 0, \quad n=0,1,\dots,\alpha-1$$

(This is the case that determines the discrete expansion coefficients in transport theory.⁴)

The Solution of the Singular Integral Equation □ Now all we have to do to find the solution to the singular integral equation (C.2) is to evaluate

$$\varphi(\mu) = \Phi^+(\mu) - \Phi^-(\mu)$$

where

$$\Phi(z) = \frac{1}{X(z)} \left[\frac{1}{2\pi i} \int_L dv \frac{X^-(v)f(v)}{(a-ib)(v-z)} + P_k(z) \right] \quad (C.9)$$

and

$$X(z) = (b-z)^{-\alpha} \exp \left[\frac{1}{\pi} \int_a^b dv \frac{\Theta(v)}{v-z} \right] \quad (C.10)$$

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□ D □

A Short Proof of the Generalized Langevin Equation^{1,2}

Let $\mathcal{L}_1$ and $\mathcal{L}_2$ be two operators (not necessarily commuting). Then

$$e^{t(\mathcal{L}_1 + \mathcal{L}_2)} = e^{t\mathcal{L}_1} + \int_0^t d\tau e^{(t-\tau)\mathcal{L}_1} \mathcal{L}_2 e^{\tau(\mathcal{L}_1 + \mathcal{L}_2)} \quad (\text{D.1})$$

To apply this result, let $\mathcal{L}_1 = iL$ and $\mathcal{L}_2 = -iPL$, where

$$P \circ \equiv \langle \circ \mathbf{a}^* \rangle \cdot \langle \mathbf{a} \mathbf{a}^* \rangle^{-1} \cdot \mathbf{a}$$

Then Eq. D.1 becomes

$$e^{it(1-P)L} = e^{itL} - \int_0^t d\tau e^{i(t-\tau)L} iPL e^{i\tau(1-P)L} \quad (\text{D.2})$$

Let us now operate with Eq. D.2 on the quantity $i(1-P)L\mathbf{a}$:

$$e^{it(1-P)L} i(1-P)L\mathbf{a} = e^{itL} i(1-P)L\mathbf{a} - \int_0^t d\tau e^{i(t-\tau)L} iPL e^{i\tau(1-P)L} i(1-P)L\mathbf{a} \quad (\text{D.3})$$

But we can identify

$$\mathbf{f}(t) = e^{it(1-P)L} i(1-P)L\mathbf{a}$$

and note

$$e^{itL} iPL\mathbf{a} = e^{itL} \langle \dot{\mathbf{a}} \mathbf{a}^* \rangle \cdot \langle \mathbf{a} \mathbf{a}^* \rangle^{-1} \cdot \mathbf{a} \equiv i\Omega \cdot \mathbf{a}(t)$$

and

$$\begin{aligned} e^{i(t-\tau)L} iPL\mathbf{f}(\tau) &= \langle \mathbf{f}(\tau) i(1-P)L\mathbf{a}^* \rangle \cdot \langle \mathbf{a} \mathbf{a}^* \rangle^{-1} \cdot \mathbf{a}(t-\tau) \\ &\equiv -\boldsymbol{\varphi}(\tau) \cdot \mathbf{a}(t-\tau) \end{aligned}$$

to rewrite Eq. D.3 in the standard form of the generalized Langevin equation

$$\frac{d\mathbf{a}}{dt} - i\boldsymbol{\Omega} \cdot \mathbf{a}(t) + \int_0^t d\tau \boldsymbol{\varphi}(\tau) \cdot \mathbf{a}(t - \tau) = \mathbf{f}(t) \quad (\text{D.4})$$

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□ E □

A Child's Primer on the Spectral Theory of Operators

To begin at the beginning, we must define more precisely the concept of an “eigenvalue” of an operator A . We usually refer to λ as an *eigenvalue* of A if there exist nontrivial solutions to

$$A\psi_\lambda = \lambda\psi_\lambda$$

But just what kind of functions ψ_λ are we going to accept as solutions? Before talking about the eigenvalues of A , it is necessary to decide just what class of functions are going to be allowed as eigenfunctions. This specification must usually be determined from the physics of the problem.

When $\psi_\lambda(v)$ is going to be used in the calculation of a particle density $N(v, t)$, almost the only physical restriction we can demand is that the corresponding detector response is bounded and nonnegative

$$0 \leq \int_0^\infty dv v \Sigma_d(v) \psi_\lambda(v) < \infty$$

This specific class of functions is referred to as a Banach class or space $\mathcal{L}_1$. Birkhoff¹ suggests that we consider an even more general class: “the space of all bounded σ -additive set functions defined on the Boolean σ -algebra of all Borel subsets of $v \in [0, \infty)$.”

But most of us are physicists and engineers, not mathematicians. Therefore we really are adept at manipulating only one class of functions, the class of all square-integrable functions $f(v)$ such that

$$\int_0^\infty dv |f(v)|^2 < \infty$$

[occasionally with a weighting function such as $M(v)$ included]. This class, of course, is just the Hilbert space of functions familiar from quantum mechanics. Hence even though physics demands a general function space such as a Banach space, mathematical convenience demands that we study

instead the eigenvalues of operators A defined on a Hilbert space of functions. We trust that most of the results we obtain for such a function space will not be altered appreciably for a more general class of functions. To this end, we begin with a definition.

Definition. Let $\mathcal{L}_2$ be the class of all complex-valued, square-integrable (in the Lebesgue sense) functions $f(v)$ defined on $v \in [0, \infty)$. Furthermore define an inner product of two functions $f(v)$ and $g(v)$ as

$$(f, g) \equiv \int_0^\infty dv f^*(v) g(v)$$

and a corresponding norm as $\|f\| = (f, f)^{1/2}$. The class of functions $\mathcal{L}_2$, when equipped with an inner product, is an example of a Hilbert space of functions.

Now we study the spectral theory of operators that act on functions contained in this Hilbert space. First we summarize some rather general concepts from the theory of Hilbert spaces.²⁻⁶

Linear Operators on Hilbert Spaces □

Definition. A Hilbert space $\mathfrak{H}$ is (i) a linear vector space over the complex field, (ii) a metric space whose metric is defined from an inner product: $\|f\| = (f, f)^{1/2}$, and (iii) a complete space (containing the limits of all Cauchy sequences).

i Properties of functions $f \in \mathfrak{H}$.

- (a) The *norm* of a function $f \in \mathfrak{H}$ is given by $\|f\| = (f, f)^{1/2}$.
- (b) Two functions f and $g \in \mathfrak{H}$ are said to be *orthogonal* if $(f, g) = 0$.
- (c) Two useful inequalities are

$$\begin{aligned} |(f, g)| &\leq \|f\| \|g\| && \text{Schwartz inequality} \\ \|f + g\| &\leq \|f\| + \|g\| && \text{Minkowski inequality} \end{aligned}$$

ii Convergence of sequences of functions $f \in \mathfrak{H}$.

- (a) A sequence of functions f_n converges *weakly* to a function f , denoted by $f_n \rightarrow f$, if (i) $\|f_n\| < \infty$, $\|f\| < \infty$, (ii) $\lim_{n \rightarrow \infty} f_n(x) = f(x)$ (componentwise convergence), (iii) $\|f_n\| < c$ for all n (uniform boundedness of norms). For a weakly convergent sequence, $f_n \rightarrow f$, and any $g \in \mathfrak{H}$, we have $(f_n, g) \rightarrow (f, g)$.
- (b) A sequence of functions f_n converges *strongly* to a function f , denoted by $f_n \rightarrow f$, if for all $n > N(\epsilon)$, we have $\|f_n - f\| < \epsilon$.

- (c) A sequence of functions f_n is said to converge in the *Cauchy sense* if given an $\epsilon > 0$, there exists an $N(\epsilon)$ such that if $n, m > N$, then $\|f_n - f_m\| < \epsilon$. (Note that strong convergence $\Leftrightarrow$ Cauchy convergence $\Rightarrow$ weak convergence, but weak convergence does *not* imply strong convergence.)

iii *Operators defined on a Hilbert space of functions.*

- (a) An *operator* A is a mapping of the function space $\mathfrak{F}$ into $\mathfrak{F}$.
 (b) A *functional* (at least as we use the concept) is a mapping of the function space $\mathfrak{F}$ into the scalar field.
 (c) The *domain* of an operator A , $\mathfrak{D}(A)$, is defined to be the class of all functions for which Af is defined.
 (d) The *range* of an operator A , $R(A)$, is the set of functions generated by letting A act on all functions $f \in \mathfrak{D}(A)$.
 (e) We define the *norm* of an operator as $\|A\| = \max\{\|Af\|/\|f\| : f \in \mathfrak{D}(A)\}$.
 (f) An operator A is *bounded* if $\|A\| < c$.
 (g) We define the *adjoint* $A^\dagger$ of an operator A by requiring that

$$(A^\dagger f, g) = (f, Ag) \quad \text{for all } f \in \mathfrak{D}(A), \quad g \in \mathfrak{D}(A^\dagger)$$

- (h) An operator A is *self-adjoint* if $A^\dagger = A$.
 (i) An operator A is *normal* if $A^\dagger A = AA^\dagger$.
 (j) An operator is *closed* if for $f_n, f \in \mathfrak{D}(A)$, $f_n \rightarrow f \Rightarrow Af_n \rightarrow Af$ and $\mathfrak{D}(A)$ is dense in $\mathfrak{F}$.
 (k) An operator A is *completely continuous* or *compact* if for $f_n, f \in \mathfrak{D}(A)$, $f_n \rightarrow f \Rightarrow Af_n \rightarrow Af$, and $\mathfrak{D}(A)$ is dense in $\mathfrak{F}$. (As an alternative definition, A is “compact” if it transforms every infinite bounded set into a compact set. Hence a compact operator is kind of a “smoothing” operator. Notice that a compact operator is tamer than a closed operator, since the former turns a weakly convergent sequence into one that converges strongly, whereas a closed operator merely ensures that a strongly convergent sequence will remain strongly convergent when acted on by the operator.)
 (l) To define the *inverse* of an operator A , consider the equation $Af = g$. Then we say that the inverse A^{-1} exists if for *any* g contained in the range $R(A)$, there exists a unique f such that $Af = g$ —that is, we can solve $Af = g$ uniquely for f for any $g \in R(A)$.

With this background involving functions and operators defined on a Hilbert space, we can proceed to study the eigenvalue problem $A\psi_\lambda = \lambda\psi_\lambda$.

The Spectral Theory of Operators Defined on $\mathfrak{H}$ □ The spectral theory of operators is approached in an indirect manner by considering the inhomogeneous problem

$$(A - \lambda)f = g \quad (\text{E.1})$$

and looking for the values of λ for which we have trouble inverting $(A - \lambda)$ to solve for f . The values of λ for which this inhomogeneous problem is “singular” make up the eigenvalue “spectrum” of the operator A . First consider those values of λ for which everything is well behaved—that is, the set of all λ for which we can invert $(A - \lambda)$ to find f with no difficulty. This set of “nice” λ is called the *resolvent set* and is defined formally as follows.

- i *Resolvent set* $\rho(A)$. The set of all λ for which
 - (a) $(A - \lambda)^{-1}$ exists.
 - (b) $(A - \lambda)^{-1}$ is a bounded operator.
 - (c) The closure of the range of $A - \lambda$, $R(A - \lambda) \equiv \mathfrak{H}$

All the rest of the complex λ -plane is defined to be in the *spectrum* of the operator A . From the three conditions necessary for λ to be in the resolvent set $\rho(A)$, we can see that there are three possible ways a point can fail to be in $\rho(A)$ —hence three types of spectrum corresponding to each of the ways in which the inhomogeneous problem of Eq. E.1 might be singular.

- ii *The spectrum* $\sigma(A)$. The set of all $\lambda \notin \rho(A)$. We can decompose $\sigma(A)$ into three disjoint sets:
 - (a) The *point spectrum* $\sigma_p(A)$. Those λ for which $(A - \lambda)^{-1}$ does not exist.
 - (b) The *continuous spectrum* $\sigma_c(A)$. Those λ for which $(A - \lambda)^{-1}$ exists, and the closure of $R(A - \lambda) \equiv \mathfrak{H}$, but $(A - \lambda)^{-1}$ is an unbounded operator.
 - (c) The *residual spectrum* $\sigma_r(A)$. Those λ for which $(A - \lambda)^{-1}$ exists, but $R(A - \lambda)$ is a proper subset of $\mathfrak{H}$.

Several comments are useful at this point to clarify these concepts. First note that all these sets are disjoint (since the definitions are mutually exclusive) and that $\rho \cup [\sigma_p \cup \sigma_c \cup \sigma_r] = C$ (the entire complex plane).

The point spectrum corresponds to what we have been calling “discrete” or “point” eigenvalues, since if $(A - \lambda)^{-1}$ does not exist for some λ , this implies that there must be a nontrivial ψ_λ such that $A\psi_\lambda = \lambda\psi_\lambda$. Actually, only $\lambda \in \sigma_p(A)$ are referred to as “eigenvalues” of A , but we will use the expression “continuous eigenvalues” from time to time.

The continuous spectrum does not correspond to the condition $A\psi_\lambda = \lambda\psi_\lambda$ and, indeed, reflects the unboundedness of $(A - \lambda)^{-1}$. Actually, the terms “point” and “continuous” are misleading because we see that the concept of a point or continuous set of λ does *not* enter into their definition. In fact it is possible to have a “point” eigenvalue in the midst of a continuous spectrum (an “embedded” eigenvalue) and a $\lambda \in \sigma_c(A)$ that is an isolated point (e.g., an eigenvalue of infinite multiplicity). Most of the time, however, $\sigma_p(A)$ corresponds to a point set and $\sigma_c(A)$ corresponds to a continuous set.

As we have noted, for $\lambda \in \sigma_c(A)$ there are no solutions ψ_λ to $A\psi_\lambda = \lambda\psi_\lambda$ that are contained in the Hilbert space. However there are solutions to this equation that lie outside the space but involve singularities such as delta functions or weak divergences (e.g., the singular eigenfunctions of Case). Hence whenever we loosely refer to the “eigenfunctions” corresponding to the continuous spectrum, we are talking about functions that are not contained in $\mathfrak{H}$ but may prove useful in expanding functions that are contained in $\mathfrak{H}$.

The residual spectrum $\sigma_r(A)$ usually does not arise in transport theory applications (fortunately). Our transport operators usually possess enough “symmetry” to avoid having a residual spectrum. This recognition stems from a theorem:² if $\lambda_1 \in \sigma_r(A)$, then $\lambda_1 \in \sigma_p(A^\dagger)$. On the other hand, if $\lambda^* \in \sigma_p(A^\dagger) \Rightarrow \lambda \in \sigma_p(A)$, then $\sigma_r(A)$ is empty.

Occasionally one encounters the term “essential spectrum” in the literature. This refers to the continuous spectrum, eigenvalues of infinite multiplicity, embedded eigenvalues, and limit points of isolated eigenvalues.

How do we go about determining whether a given point λ is in the point, continuous, or residual spectrum of an operator? There are several useful tests.

- i To determine whether λ is in the *spectrum* of A . Consider a sequence of functions $\{\varphi_\delta\} \in \mathfrak{D}(A)$ such that $\|\varphi_\delta\| \geq c > 0$ and $\varphi_\delta \rightarrow 0$. Then if

$$\|(A - \lambda)\varphi_\delta\| \rightarrow 0 \quad \text{as } \delta \rightarrow 0$$

we can conclude that $\lambda \in \sigma(A)$.

- ii To determine whether λ is in the *continuous spectrum* of A . Consider a sequence of functions $\{\varphi_\delta\} \in \mathfrak{D}$ such that $\|\varphi_\delta\| \geq c > 0$ and $\varphi_\delta \rightarrow 0$. Then if

$$\|(A - \lambda)\varphi_\delta\| \rightarrow 0 \quad \text{as } \delta \rightarrow 0$$

we conclude that $\lambda \in \sigma_c(A)$. (Notice that to demonstrate that a point is in the continuous spectrum, we must construct a test sequence that is weakly convergent. Without the weak convergence, all we

can say is that a point λ is in the spectrum of A .) This test is sometimes referred to as the *Weyl criterion*.⁵

- iii To determine whether λ is in the *point spectrum* of A , just demonstrate that there exist nontrivial solutions $\psi_\lambda \in \mathfrak{H}$ to

$$A\psi_\lambda = \lambda\psi_\lambda$$

- iv To determine whether there is a *residual spectrum*, apply the theorem mentioned earlier[i.e., check to see whether $\lambda^* \in \sigma_p(A^\dagger)$ implies that $\lambda \in \sigma_p(A)$]. (Notice that this implies that self-adjoint and normal operators have no residual spectrum.)
- v A self-adjoint operator possesses a real spectrum $\sigma = \sigma_p \cup \sigma_c$.
- vi A completely continuous (compact) operator has only a point spectrum. (In this sense, a compact operator is the direct analogue to a matrix.)
- vii A completely continuous self-adjoint or normal operator possesses only a point spectrum, and it also is characterized by a complete, orthonormal set of eigenfunctions (provided we include the “null space” corresponding to the eigenvalue $\lambda = 0$).
- viii *The Weyl–von Neumann Theorem*.⁵ If a compact, self-adjoint operator B is added to a closed operator A , the continuous spectrum of A remains unaltered: $\sigma_c(A + B) = \sigma_c(A)$.

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