THE UNIVERSITY OF MICHIGAN

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THE THEORY OF NEUTRON SLOWING DOWN IN NUCLEAR REACTORS

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PREFACE

In this book, one small facet of nuclear reactor design is considered - the slowing down (or moderation) of neutrons from the high energies with which they are born in fission to the energies at which they ultimately are absorbed. In conjunction with the study of neutron moderation, however, some remarks must of necessity be made concerning the calculation of reactor criticality, for the raison d'être of slowing-down calculations (or experiments) is to provide information for criticality calculations. A criticality calculation is the computation of the amount of fuel and/or geometrical configuration required to bring a chain reacting system to steady state operation.

It is true that reactors can be built - and indeed have been built - with neither slowing down, criticality, nor almost any other type of calculation having been performed. But the present demands of nuclear power plant performance no longer permit this engineering lèsé majesté. Today reactors fall into three broad categories: experimental reactors, built to obtain information for future designs; high performance propulsion or auxiliary power systems (as for submarines, rocket engines, or satellites); and plants for the production of commercial power.

The first of these, the experimental reactor, while possibly amenable to slipshod design, must be analyzed rather carefully once it is operating, or else the sought-after information, which the reactor was built to obtain, will not be forthcoming. The second type clearly

must be designed to high performance specifications including maximum power production and minimum weight and size, while the third type of plant, that designed to produce commercial power, must be optimized from the point of view of economics. In every case sophisticated mathematical techniques for the analysis of the reactor system are called into play, and the history of the world's atomic energy program since the end of the World War II includes a not insignificant portion devoted to the development of these techniques.

The names of the many scientists who contributed to the development of the methods described in subsequent chapters of this book could never be enumerated. However, the authors would like to recognize particularly the many contributions of Dr. Henry Hurwitz, Jr., and Dr. Alvin Weinberg, to whom this book is dedicated.

The authors would also like to thank the many people who made this book possible. This book was first written as lecture notes for an ASEE-AEC Summer Institute at The University of Michigan in the summer of 1959; the reactor physics portion of the course was taught by the authors and Mr. Sidney Yip, whose contribution to this work is quite significant. Thanks for aid at this phase of the work are due to the sponsors of the institute, the "students", who acted as guinea pigs for the first draft, and to Mrs. Beverly Doane and Miss Linda Berns who did the typing. Later this book was much expanded as a doctoral dissertation for one of the authors (Joel H. Ferziger). At this stage, we were deeply indebted not only to Professor R. K. Osborn and Professor K. M. Case for their invaluable comments, but also to Professors H. J. Gomberg, J. S. King, and K. M. Siegel who acted on

the doctoral committee, to Dean Ralph A. Sawyer who made this work possible, and to Miss Hariett L. Gluckstein,* who as the typist also made an excellent editor. Finally, the authors want to express their thanks to Pergamon Press Inc., the publisher, whose patience has been nearly inexhaustible.

* Now Mrs. Joel H. Ferziger.

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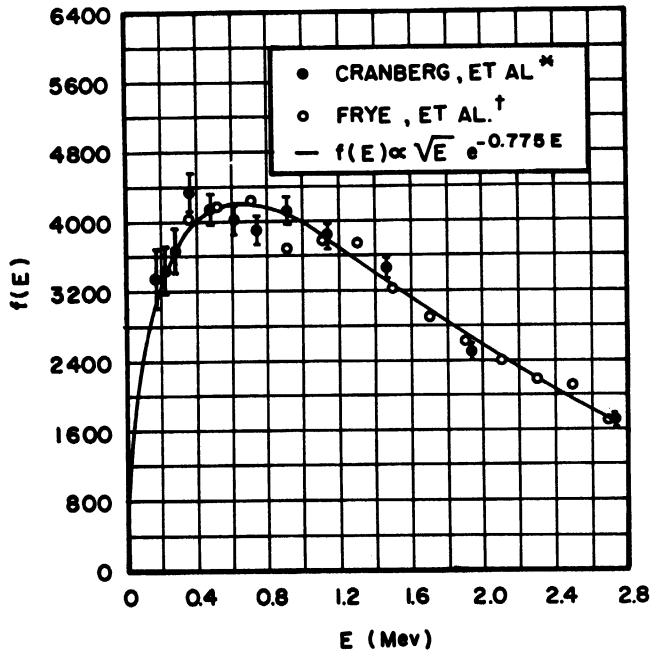
A. The Role of Slowing Down

1. The Need for Neutron Moderation

In all reactor designs, the mean energy of the neutrons which cause fission is lower than the energy with which neutrons are born as fission neutrons. (The fission spectrum of U-235 is shown in Figure 1, and has a mean value of 1.98 mev. The spectra of other fissionable isotopes is not too different.)

In some reactors (called fast reactors) the mean fission energy is very high - sometimes above 100 kev. In such reactors, neutron slowing down is accomplished primarily by inelastic scattering in the fuel and structural materials of the reactor core; a smaller contribution comes from elastic and inelastic scattering by the coolant (usually a liquid metal, e.g., sodium). In other reactor types the mean energy of the fission-inducing neutrons may range anywhere from that of a fast reactor down to the mean energy associated with the thermal motion of the atoms of the materials comprising the reactor core (kT, at 20° C = 0.0253 ev.). This last type of reactor is called a thermal reactor, while those in which the mean energy of fission inducing neutrons is between those of thermal and fast reactors are intermediate reactors. This distinction is, of course, arbitrary, but is nevertheless a useful guide.

In order to construct an intermediate reactor, one needs only to add quantities of light elements (e.g., hydrogen, deuterium, beryllium,



*The dotted points are from Lawrence Canberg and Norris G. Nereson, Fission Neutron Spectrum of U-235 from 0.2 to 3 Mev (Los Alamos Scientific Laboratory, LA-1916 [May, 1955]).

+The triangles are from Glenn M. Frye, Jr., Juanita H. Gammel, and Louis Rosen, Energy Spectrum of Neutrons from Thermal Neutron Fission of U-235 and from an Untamped Multiplying Assembly of U-235 (Los Alamos Scientific Laboratory, LA-1670 [May, 1954]).

Figure I-1 Fission Spectrum of U-235 Obtained from Time-of-Flight Experiments, After Weinberg and Wigner. p. 113

and carbon or their compounds) called moderators to the core of a fast reactor. Elastic collisions between the neutrons and the moderator nuclei degrade the energy of the neutrons before fissions occur. The more moderator one adds, the lower the mean energy of fission inducing neutrons will be (see Figure 2).

Generally speaking, the energy spectrum of neutrons in a reactor has the following characteristics. In all reactor types the neutron population is high near the fission spectrum energies. In fast reactors, the neutron population falls off at lower energies, although there are always some neutrons at energies well below the fission spectrum. As moderator is added and elastic scattering becomes the predominant means of moderation, the neutron spectrum contains a larger proportion of intermediate (1 ev to 100 kev) neutrons. Any neutrons that survive long enough to reach thermal energies tend to diffuse towards equilibrium with the moderator and hence towards a Maxwellian spectrum, which is

$$M(E) = \frac{2\pi}{(\pi kT)^{3/2}} E^{1/2} e^{-E/kT} \qquad (1.1)$$

where $M(E)dE$ is the number of neutrons with energies between E and E + dE, k is Boltzmann's constant and T is the absolute temperature. Addition of sufficient moderator makes the reactor thermal; the neutron spectrum still shows a peak near fission spectrum energies; it has approximately a "1/E" shape at intermediate energies and closely approximates a Maxwellian spectrum (Equation (1.1))at thermal energies. Most of the fissions are induced by the neutrons in the Maxwellian component.

After a certain point, the introduction of more moderator only dilutes the fuel concentration without slowing the neutrons down any

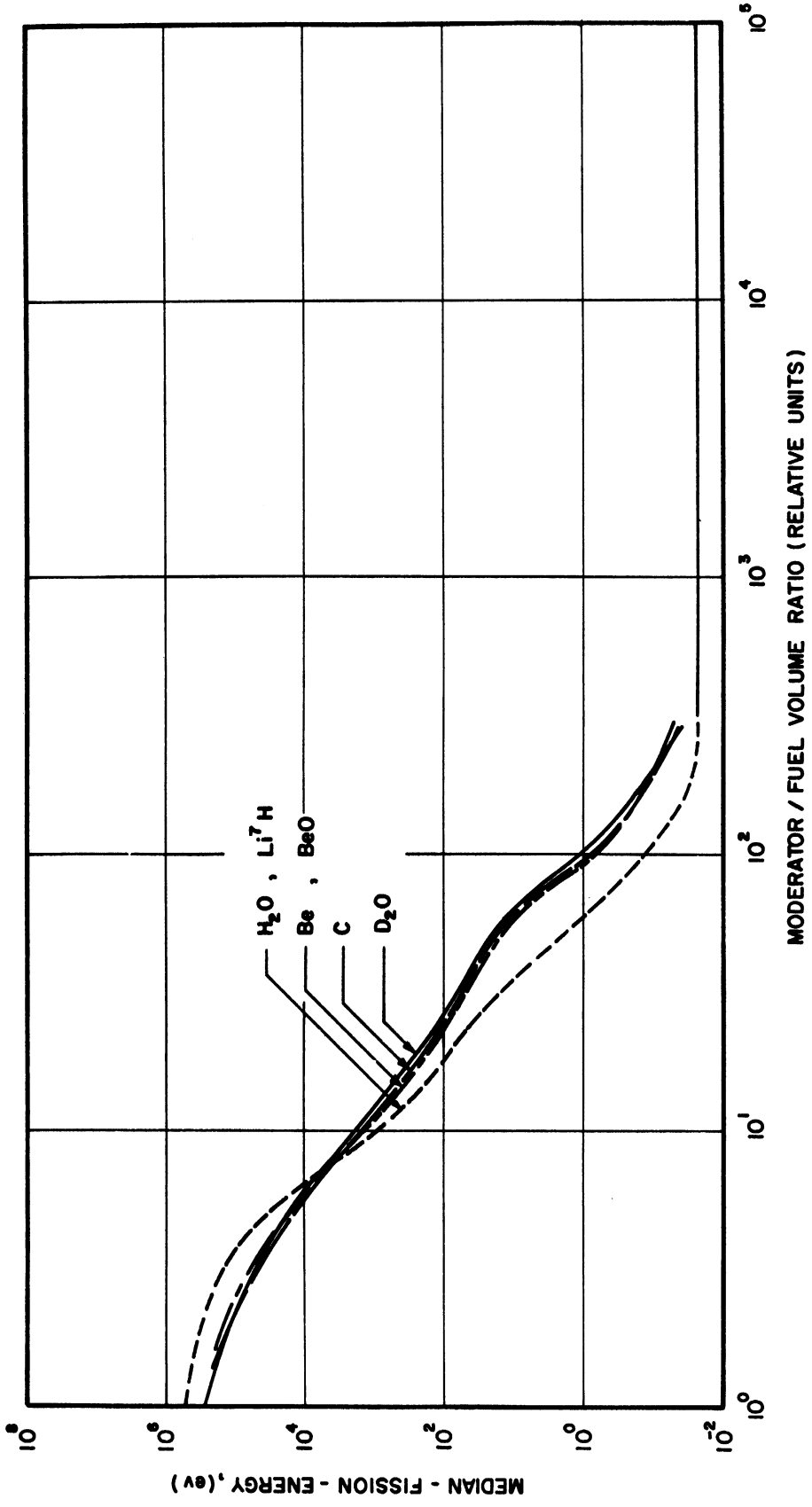


Figure I-2 Variation of Median Fission Energy with Moderator to Fuel Ratio, Adapted from Rand Corp. Report RM-2280 by B. Pinkus and G. Young.

further (see Figure 3). This results from the fact that neutrons cannot be moderated to a spectrum lower than that of Equation (1-1). In practice, the thermal neutron spectrum is actually somewhat shifted toward higher energies than the Maxwellian because the presence of neutron sources and sinks prevents the neutrons from attaining a true equilibrium distribution.[1]

The advantage of decreasing the mean neutron fission energy is that the microscopic fission cross section (a measure of the probability of a fission event occurring, defined in the next section) of U-235 (and of other fissionable isotopes as well) is, in the large, a decreasing function of energy (see Figure 4). Thus, as the mean fission energy decreases, the fuel loading necessary to maintain the chain reaction decreases (compare Figures 2 and 3). This saving in fuel is of more importance in reactors designed to produce economic power than in high performance propulsion and/or auxiliary power reactors. However, as was pointed out previously, even in fast reactors, which contain no moderator, some neutron moderation does occur, and must be taken into account if a proper design is to be obtained.

Because much of the cost of nuclear power is directly attributable to the fuel (including fuel fabrication costs, reprocessing costs, and inventory charges) thermal reactors, which have the lowest fuel loading, are most practical for commercial power purposes at present. Such reactors also have the tremendous advantage that they alone can be fueled with natural uranium (containing 0.7% U-235). At higher

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[1] Wigner, E. P. and J. E. Wilkins, Jr., Report AECD-2275, (1944).

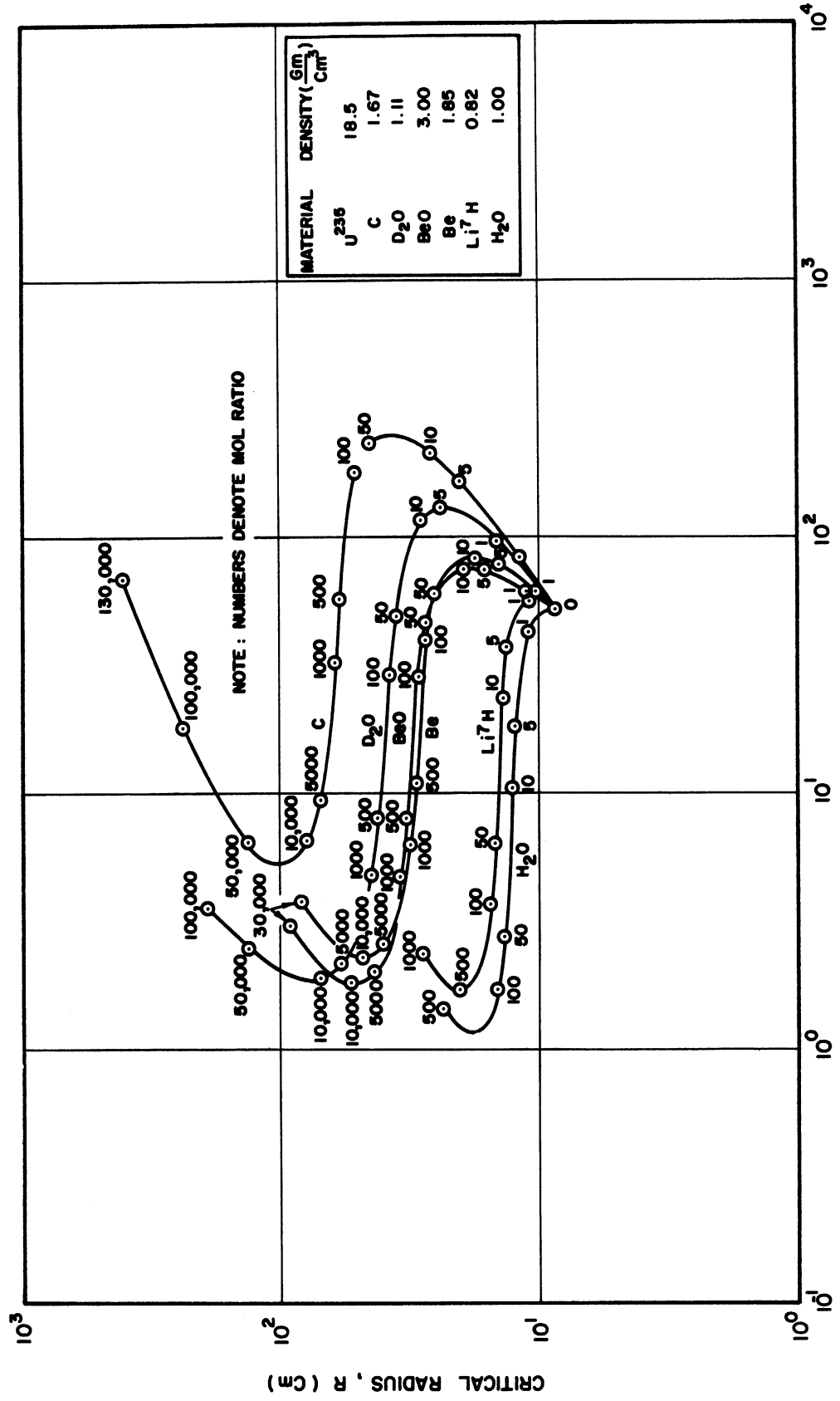

Figure I-3 Relationship Between Size and Fuel (Uranium) Investment Required for Criticality, Adapted from Rand Corp. Report RM-2280 by B. Pinkus and G. Young.

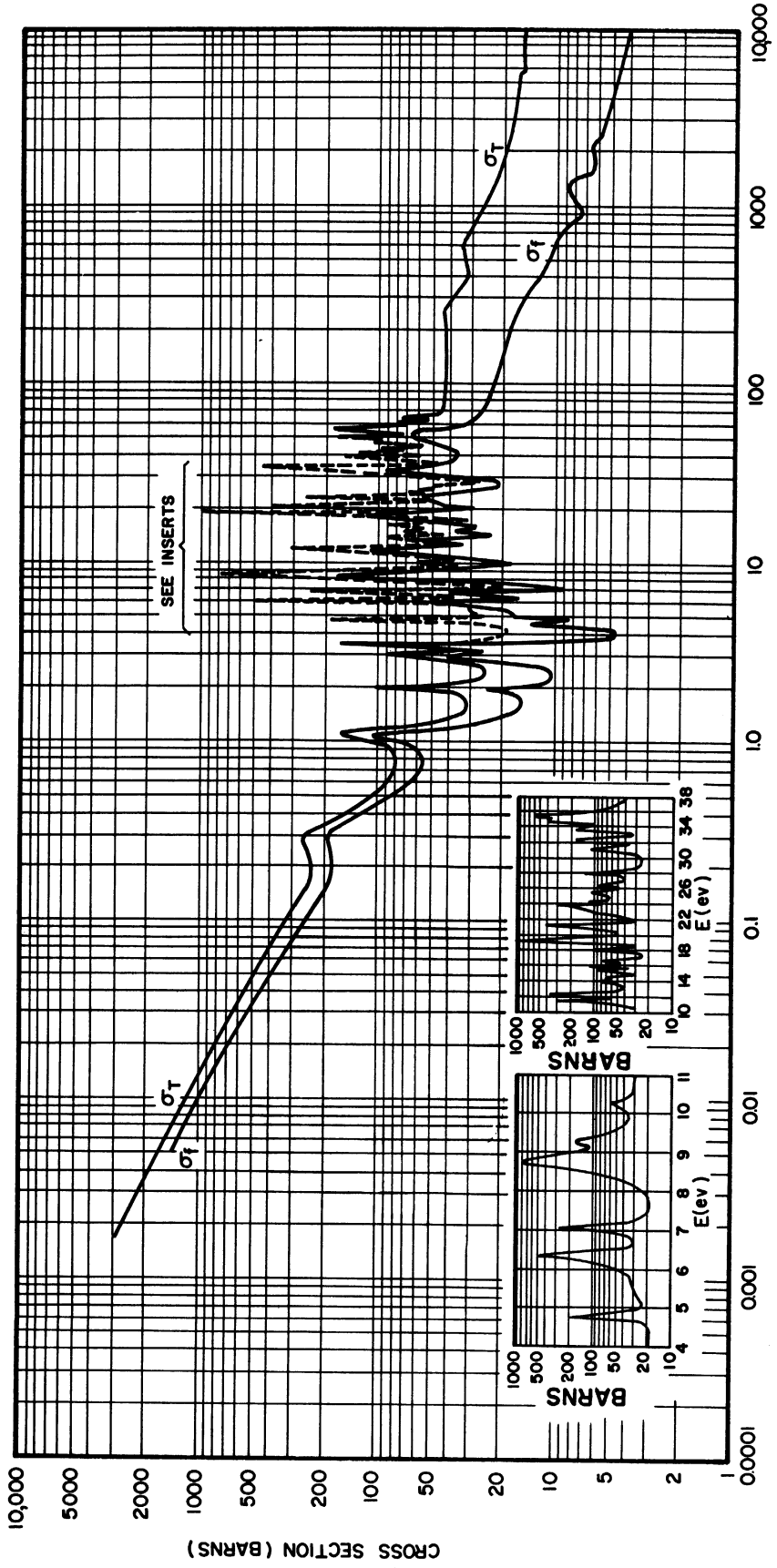

Figure I-4 Total (σ_T) and Fission (σ_f) Cross-Section of U-235 at Low Energies.

neutron energies, the fission cross section of U-235 is too low compared with the absorption cross section of the U-238 (99.3%) to maintain a chain reaction in natural uranium. Since natural uranium is far less expensive than enriched (> .7% U-235) fuel, the possibility of using natural uranium fuel should be exploited whenever feasible. In many nations enriched fuel is unavailable, so this choice is reduced to a necessity.

Balanced against this is the fact that reprocessing and fuel fabrication costs are so high that long burn-up is desirable. Clearly, enriched fuel will last longer than unenriched fuel, although the conversion of U-238 by neutron capture and two subsequent beta decays into Pu-239, a fissionable isotope, increases the lifetime of reactors containing U-238. In fact, in some designs, more fissionable isotope is produced than is destroyed, in which case one speaks of breeding.* In practical reactor design, all of these considerations must be taken into account, and the associated problems of analysis are quite formidable.

The discussion of this section has attempted to point out that the problems of neutron moderation are important in all types of reactors. In the rest of the book a mathematical description of the slowing-down process is given, with particular emphasis on the problems encountered in the design of thermal reactors. This is done because of the greater mathematical elegance possible in treating such reactors (i.e., those

* Only fast reactors can breed Pu-239 from U-235 because the ratio of fission to capture cross sections in U-235 is too low at thermal and intermediate energies to permit breeding. However, U-233 can be bred from Th-232 even in a thermal reactor, but here too the advantage is greater in a fast reactor.

in which slowing down is predominantly due to elastic scattering). Many of the methods may be applied to any reactor type, however, as will be discussed in Chapter IV.

B. The Mathematical Description of the Neutron Density in a Reactor

2. The Boltzmann Equation

As has probably become clear by now, the primary problem of reactor physics is the prediction of the conditions under which a given reactor configuration will be critical. The most general manner of solving this problem is to set up an equation which describes the time behavior of the neutron population in a reactor and to determine the conditions necessary for the existence of a steady state.* This equation is a simple statement of neutron conservation and is usually called the Boltzmann Equation, and sometimes the Transport Equation. The derivation given here will be rather brief.

We define the angular neutron flux $\Phi(\underline{r}, E, \underline{\Omega}, t)$ relative to a fixed set of coordinates such that the number of neutrons in the volume element d^3r (= dxdydz) at $\underline{r}$ with energies between E and E + dE and with velocity vectors in the solid angle element $d\underline{\Omega}$ ($\sin\theta\, d\theta d\phi$) about the unit vector $\underline{\Omega}$ at time t is given by

$$n(\underline{r}, E, \underline{\Omega}, t) = \frac{1}{v(E)} \Phi(\underline{r}, E, \underline{\Omega}, t) d^3r\, dE\, d\underline{\Omega} \qquad (1\text{-}2a)$$

Here v(E) is the speed of a neutron of energy E:

$$v(E) = \left(\frac{2E}{m}\right)^{1/2} \qquad (1\text{-}2b)$$

* Some non-steady state problems are treated in Appendix A.

where m is the neutron mass, so that the velocity of the neutron is given by

$$\underline{v}(E) = \underline{\Omega} v(E) \qquad (1\text{-}2c)$$

To obtain the Boltzmann equation, we consider the conservation of those neutrons which are in a small volume element d^3r, whose energies are between E and E + dE and whose velocities are directed in $d\underline{\Omega}$ about $\underline{\Omega}$. The expression of neutron conservation obtained must apply for every $\underline{r}$, every E and every $\underline{\Omega}$ (see Figure 5).

If we consider the neutron balance in a small time interval Δt, we must have

Change of neutron density during Δt (in $d^3r\ dE\ d\underline{\Omega}$) = Sources - Sinks (in $d^3r\ dE\ d\underline{\Omega}\ \Delta t$)

The change of neutron density during Δt is

$$\frac{\partial}{\partial t}\left[\frac{\Phi(\underline{r},E,\underline{\Omega},t)}{v(E)}\, d^3r\, dE\, d\underline{\Omega}\right]\Delta t$$

for sufficiently small Δt. Thus:

$$\frac{1}{v}\frac{\partial}{\partial t}\left[\Phi(\underline{r},E,\underline{\Omega},t)\right] d^3r\, dE\, d\underline{\Omega}\, \Delta t = \text{Sources} - \text{Sinks} \quad (\text{in } d^3r\, dE\, d\underline{\Omega}\, \Delta t) \qquad (1\text{-}3)$$

Consider the right-hand side of the above equation. The sinks include two terms:

(1) Any neutron-nuclear interaction will, by definition, change the energy and/or direction of the neutron involved and hence remove the neutron from dE or $d\underline{\Omega}$ or both and the neutron will thus

be lost to the region under consideration. In order to calculate this term, it will be necessary to introduce the concept of cross section.

We define the microscopic cross-section for an event of type i* (e.g., scattering, absorption, or fission) in the following manner. Consider a fictitious target containing one target atom/cm^3 with a cross-sectional area of one cm^2. If a neutron beam is directed normal to the target such that I_o neutrons enter the target each second (see Figure 6) then the number of events of type i occurring between x and x + dx will be $\sigma_i I(x)\, dx$. Here x is the distance from the surface and I(x) is the uncollided neutron intensity reaching the plane at x. Mathematically

$$dI(x) = -\sigma_i\, I(x)\, dx \tag{1-4a}$$

Solving Equation (1-4a), we have

$$I(x) = I_o e^{-\sigma_i x} \tag{1-4b}$$

For a target containing N nuclei/cm^3, we have

$$I(x) = I_o e^{-\Sigma_i x} \tag{1-4c}$$

where

$$\Sigma_i = N\sigma_i \tag{1-4d}$$

Σ_i is called the macroscopic cross section. An important quantity is the probability per unit path, for small paths, that a neutron will suffer a collision of the type i. This is clearly given by

* Subscripts (i) will be a, absorption; c, capture; f, fission; s, scattering; t, total; and tr, transport (defined later). Superscripts will denote the fact that a particular nuclide is referred to, e.g., σ_a^u represents the absorption cross section of uranium.

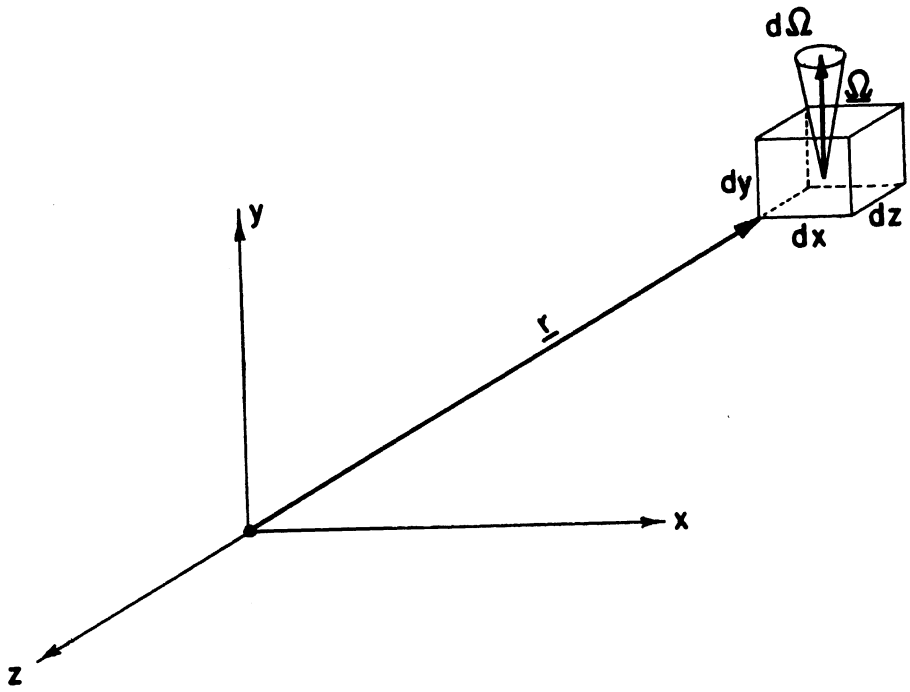

Figure I-5 Coordinates for Boltzmann Equation.

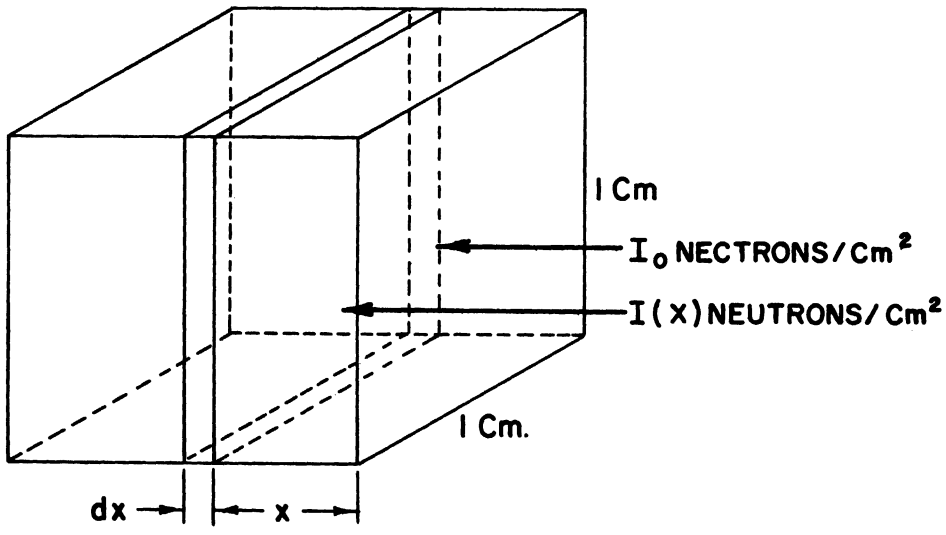

Figure I-6 Attenuation of Neutrons in a Slab.

$$\frac{1}{I(x)} \frac{I(x) - I(x+dx)}{dx} = -\frac{d}{dx} \ln I(x) = \Sigma_i \quad (1\text{-}4e)$$

when only events of type i are considered to remove neutrons from the beam. The mean free path, i.e., the expected distance a neutron will travel before suffering a collision of type i is Σ_i^{-1}.

The total number of neutron-nuclear events in d^3r per second will be the product of $\Sigma_t = \sum_i \Sigma_i$ with the total path length traveled by all neutrons in $d^3r\, d\underline{\Omega}\, dE$ per second. Since a neutron of speed v travels v centimeters in one second, this path length is just

$$v\, n(\underline{r}, E, \underline{\Omega}, t)\, d^3r\, dE\, d\underline{\Omega} = \Phi(\underline{r}, E, \underline{\Omega}, t)\, d^3r\, dE\, d\underline{\Omega}$$

and the required number of events is:

$$\Sigma_t(r, E)\, \Phi(\underline{r}, E, \underline{\Omega}, t)\, d^3r\, dE\, d\underline{\Omega}\, \Delta t \quad (1\text{-}4f)$$

(2) Neutrons which flow or leak from d^3r without collision in time Δt. Since the number of neutrons in $d\underline{\Omega}$ entering a small element $\underline{ds}$ of the surface in time Δt are those in the cylinder whose height $v\Delta t$ and whose cross section is $\underline{\Omega} \cdot \underline{ds}$ (see Figure 7), the net leakage can be written

$$\left[\int_S \underline{\Omega} \cdot \underline{ds}\, \Phi(\underline{r}, E, \underline{\Omega}, t)\right] d\underline{\Omega}\, dE\, dt = \text{Leakage}$$

where S is the surface of d^3r. Applying the divergence theorem we have

$$\left[\int \nabla \cdot (\underline{\Omega}\, \Phi(\underline{r}', E, \underline{\Omega}, t)\, d^3r'\right] d\underline{\Omega}\, dE\, dt = \text{Leakage}$$

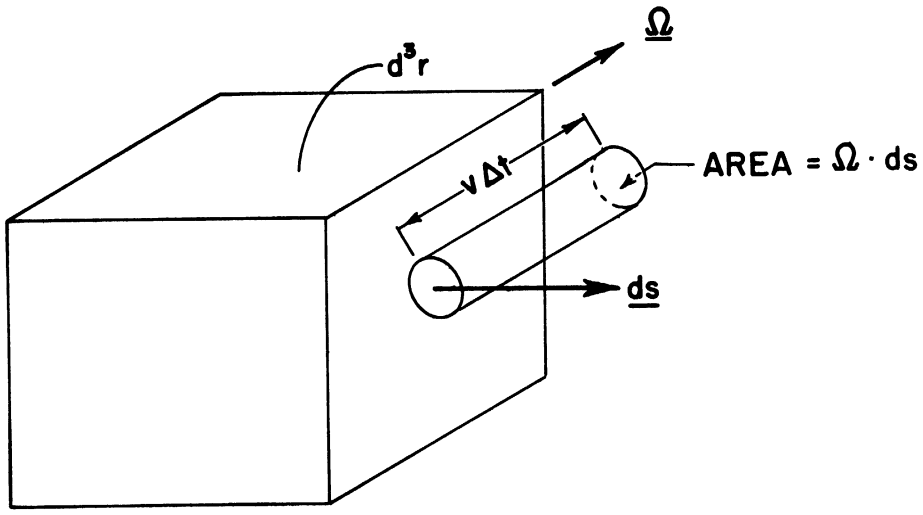

Figure I-7 Geometry for Calculation of Neutron Leakage.

where now the integration is over the interior of d^3r. If d^3r is small enough, the integral may be approximated by

$$\nabla \cdot \underline{\Omega}\, \Phi(r, E, \underline{\Omega}, t) d^3r\, d\underline{\Omega} dE \Delta t$$

or, applying a vector identity, this becomes

$$\underline{\Omega} \cdot \nabla \Phi(r, E, \underline{\Omega}, t)\, d^3r\, d\underline{\Omega}\, dE \Delta t \qquad (1\text{-}5)$$

since $\underline{\Omega}$ is independent of $\underline{r}$. If we consider the balance we are setting up as one in a phase space with coordinates x, y, z, v_x, v_y, v_z and volume element

$$d\tau = d^3r\, dE\, d\underline{\Omega}$$

(1-4f) represents the loss of neutrons in the velocity space without change in the space coordinates; while (1-5) represents the loss of neutrons in configuration space without change in the velocity coordinates.

We now consider the sources required in Equation (1-3). These also consist of two terms:

(1) Direct ("virgin") sources of neutrons - those produced, for example, by fission or by the (γ,n) reaction on deuterium or beryllium. We define a function $S(\underline{r}, E, \underline{\Omega}, t)$ such that

$$\text{Direct source (in } d^3r dE d\underline{\Omega}\, \Delta t) = S(\underline{r}, E, \underline{\Omega}, t)\, d^3r dE d\underline{\Omega}\, \Delta t \qquad (1\text{-}6)$$

(2) Scattering in of neutrons from other energies and/or other directions into $dE d\underline{\Omega}$. Here, we define a scattering function $F(E' \rightarrow E, \underline{\Omega}' \rightarrow \underline{\Omega})$ such that this term is given by

$$\text{Scattering in} = \int dE' \int d\underline{\Omega}' \, \Sigma_s(\underline{r}, E') \Phi(\underline{r}, E', \underline{\Omega}', t) F(E' \to E, \underline{\Omega}' \to \underline{\Omega}) \quad (1\text{-}7)$$
$$d^3r \, dE \, d\underline{\Omega} \, dt$$

from which it may be seen that $F(E' \to E, \underline{\Omega}' \to \underline{\Omega}) d\underline{\Omega} dE$ represents the probability that a neutron which was scattered with energy E' and while traveling in direction $\underline{\Omega}'$ have an energy between E and E + dE and direction in $d\underline{\Omega}$ about $\underline{\Omega}$ after that collision.

Subsituting the source and sink terms (1-4f), (1-5), (1-6) and (1-7) into the balance relation (1-3) and eliminating the common differentials, we have the Boltzmann Equation:

$$\frac{1}{v} \frac{\partial \Phi(\underline{r}, E, \underline{\Omega}, t)}{\partial t} = S(\underline{r}, E, \underline{\Omega}, t) + \int dE' \int d\underline{\Omega}' \, \Sigma_s(\underline{r}, E') \Phi(\underline{r}, E', \underline{\Omega}', t) F(E' \to E, \underline{\Omega}' \to \underline{\Omega}) - \underline{\Omega} \cdot \nabla \Phi(\underline{r}, E, \underline{\Omega}, t) - \Sigma_t(\underline{r}, E) \Phi(\underline{r}, E, \underline{\Omega}, t) \quad (1\text{-}8)$$

In this derivation, the possibility of neutron-neutron interactions has been neglected. The justification for this lies in the fact that neutron densities are normally no greater than about 10^9 per cm^3 whereas atomic densities are of the order of 10^{22} per cm^3.

3. An Alternate Form of the Boltzmann Equation

For some purposes, the form (1-8) of the Boltzmann equation will be most convenient, while for others, it will be rather clumsy. In particular, the scattering-in term, which is really a slowing down term,* is rather difficult to treat in general; a particular functional form must be obtained for the scattering frequency, $F(E' \to E, \underline{\Omega}' \to \underline{\Omega})$ before any calculations can be carried out.

Instead of writing the slowing-down contribution to the angular flux $\Phi(\underline{r}, E, \underline{\Omega}, t)$ in terms of the angular flux prior to the last collision, we can formulate it in terms of the sources at other energies and positions. To do this we must first define the slowing-down kernel, $P(\underline{r}' \to \underline{r}, E' \to E, \underline{\Omega}' \to \underline{\Omega}, t' \to t)$ such that $P(\underline{r}' \to \underline{r}, E' \to E, \underline{\Omega}' \to \underline{\Omega}, t' \to t) d^3r dE d\underline{\Omega} \Delta t$ is the probability that a neutron which was born at time t' at point $\underline{r}'$ in the reactor with energy E', with velocity in direction $\underline{\Omega}'$ will appear in (or in the case of fast neutrons, be slowed down into) the energy range dE about E in d^3r about $\underline{r}$ while traveling in direction $d\underline{\Omega}$ about $\underline{\Omega}$ in the time interval Δt at t. Then the slowing-down or scattering-in contribution to $\Phi(\underline{r}, E, \underline{\Omega}, t)$ may be written as*

$$\int_R d^3r' \int dE' \int d\underline{\Omega}' \int_{-\infty}^{\infty} dt' \; S(\underline{r}', E', \underline{\Omega}', t') \, P(\underline{r}' \to \underline{r}, E' \to E, \underline{\Omega}' \to \underline{\Omega}, t' \to t)$$

and the Boltzmann Equation is then written as

$$\frac{1}{v} \frac{\partial \Phi}{\partial t} + \underline{\Omega} \cdot \underline{\nabla} \Phi + \Sigma_t \Phi = S + \int_R d^3r' \int dE' \int d\Omega' \int_{-\infty}^{t} dt' \; S(\underline{r}', E', \underline{\Omega}', t') \, P(\underline{r}' \to \underline{r}, E' \to E, \underline{\Omega}' \to \underline{\Omega}, t' \to t)$$

Throughout this book we shall be interested only in critical reactors, i.e., those in which a time independent neutron population is possible. Furthermore, the only neutron source considered, except for a brief discussion of non-critical systems, will be fission, in which case the source is proportional to the neutron density. Thus, the basic

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* It is possible to incorporate the direct source contribution $S(\underline{r}, E, \underline{\Omega})$ into this term if desired. This is mostly a matter of taste, but as formulated here the function P will have greater mathematical simplicity.

problem of the book will be one of solving a homogeneous linear integro-differential equation for the time independent neutron flux $\Phi(\underline{r}, E, \underline{\Omega})$ with the boundary condition (for a finite convex assembly) that no neutrons enter the system from the surroundings:

$$\Phi(\underline{r}_s, E, \underline{\Omega}) = 0 \qquad (1\text{-}10)$$

at all points $\underline{r}_s$ on the boundary if $\underline{\Omega}$ points into the body (i.e., for $\underline{\Omega} \cdot \underline{n} < 0$ where $\underline{n}$ is a unit normal to the surface). This leads to an eigenvalue problem which will yield a time-independent solution only for certain combinations of the physical parameters and geometry of the system. The determination of this relationship (the critical condition) in terms of the yet unknown slowing-down kernel will be the major interest of the first part of this chapter. Reduction of Equation (1-9) to the time-independent case is readily carried out by setting

$$\Phi(\underline{r}, E, \underline{\Omega}, t) = \Phi(\underline{r}, E, \underline{\Omega})$$

which is constant in time. Then Equation (1-9) becomes, since the source is also time independent,

$$\underline{\Omega} \cdot \nabla \Phi(\underline{r}, E, \underline{\Omega}) + \Sigma_t(\underline{r}, E)\Phi(\underline{r}, E, \underline{\Omega}) = S(\underline{r}, E, \underline{\Omega})$$

$$+ \int_R d^3r' \int dE' \int d\underline{\Omega}' \, S(\underline{r}', E', \underline{\Omega}') \, P(\underline{r}' \to \underline{r}, E' \to E, \underline{\Omega}' \to \underline{\Omega}) \qquad (1\text{-}11)$$

where the new kernel is defined by

$$P(\underline{r}' \to \underline{r}, E' \to E, \underline{\Omega}' \to \underline{\Omega}) = \int_{t'=0}^{t} dt' \, P(\underline{r}' \to \underline{r}, E' \to E, \underline{\Omega}' \to \underline{\Omega}, t' \to t)$$

This new kernel is time-independent since the time-dependent kernel may be expected to depend only on the time interval t-t'. Thus, the

integration over t' may be converted into an integration over a new variable, $\tau = t - t'$, with limits zero and infinity, which plainly has no time dependence. The new kernel represents the probability per unit volume, energy and $\underline{\Omega}$, that a neutron born with energy E' and direction $\underline{\Omega}'$ at $\underline{r}'$ will appear with energy E and direction $\underline{\Omega}$ at $\underline{r}$.

The difference between the two forms of the Boltzmann Equation (1-8) and (1-9) is, of course, only a formal one. Equation (1-9) proves to be more amenable to the extraction of a general critical condition (in terms of the slowing down kernel P), but the derivation of the slowing down kernel is extremely difficult and can generally be carried out in terms of the scattering frequency. On the other hand, the scattering frequency F is readily derived from existing cross section data. Hence our program will be first to develop a critical condition (to some approximation) from Equation (1-9) and then to calculate the slowing down kernel in terms of the scattering frequency (again, to some approximation).

In treating time-dependent problems it is frequently assumed that the time behavior is exponential, say e^{-st}, and that the neutron flux is separable into the product of a function of time and a function of the other variables.[2] This procedure effectively adds a term s/v to the total cross section. The problem can then be treated formally as a time independent problem, except that s is to be determined rather than a critical condition derived.

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[2] See, for example, B. Davison, Neutron Transport Theory Oxford 1955 .

4. The Total Neutron Flux and Current

As it stands, Equation (1-9) is difficult to solve; indeed, analytical solutions have been found only for a few special cases. These, however, will be useful as standards for comparison of any approximations that we may develop to treat more general cases. As a starting point, we may note that in an infinite, homogeneous medium with uniform, isotropic neutron sources (such as fission), the angular flux must be isotropic since there exists no preferred direction in space. At a reactor-vacuum interface as in a bare (unreflected) reactor the boundary condition (1-10) must be obeyed; thus the angular flux will be grossly anisotropic there. Physically, this anisotropy can be expected to be propagated into the system up to a few mean free paths from the surface. When the reactor becomes very large with respect to a mean free path (as is usually required for criticality*) the flux far from the boundary is almost isotropic. Thus, as a starting point we may say that the angular flux is almost isotropic throughout the reactor; hence we shall deal only with large reactors for the present. It would be folly to assume an isotropic flux, as it can predict no net neutron transport. Thus, in order to account for neutron flow out of the system, calculations in a finite assembly require an anisotropic component of the angular flux. The simplest representation of such a component is an expansion in spherical harmonics up to the first order (using the first four

* Since only slightly greater than two neutrons are released per absorption of a neutron in U-235, no more than half of these can be allowed to leak out if the system is to be critical. In turn, this requires that the system be several mean free paths thick, since a neutron generally makes many collisions before it is absorbed.

harmonics), which may be written compactly as

$$\underline{\Phi}(\underline{r},E,\underline{\Omega}) = \frac{\phi_0(\underline{r},E)}{4\pi} + \frac{3}{4\pi}\,\underline{\phi}_1(\underline{r},E)\cdot\underline{\Omega} \qquad (1\text{-}12a)$$

The second term is equivalent to an expansion in the three spherical harmonics of order unity:

$$\underline{\phi}_1\cdot\underline{\Omega} = \sum_{m=-1}^{+1} \phi_{1m}(\underline{r},E)\,Y_1^m(\underline{\Omega}) \qquad (1\text{-}12b)$$

where the $Y_\ell^m(\underline{\Omega})$ are the normalized spherical harmonics

$$Y_\ell^m(\underline{\Omega}) = \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}}\;P_\ell^m(\mu)\,e^{im\varphi} \qquad (1\text{-}12c)$$

and the $P_\ell^m(\mu)$ are the associated Legendre Polynomials.[3] An expression of the form (1-12b) is possible because the components of a unit vector can be written in terms of the $Y_1^m(\Omega)$:

$$\begin{aligned}
\Omega_x &= \sin\theta\cos\varphi = \sqrt{\frac{4\pi}{3}}\left[Y_1^1(\underline{\Omega}) + Y_1^{-1}(\underline{\Omega})\right] \\
\Omega_y &= \sin\theta\sin\varphi = \sqrt{\frac{4\pi}{3}}\,i\left[Y_1^1(\underline{\Omega}) - Y_1^{-1}(\underline{\Omega})\right] \qquad (1\text{-}12d) \\
\Omega_z &= \cos\theta = \sqrt{4\pi}\,Y_1^0(\underline{\Omega})
\end{aligned}$$

Before applying (1-12a), it will be informative to inquire as to the physical meaning of the quantities $\phi_0(\underline{r})$ and $\underline{\phi}_1(\underline{r})$.

First we define the <u>total neutron flux</u> (usually simply called the flux), $\phi(\underline{r}, E)$ such that $\phi(\underline{r},E)\,d^3r\,dE$ is the sum of the path lengths travelled per second by all neutrons with energies between E and E+dE

[3] For definitions and properties of these functions, see any of the standard mathematical texts, for example, E. T. Whittaker and G. N. Watson <u>Modern Analysis</u>, Oxford, 1927 .

contained within a volume element d^3r at $\underline{r}$.* Since $\Phi(\underline{r}, E, \underline{\Omega})$ is the path length of those neutrons traveling in directions $d\underline{\Omega}$ aboout $\underline{\Omega}$, this quantity is

$$\phi(\underline{r},E) = \int d\underline{\Omega}\, \Phi(\underline{r},E,\underline{\Omega}) \equiv n(\underline{r},E)\, v(E) \qquad (1\text{-}13a)$$

where $n(\underline{r},E)$ is the density of neutrons per unit volume at $\underline{r}$ per unit energy at E, and v(E) is the neutron speed defined by Equation (1-2b). By integration of Equation (1-12a) over $\underline{\Omega}$ we find

$$\phi(\underline{r},E) \equiv \phi_o(\underline{r},E) \qquad (1\text{-}13b)$$

since**

$$\int d\underline{\Omega} = 4\pi \qquad (1\text{-}13c)$$

$$\int \underline{A}\cdot\underline{\Omega}\, d\underline{\Omega} = 0 \qquad (1\text{-}13d)$$

for any constant vector $\underline{A}$.

Secondly, we define the angular neutron current $\underline{j}(\underline{r},E,\underline{\Omega})$ such that

$$\underline{j}(\underline{r},E,\underline{\Omega})\cdot d\underline{s}\, dE\, d\underline{\Omega} \qquad (1\text{-}14a)$$

represents the number of neutrons per second which cross area element $\underline{ds}$ located at $\underline{r}$ with energies in dE about E and velocities in $d\underline{\Omega}$ about $\underline{\Omega}$. By using the artifice used in the derivation of the Boltzmann Equation, namely considering all neutrons in the cylinder of volume $(v\underline{\Omega}\cdot ds)$ as crossing $\underline{ds}$ in one second, we find that this term is also:

$$\Phi(\underline{r},E,\underline{\Omega})\,(\underline{\Omega}\cdot d\underline{s})\,dE\,d\underline{\Omega}$$

---

* Then $\Sigma_t(\underline{r})\phi_o(\underline{r})$ is the total reaction rate per unit volume at $\underline{r}$ for neutrons with energies in dE. Cf. Equation (1-4f).

**Proof of these and the vector identities to follow are given in Appendix B.

so that comparison with the definition of $\underline{j}(\underline{r}, E, \underline{\Omega})$ gives:

$$\underline{j}(\underline{r}, E, \underline{\Omega}) = \underline{\Omega}\,\Phi(\underline{r}, E, \underline{\Omega}) = \underline{v}\, n(\underline{r}, E, \underline{\Omega}) \quad (1\text{-}14b)$$

By analogy to the total neutron flux we define the total neutron current (or simply the current) $\underline{J}(\underline{r}, E)$ so that

$$\underline{J}(\underline{r}, E) \cdot \underline{ds}\, dE \quad (1\text{-}14c)$$

represents the net number of neutrons which cross the area element $\underline{ds}$ at $\underline{r}$ per second with energies in dE about E. Clearly

$$\begin{aligned} \underline{J}(\underline{r}, E) &= \int d\underline{\Omega}\, \underline{j}(\underline{r}, E, \underline{\Omega}) \\ &= \int d\underline{\Omega}\, \underline{\Omega}\, \Phi(\underline{r}, E, \underline{\Omega}) \end{aligned} \quad (1\text{-}14d)$$

Multiplying Equation (1-12) by $\underline{\Omega}$ and integrating over $\underline{\Omega}$, we find

$$\underline{J}(r, E) \equiv \underline{\phi}_1(r, E) \quad (1\text{-}14e)$$

where the results

$$\int \underline{\Omega}\, d\underline{\Omega} = 0 \quad (1\text{-}14f)$$

and

$$\int d\underline{\Omega}\, \underline{A} \cdot \underline{\Omega}\, \underline{\Omega} = \frac{4\pi}{3} \underline{A} \quad (1\text{-}14g)$$

have been employed. This argument also shows that an isotropic flux would yield $\underline{J}(\underline{r}, E) = 0$ and hence no net neutron transport.

5. Reduction of the Boltzmann Equation

With these interpretations of the expansion coefficients in Equation (1-12), we are ready to insert the expansion into the Boltzmann Equation (1-8). A scalar equation may be obtained by integrating over all $\underline{\Omega}$:

$$\int d\underline{\Omega}\, \underline{\Omega}\cdot\nabla\Phi(\underline{r},E,\underline{\Omega}) + \Sigma_t(\underline{r},E)\int d\underline{\Omega}\,\Phi(\underline{r},E,\underline{\Omega}) = \int d\underline{\Omega}\, S(\underline{r},E,\underline{\Omega}) + \int d\underline{\Omega}\int dE' \int d\underline{\Omega}'\, \Sigma_s(\underline{r},E')\,\Phi(\underline{r},E',\underline{\Omega}')\,F(E'\to E,\underline{\Omega}'\to\underline{\Omega}) \quad (1\text{-}15a)$$

Inserting Equation (1-12) in the first term of Equation (1-15a) and applying (1-13d) and

$$\int d\underline{\Omega}\ (\underline{A}\cdot\underline{\Omega})(\underline{B}\cdot\underline{\Omega}) = \underline{A}\cdot\underline{B} \quad (1\text{-}15b)$$

(treating the gradient operator $\underline{\nabla}$ as a vector) we obtain just $\underline{\nabla}\cdot\underline{J}(\underline{r},E)$. The integral appearing in the second term on the left side of Equation (1-15a) is the definition of $\phi(\underline{r}, E)$ so that this term becomes $\Sigma_t(\underline{r}, E)\phi(r, E)$. Under the assumption of isotropic sources, the second term on the right hand side is simply

$$S_0(\underline{r},E) = \int S(\underline{r},E,\underline{\Omega})\,d\underline{\Omega} = 4\pi S(\underline{r},E,\underline{\Omega}) \quad (1\text{-}15c)$$

In the first term on the right-hand side of Equation (1-15a) the integral

$$\int d\underline{\Omega}\ F(E'\to E,\underline{\Omega}'\to\underline{\Omega}) \quad (1\text{-}15d)$$

occurs. In most cases, anisotropies due to crystalline effects are absent and the scattering frequency $F(E'\to E,\ \Omega'\to\Omega)$ is rotationally invariant; that is, it depends only on the angle between $\underline{\Omega}'$ and $\underline{\Omega}$ (i.e., only on $\underline{\Omega}'\cdot\underline{\Omega} = \mu$) and not on $\underline{\Omega}'$ and $\underline{\Omega}$ individually:

$$F(E'\to E,\underline{\Omega}'\to\underline{\Omega}) = F(E'\to E,\underline{\Omega}'\cdot\underline{\Omega})$$

Then the integral (1-15d) will be independent of $\underline{\Omega}'$ and it is possible

to write:*

$$\int d\underline{\Omega}\, F(E' \to E, \underline{\Omega}' \cdot \underline{\Omega}) = F_0(E \to E) \qquad \text{(1-15e)}$$

which is the zeroth moment of the scattering frequency. The remainder of the second term on the right-hand side of Equation (1-15d) is

$$\int dE'\, F_0(E' \to E)\, \Sigma_s(\underline{r}, E') \int d\underline{\Omega}'\, \Phi(\underline{r}, E', \underline{\Omega}')$$

which, in light of the definition of $\phi(\underline{r}, E)$ becomes

$$\int dE'\, F_0(E' \to E)\, \phi(\underline{r}, E)\, \Sigma_s(\underline{r}, E') \qquad \text{(1-15f)}$$

Combining all of these results, Equation (1-15a) can be rewritten as:

$$\underline{\nabla} \cdot \underline{J}(\underline{r}, E) + \Sigma_t(\underline{r}, E)\, \phi(\underline{r}, E) = \int dE'\, \Sigma_s(\underline{r}, E')\, \phi(\underline{r}, E')\, F_0(E' \to E) + S(\underline{r}, E) \qquad \text{(1-15g)}$$

Another equation between $\phi(\underline{r}, E)$ and $\underline{J}(\underline{r}, E)$ is obtained by multiplying Equation (1-9) by $\underline{\Omega}$ before integrating.

$$\int d\underline{\Omega}\, \underline{\Omega} \cdot \underline{\nabla} \Phi(\underline{r}, E, \underline{\Omega}) + \Sigma_t(\underline{r}, E) \int d\underline{\Omega}\, \underline{\Omega}\, \Phi(\underline{r}, E, \underline{\Omega}) = \int d\underline{\Omega}\, \underline{\Omega}\, S(\underline{r}, E, \underline{\Omega})$$

$$+ \int \underline{\Omega}\, d\underline{\Omega} \int dE' \int d\underline{\Omega}'\, \Sigma_s(\underline{r}, E')\, \Phi(\underline{r}, E', \underline{\Omega}')\, F(E' \to E, \underline{\Omega}' \cdot \underline{\Omega}) \qquad \text{(1-16a)}$$

The source term is seen to vanish in light of the assumed isotropy of $S(\underline{r}, E, \underline{\Omega})$ and Equation (1-14f), while the first term is readily evaluated by means of Equation (1-14g) and the identity:

$$\int d\underline{\Omega}\, (\underline{A} \cdot \underline{\Omega})(\underline{B} \cdot \underline{\Omega})\underline{\Omega} = 0 \qquad \text{(1-16b)}$$

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* Physically, $F_0(E' \to E)dE$ is the probability that a neutron scattered at E' will have an energy in dE about E after the collision.

with $\underline{\nabla}$ again treated as a vector: the result is $(1/3)\,\underline{\nabla}\,\phi(r,E)$. The integral in the second term on the left is just the definition of $\underline{J}(\underline{r}, E)$. Now the last term on the right-hand side contains the integral

$$\int d\underline{\Omega}\;\underline{\Omega}\;F(E'\to E, \underline{\Omega}'\cdot\underline{\Omega}) \qquad (1\text{-}16c)$$

where the rotational invariance already assumed is explicitly exhibited. This integral must be a vector proportional to $\underline{\Omega}'$, since $\underline{\Omega}$ is integrated out. Call the result $A\underline{\Omega}'$. Then, taking the scalar product of (1-16c) with $\underline{\Omega}'$, we obtain (note that $\underline{\Omega}' \cdot \underline{\Omega}' = 1$ since $\underline{\Omega}'$ is a unit vector):

$$A = \int d\underline{\Omega}\;\underline{\Omega}\cdot\underline{\Omega}'\,F(E'\to E, \underline{\Omega}\cdot\underline{\Omega}') \equiv F_1(E'\to E) \qquad (1\text{-}16d)$$

which cannot depend on $\underline{\Omega}'$ as a result of the assumed rotational invariance of $F(E'\to E,\ \underline{\Omega}'\to\underline{\Omega})$.* Thus,

$$\int d\underline{\Omega}\;\underline{\Omega}\;F(E'\to E, \underline{\Omega}'\cdot\underline{\Omega}) = \underline{\Omega}'\,F_1(E'\to E) \qquad (1\text{-}16e)$$

and the triple integral (1-16a) reduces to

$$\int dE'\,\Sigma_s(r,E')\,F_1(E'\to E)\int d\underline{\Omega}'\,\underline{\Omega}'\,\Phi(r,E,\underline{\Omega}') = \int dE'\,\Sigma_s(r,E')\,\underline{J}(r,E')\,F_1(E'\to E) \qquad (1\text{-}16f)$$

where the definition of $\underline{J}(\underline{r}, E)$, Equation (1-14d) has been used. Equation (1-16a) can now be written in the following form:

$$\frac{1}{3}\underline{\nabla}\,\phi(r,E) + \Sigma_t(r,E)\,\underline{J}(r,E) = \int \Sigma_s(r,E')\,\underline{J}(r,E')\,F_1(E'\to E)\,dE' \qquad (1\text{-}16g)$$

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* Unfortunately $F_1(E'\to E)$, the first moment of the scattering function, does not have the simple physical significance that the zeroth moment $F_0(E'\to E)$ has.

6. Thermal Neutrons

At thermal neutron energies, i.e., those energies of the same order as the energies associated with the thermal motion of the atoms of the media in which the neutron are diffusing, neutrons gain or lose energy in collisions with nuclei with roughly equal probability. Certainly, the behavior of neutrons with thermal energies is considerably different than that of high energy (fast) neutrons, which lose energy in every collision with a nucleus. Of course, there is no really clear-cut energy at which a neutron can be said to be transformed from a fast neutron into a thermal neutron, but the distinction is an intuitively clear one and a "cutoff", above which a neutron is a fast neutron and below which it is a "thermal" neutron, can generally be chosen without introducing a great deal of error.[4] Since this book will deal with the behavior of fast neutrons almost exclusively, the treatment of thermal neutrons will be disposed of now. The approximations introduced will make it possible to relate the basic problem of reactor criticality to calculations involving only fast neutrons. Equations (1-15g) and (1-16g) will provide the starting point in our treatment of thermal neutrons. Before proceeding, we define the thermal neutron flux:

$$\phi_T(\underline{r}) = \int_0^{E_T} \phi(\underline{r}, E)\, dE \qquad (1\text{-}17a)$$

[4] A convenient cutoff is that energy above which the neutron has no appreciable probability of gaining energy in a collision; this definition will be adopted here. The determination of this energy and many other problems concerning thermal neutrons, which are but briefly mentioned in this book, are discussed at great length by N. Corngold in his book Neutron Thermalization, to be published. Other material may be found in some of the work of M. Nelkin.

the thermal neutron current:

$$\underline{J}_T(\underline{r}) = \int_0^{E_T} \underline{J}(\underline{r}, E)\, dE \qquad (1\text{-}17b)$$

and the thermal average total macroscopic cross section:

$$\Sigma_{t_T}(\underline{r}) = \frac{\int_0^{E_T} \Sigma_t(\underline{r}, E)\, \phi(\underline{r}, E)\, dE}{\int_0^{E_T} \phi(\underline{r}, E)\, dE} \qquad (1\text{-}17c)$$

with similar definitions for the thermal average absorption, fission, and scattering cross sections. Integrating Equation (1-15f) from $E = 0$ to $E = E_T$, and noting that fission produces essentially no neutrons at thermal energies, we obtain:

$$\int_0^{E_T} \nabla \cdot \underline{J}(\underline{r}, E)\, dE + \int_0^{E_T} \Sigma_t(\underline{r}, E)\, \phi(\underline{r}, E)\, dE = \int_0^{E_T} dE \int_0^{\infty} \Sigma_s(\underline{r}, E')\, \phi(\underline{r}, E')\, F_0(E' \to E)\, dE' \qquad (1\text{-}18a)$$

The first term is simply the divergence of the thermal current $\nabla \cdot \underline{J}_T(\underline{r})$, since we expect $\underline{J}(\underline{r}, E)$ to be sufficiently well behaved to allow interchange of the integration and divergence operations. The second term is easily evaluated using definition (1-17c) and is $\Sigma_{t_T}(\underline{r})\, \phi_T(\underline{r})$, the thermal collision density or the total number of thermal neutron-nuclear interactions per second per unit volume at $\underline{r}$. Only the term on the right-hand side causes any difficulty. To treat that term, we first decompose it as follows:

$$\int_0^{E_T} dE \int_0^{\infty} dE'\, \Sigma_s(\underline{r}, E')\, \phi(\underline{r}, E')\, F_0(E' \to E) = \int_0^{E_T} dE \int_0^{E_T} dE'\, \Sigma_s(\underline{r}, E')\, \phi(\underline{r}, E')\, F_0(E' \to E) + \int_0^{E_T} dE \int_{E_T}^{\infty} dE'\, \Sigma_s(\underline{r}, E')\, \phi(\underline{r}, E')\, F_0(E' \to E) \qquad (1\text{-}18b)$$

In the first term on the right-hand side of Equation (1-18b), consider first the integral

$$\int_0^{E_T} F(E' \to E) dE$$

which is the probability that a thermal neutron which has scattered (note the limits on the E' integral) will remain within the thermal group after that collision. Now E_T can be chosen such that the number of neutrons with energies less than E_T which scatter to energies above E_T is vanishingly small. Clearly, the optimum choice of E_T will be the lowest energy for which this statement holds to some desired approximation.[5] With this choice of E_T the above integral is unity by definition and the first term on the right hand side of Equation (1-18b) becomes:

$$\int_0^{E_T} \Sigma_S(\underline{r}, E) \phi(\underline{r}, E) dE = \Sigma_{ST}(\underline{r}) \phi_T(\underline{r}) \qquad (1\text{-}18c)$$

as a consequence of the definition of Σ_{ST}.

Returning to the last term of Equation (1-18b), we note that it represents physically the number of neutrons entering the thermal group due to collisions at higher energies. In order to obtain a more convenient form of the equation for thermal neutrons, we formally introduce a thermalization kernel $P_T(\underline{r}' \to \underline{r}, E', \underline{\Omega})$ defined such that

$$P_T(\underline{r}' \to \underline{r}, E', \underline{\Omega}) d\underline{\Omega}\, d^3r \qquad (1\text{-}19a)$$

is the expected number of neutrons traveling in directions in $d\underline{\Omega}$ about $\underline{\Omega}$ thermalized (i.e., entering the thermal group or, equivalently,

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[5] See N. Corngold, op. cit.

slowing down past E_T) in d^3r at $\underline{r}$ per neutron born isotropically with energy E' at $\underline{r}'$. Then

$$\int_R d^3r' \int_{E_T}^{\infty} dE' \, S_0(\underline{r}', E') \, P_{T_0}(\underline{r}' \to \underline{r}, E') \qquad (1\text{-}19b)$$

is the total number of neutrons thermalized per second per unit volume at $\underline{r}$ and is equal to the last term of Equation (1-18b) by physical identity. Here, $P_{T_0}(\underline{r}' \to \underline{r}, E')$ is the zeroth moment,

$$P_{T_0}(\underline{r}' \to \underline{r}, E') = \int P_T(\underline{r}' \to \underline{r}, E', \underline{\Omega}) \, d\underline{\Omega} \qquad (1\text{-}19c)$$

and S is the zeroth moment of the source. Hence, we arrive at the first thermal equation:

$$\underline{\nabla} \cdot \underline{J}_T(\underline{r}) + \Sigma_{a_T}(r) \phi_T(\underline{r}) = \int_R d^3r' \int dE' \, S(\underline{r}', E') \, P_{T_0}(\underline{r}' \to \underline{r}, E') \qquad (1\text{-}20)$$

The adaptation of Equation (1-16g) to the thermal group proceeds in a like manner. Integration from E = 0 to $E = E_T$ yields:

$$\frac{1}{3} \int_0^{E_T} \underline{\nabla} \phi(\underline{r}, E) \, dE + \int_0^{E_T} \Sigma_t(\underline{r}, E) \underline{J}(\underline{r}, E) dE = \int_0^{E_T} dE \int_0^{\infty} dE' \, \Sigma_s(\underline{r}, E') \underline{J}(\underline{r}, E') F_1(E' \to E) \qquad (1\text{-}21a)$$

The first term on the left-hand side is simply $\frac{1}{3} \underline{\nabla} \phi_T(\underline{r})$, again provided the functions are sufficiently well behaved to permit the interchange of operations. Consideration of the second term is delayed for the present. Again, the scattering-in term is decomposed.

$$\int_0^{E_T} dE \int_0^{\infty} dE' \, \Sigma_s(\underline{r}, E') \, \underline{J}(\underline{r}, E') \, F_1(E' \to E) =$$

$$\int_0^{E_T} dE \int_0^{E_T} dE' \, \Sigma_s(\underline{r}, E') \, \underline{J}(\underline{r}, E') F_1(E' \to E)$$

$$+ \int_0^{E_T} dE \int_{E_T}^{\infty} dE' \, \Sigma_s(\underline{r}, E') \, \underline{J}(\underline{r}, E') \, F_1(E' \to E) \qquad (1\text{-}21b)$$

In the first term of the right-hand side, the integral

$$\int_0^{E_T} F_1(E' \to E) dE = \int_0^{E_T} dE \int d\Omega \, (\underline{\Omega} \cdot \underline{\Omega}') F(E' \to E, \underline{\Omega}' \to \underline{\Omega})$$

is encountered. From the definition of $F(E' \to E, \underline{\Omega}' \to \underline{\Omega})$, this term is seen to be the average value of $\mu = \underline{\Omega} \cdot \underline{\Omega}'$ for neutrons which scatter while traveling in direction $\underline{\Omega}'$ with energy E'. We denote this quantity by $\bar{\mu}(E')$. The remaining integral over E' may be combined with the second term on the left-hand side of Equation (1-21a) and after defining the transport cross section by

$$\Sigma_{tr}(\underline{r}, E) = \Sigma_t(\underline{r}, E) - \Sigma_s(\underline{r}, E) \, \bar{\mu}(\underline{r}, E) \qquad (1\text{-}21c)$$

we have

$$\int_0^{E_T} \left(\Sigma_t(\underline{r}, E) - \Sigma_s(\underline{r}, E) \, \bar{\mu}(\underline{r}, E) \right) \underline{J}(\underline{r}, E) dE = \Sigma_{tr_T} \underline{J}(\underline{r}, E) \qquad (1\text{-}21d)$$

which defines the thermal average cross section $\Sigma_{tr_T}(\underline{r})$. Note that $\Sigma_{tr_T}(\underline{r})$ is obtained by averaging over the current as opposed to the flux averaging used for the other cross sections. The second term on the right-hand side of Equation (1-21b) can be expressed in terms of

the first Legendre moment $\underline{P}_{T1}(r' \rightarrow r, E')$ of the thermalization kernel $P_T(\underline{r}' \rightarrow \underline{r}, E', \underline{\Omega})$ just as the zeroth moment was introduced into Equation (1-20). In this fashion Equation (1-21b) reduces to

$$\frac{1}{3}\nabla \phi_T(r) + \Sigma_{tr_T} \underline{J}_T(r, E) = \int d^3r' \int dE' \, S(r', E') \underline{P}_{T_1}(r' \rightarrow r, E) \tag{1-21e}$$

Equations (1-20) and (1-21e) are then the two simultaneous (P_1) thermal group equations for the two unknowns -- the thermal flux and the thermal current.

7. The Thermal Diffusion Equation

The pair of equations (1-20) and (1-21e) (or the pair (1-15f) and (1-16g) from which Equations (1-20) and (1-21e) were obtained by specialization to the thermal group) are sometimes called the (consistent) P_1 approximation (see Chapter III, Section 5) because the angular flux was assumed to contain only the first order terms in a spherical harmonics expansion (i.e., Legendre Polynomials up to P_1). To obtain the thermal diffusion approximation it is necessary to approximate further by ignoring the integral term on the right hand side of Equation (1-21e).* If this is done we obtain Fick's Rule which is the basic equation of diffusion theory.

$$\underline{J}_T(r, E) = -D_T(r) \nabla \phi_T(r) \tag{1-21f}$$

Here D_T, the thermal diffusion coefficient, is defined by

$$D_T(r) = \frac{1}{3\Sigma_{tr_T}(r)} \tag{1-21g}$$

* Equivalently this assumes the neutron slowing down into the thermal group to be distributed isotropically. For a discussion of the error introduced by this neglect, see Appendix D.

The term "diffusion" arises out of the similarity of Equation (1-21f) to other diffusion equations, e.g., these encountered in the kinetic theory of gases. The more often quoted result

$$D_T(\underline{r}) = \frac{\int_0^{E_T} D(\underline{r},E)\phi(\underline{r},E)\,dE}{\int_0^{E_T} \phi(\underline{r},E)\,dE} \qquad (1\text{-}21h)$$

with

$$D(\underline{r},E) = [3\Sigma_{tr}(\underline{r},E)]^{-1}$$

is obtained only if the neutrons are assumed to obey Fick's Rule at every energy in the thermal region. The diffusion equation for thermal neutrons is then obtained by combining Equation (1-20) and (1-21f):

$$-\underline{\nabla}\cdot D_T(\underline{r})\underline{\nabla}\phi_T(\underline{r}) + \Sigma_{aT}(\underline{r})\phi_T(\underline{r}) = \int_R d^3r' \int dE' S(\underline{r},E') P_0(\underline{r}'\rightarrow\underline{r},E') \qquad (1\text{-}21i)$$

For assemblies in which the application of diffusion theory to the thermal neutron group is not valid, a "thermal transport equation" can be derived in the same manner as the thermal diffusion equation, i.e., by integrating the transport equation over the thermal group. This procedure again leads to the same two difficulties which appear in the derivation of the thermal diffusion equation:

a. Cross section averages over the angularly-dependent flux appear which means that unless the flux is separable in energy and angle the cross section becomes a function of direction. Alternatively, if one uses a spherical harmonics expansion of the angular flux, cross-sections appear averaged over the various spherical harmonics components of the flux, just, as in the case of the diffusion equation, the total cross section appears as a flux average while the transport cross section

is current averaged. This problem has never been answered satisfactorily and, indeed, may be the reason that higher order approximations to the Boltzmann Equation for thermal neutrons frequently provide less accurate answers than does diffusion theory. In the case of the diffusion equation, one can argue approximately to yield Equation (1-21h). In this case one finds $\Sigma_{tr_T} = < \lambda_{tr} >^{-1}$ where the bracket represents a flux average.

b. The other difficulty is in the higher order anisotropies associated with neutron slowing down into the thermal group. However, since (see Appendix D) it may be argued that these anisotropy terms are usually smaller than those terms included in the diffusion approximation, their neglect in higher order calculations is probably not a severe error.

C. Asymptotic Reactor Theory

8. The Asymptotic Reactor Model

It would be desirable to obtain a simple mathematical expression which would tell one when any reactor is critical, but unfortunately, this is impossible. However, one specific reactor class, for which the critical conditions can be formulated simply, does exist. This type of reactor called an "asymptotic reactor," is not a practical reactor design, but it is a useful first approximation to many reactors. We shall consider it in detail because it is a useful first approximation and it provides considerable insight into more complex and hence, more realistic, reactor designs. Critically calculations for actual reactors are generally done numerically by the methods discussed in Chapter IV,

but even in these calculations, frequent recourse is made to the results of the analytical theory.

An asymptotic reactor is defined as follows:

(a) The reactor is composed of a single, convex region in which all materials are distributed homogeneously.

(b) The reactor must be large compared to a neutron mean free path. This is generally a requirement for criticality, however (see footnote, p.20).

It would be natural, at this point, to question the assumption of homogeneity so off-handedly made above, in view of the fact that most reactors today consist of solid fuel elements, separate solid or liquid moderators, and, when the moderator is not also the coolant, a fluid coolant. However, if the dimensions of the inhomogeneities (fuel plates, coolant channels, etc.) are small compared to the mean free path of a neutron, the neutron "does not know" that the system is inhomogeneous and treatment of the system as homogeneous can be justified. If this is not true, but the inhomogeneities are periodic within the core, it is frequently possible to find a set of physical constants which yield the same overall reactor behavior (critical mass, outer dimensions, etc.) while destroying only the details of the neutron behavior within one periodic substructure (cell). For reactors which fall in neither of these categories, or vary in other ways from the simple model given below, analytical techniques of general applicability have not been developed and it is necessary to fall back upon the numerical methods to be described in Chapter IV.

The physical model of the neutron processes in an ideal thermal asymptotic reactor is as follows:

A fast neutron, born as a result of fission, suffers scattering events with moderator nuclei until it reaches an energy comparable to that of the moderator nuclei themselves. In the process of slowing down, neutrons may leak out or be absorbed but cannot cause fission. As long as a neutron is moving much faster than the moderator nucleus with which it collides, it will always lose energy in the collision; when the energies of the neutron and nucleus are comparable, i.e., when the neutron is in the thermal group, both loss and gain of energy are possible and the neutron diffuses at thermal energies until it is either leaks out or is absorbed, possibly to cause a fission.

It will be possible to treat fissions caused by neutrons at energies above E_T, without only slight loss of generality. This case is discussed in Appendix C. Some further restrictions will be required, but we shall reserve their application until the need for them is apparent.

9. Fission Sources

Up to now, the nature of the neutron source has been left unspecified. While it has been mentioned that fission is the only neutron source in a critical reactor, a general source has been retained for simplicity. In subcritical assemblies, which can have steady state neutron fluxes only when an "extraneous" (e.g., $P_o(\alpha,n)Be$) source is present, a more general source term is required. (During reactor start up such sources are almost always present.)

Returning to consideration of the fission sources, we first note that the number of fissions caused by neutrons with energies in dE about E per second in a volume element d^3r at $\underline{r}$ is

$$\Sigma_f (\underline{r}, E) \phi (\underline{r}, E) d^3r \, dE$$

so that the total fission rate per unit volume at $\underline{r}$ is

$$F(\underline{r}) = \int_0^\infty \Sigma_f (\underline{r}, E) \phi (\underline{r}, E) dE = \Sigma_{fT} \phi_T (\underline{r}) + \int_{E_T}^\infty \Sigma_f (\underline{r}, E) \phi (\underline{r}, E) dE \quad (1\text{-}22a)$$

where $\Sigma_{fT}(\underline{r})$ is the thermal fission cross section. If ν is the <u>mean number of neutrons produced per fission</u>* the number of neutrons produced in d^3r at $\underline{r}$ per second is just ν times either side of (1-22a).

Finally we define the <u>fission spectrum</u> f(E) such that f(E)dE is the probability that a fission neutron will have energy in dE about E. This function is given (for U-235) in Figure 1.[6] Then, the source in a critical reactor may be represented by

$$S(\underline{r}, E) = \nu f(E) \left[\Sigma_{fT} \phi_T (\underline{r}) + \int_{E_T}^\infty \Sigma_f (\underline{r}, E) \phi (\underline{r}, E) dE \right] \quad (1\text{-}22b)$$

The case of the general source given by Equation (1-24b) is discussed in Appendix D. In the remainder of this chapter we consider only the case in which all fissions occur at thermal energies so that the source becomes

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* ν is only slightly sensitive to the energy of the fission-inducing neutron and will be assumed constant. If it is not constant, one can treat $\nu\Sigma_f(E)$ as a "neutron production" cross section and carry through the same analysis without loss of generality.

6 It is frequently given by the semiempirical formula $f(E) = .484\, e^{-E} \sinh \sqrt{2E}$ (E in mev) which is called the Watt spectrum B. E. Watt, Phys. Rev., 87, 1037 (1952).

$$S(\underline{r},E) = \nu f(E)\Sigma_f \phi_T(\underline{r}) \qquad (1\text{-}22c)$$

Not all neutrons are emitted simultaneously with a fission event. Some are produced as a result of radioactive decay some time after the fission events responsible for creating them. These neutrons, called delayed neutrons, have no effect on criticality, since at steady state the ratio of delayed neutron production to prompt neutron (those produced simultaneously with a fission event) production is constant. Nor do they effect time dependent solutions of the type considered in Appendix A, which do not include fission sources. Only in a reactor in which the neutron population is changing in time are their effects important. In that case their effect is solely on the rate of increase of power level (i.e., on the time constants) and not on the direction in which the power level changes. Since we shall only be interested qualitatively in reactor kinetics, per se, delayed neutron effects may be ignored in this discussion.

10. The Asymptotic Reactor Equations

It was argued in an earlier section that in a large reactor, the angular neutron flux is nearly isotropic throughout a large portion of the reactor core. In such reactors, the system "looks" infinite to neutrons near the center, it might be possible to replace the slowing down and thermalization kernels (Equation (1-19a)) by the infinite medium kernels which we denote by subscript "∞". Since these kernels, in general, decrease rapidly with increasing source to field point distance, the integrals may be extended to all space, to a good

approximation. The question of defining a "neutron flux" outside of the reactor system is deferred until later.

The major point is that the slowing down and thermalization kernels for an infinite homogeneous medium have definite symmetry properties. In particular, they are functions of the vector $(\underline{r} - \underline{r}')$ only.* The proof of this is obtained by noting the invariance properties of the Boltzmann Equation for an infinite homogeneous medium; e.g., it is invariant under the transformation $\underline{r} \rightarrow \underline{r} - \underline{r}'$.

Under the approximation considered here, i.e., that all fissions take place at thermal energies and that the diffusion equation be used to describe the thermal flux, only the zeroth Legendre moment of $P_{\infty T}$, the infinite medium thermalization kernel averaged over a fission spectrum, is required. Since P_{∞_T} depends on $|\underline{r} - \underline{r}'|$ and $(\underline{r} - \underline{r}') \cdot \underline{\Omega}$,

$$P_{T\infty}(\underline{r}-\underline{r}') = \int d\underline{\Omega}\, P_{T\infty}(|\underline{r}-\underline{r}'|, (\underline{r}-\underline{r}')\cdot\underline{\Omega}) = \int d\underline{\Omega} \int dE'\, f(E') \cdot P_{T\infty}(|\underline{r}-\underline{r}'|, (\underline{r}-\underline{r}')\cdot\underline{\Omega}, E') \qquad (1\text{-}23a)$$

depends only on $|\underline{r} - \underline{r}'|$. In order to limit the number of subscripts, we will write $P_{\infty_{T_o}} = P_\infty$. We can now substitute (1-22a) and (1-23a) into (1-21c) to obtain the asymptotic reactor thermal diffusion equation

$$-\underline{\nabla} \cdot D_T(\underline{r})\underline{\nabla}\phi_T(\underline{r}) + \Sigma_{aT}(\underline{r})\phi_T(\underline{r}) = \nu \int \Sigma_{f_T}(\underline{r}')\phi_T(\underline{r}') P_\infty(|\underline{r}-\underline{r}'|)\, d\underline{r}' \qquad (1\text{-}23b)$$

or, if D_T, Σ_{a_T}, and Σ_{f_T} are not functions of $\underline{r}$

$$-D_T \nabla^2 \phi_T(\underline{r}) + \Sigma_{aT}\phi_T(\underline{r}) = \nu\Sigma_{f_T} \int \phi_T(\underline{r}') P_\infty(|\underline{r}-\underline{r}'|) d^3r' \qquad (1\text{-}23c)$$

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* In fact, because of rotational invariance, the kernels are functions of $|\underline{r} - \underline{r}'|$ and $(\underline{r} - \underline{r}') \cdot \underline{\Omega}$ only. This fact will be used when it is needed (see Figure 8).

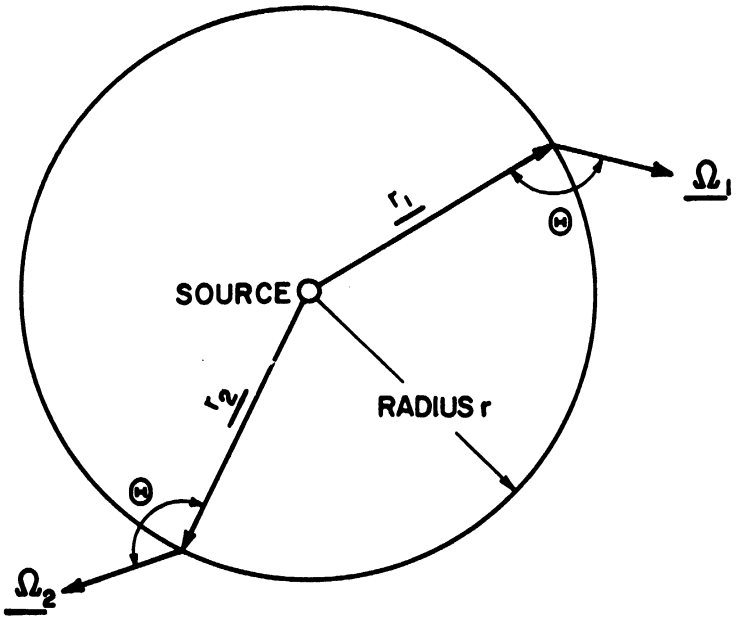

Figure I-8 For an Isotropic Source in a Uniform Isotropic Medium, the Flux at any Point on a Given Sphere Will be the Same in all Directions Which Make the Same Angles with the Radius Vector.

Equation (1-23c) can be written only if the neutron flux at thermal energies is separable into a product of a function of energy and a spatial distribution function. For, if this condition did not obtain the thermal average cross sections might be functions of position even though the energy dependent cross sections were not (see Equation (1-17c)). This assumption will later be seen to be justifiable for the idealized type of reactor considered here.

11. Critical Conditions

While assumptions made above are rather arbitrary, they do lead to significant and accurate results. On examination, the spatial integral in Equation (1-23c) is seen to be a convolution integral in the context of the Fourier Transform.[7] Since this equation is linear and homogeneous in $\phi_T(\underline{r})$ we can expect to arrive at a linear homogeneous algebraic equation in Fourier Transform space. The condition that the Fourier Transform of $\phi_T(\underline{r})$ not vanish will then lead to a critical condition.

The Fourier Transforms of the essential quantities are defined by

$$\overline{\phi}_T(\underline{k}) = \int_{\text{all space}} e^{i\underline{k}\cdot\underline{r}}\, \phi(\underline{r}, E)\, d^3r \qquad (1\text{-}24a)$$

$$\overline{P}_\infty(k^2) = \int_{\text{all space}} e^{i\underline{k}\cdot\underline{r}}\, P(|\underline{r}|)\, d^3r \qquad (1\text{-}24b)$$

Note that $\overline{P}_\infty(\underline{k})$ is a function only of $|\underline{k}|$ (or k^2) since $P_\infty(r)$ depends on $|\underline{r}|$. Now, taking the Fourier Transform of Equation (1-23c), that is, multiplying it by $e^{i\underline{k}\cdot\underline{r}}$ and integrating over all space we have

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[7] For a discussion of the properties of Fourier Transforms see, for example, Sneddon, Fourier Transforms, New York: McGraw-Hill, 1957.

$$\left(D_T k^2 + \Sigma_{aT}\right)\bar{\phi}_T(\underline{k}) = \nu\Sigma_{fT}\,\bar{P}_\infty(k^2)\,\bar{\phi}_T(\underline{k}) \qquad (1\text{-}25a)$$

so that if $\bar{\phi}_T(\underline{k})$ is to be non-vanishing, it follows that

$$\frac{\left(\nu\Sigma_{fT}/\Sigma_{aT}\right)\bar{P}_\infty(k^2)}{1 + L^2 k^2} \equiv k_{eff} = 1 \qquad (1\text{-}25b)$$

Here $L^2 = D_T/\Sigma a_T$ is called the thermal diffusion area and can be shown to be equal to one sixth the mean square distance traveled by a neutron from the time it is thermalized until the time it is absorbed in an infinite medium.[8]

Equation (1-25b) is sometimes written in terms of the two quantities

$$\eta = \nu\,\frac{\Sigma^u_{fT}}{\Sigma^u_{aT}} \qquad (1\text{-}25c)$$

and

$$f = \frac{\Sigma^u_{aT}}{\Sigma_{aT}} \qquad (1\text{-}25d)$$

Here Σ^u_{aT} is the total absorption (fission plus capture) cross section of the fuel. η is called the fuel efficiency and f the thermal utilization; the advantage of the introduction of these quantities is that η is a function only of the type of fuel and that any geometrical effects which may be present in the case of heterogeneous reactors,[9] and for which cell

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[8] See, for example, S. Glasstone and M. Edlund, The Elements of Nuclear Reactor Theory. Van Nostrand (1952).

[9] In this case space averaged cross section must be used in the critical equation. See, for example, A. M. Weinberg and E. P. Wigner, The Physical Theory of Neutron Chain Reactors, University of Chicago (1958).

averages must be taken before asymptotic reactor theory can be applied, are contained in f. With these definitions Equation (1-25b) becomes

$$\frac{\eta f \, \overline{P}_{\infty}(k^2)}{1 + L^2 k^2} = 1 \qquad (1\text{-}25e)$$

This equation has a simple physical interpretation. η represents the number of fission neutrons emitted per neutron absorbed in the fuel. Since f is the fractional number of neutrons absorbed in the fuel, ηf is the number of fission neutrons emitted per thermal neutron absorbed.

$\overline{P}_{\infty_o}(k^2)$ will be shown to be the total number of neutrons thermalized in the reactor per fast neutron born and $(1 + L^2 k^2)^{-1}$ will be shown to be the probability that a neutron thermalized will be absorbed before it leaks from the system. Clearly then

$$\frac{\eta f \, \overline{P}_{\infty}(k^2)}{1 + L^2 k^2}$$

represents the number of thermal neutrons absorbed per thermal neutron absorbed in the preceding generation which quantity must equal unity if a steady state is to be maintained. If $k_{eff} < 1$, the reactor is subcritical while if $k_{eff} > 1$ the reactor is supercritical. In either case no steady state neutron flux can exist.

12. The Material Buckling

Equation (1-25e), the critical equation, is an implicit equation for k^2 which has at most one positive root $k^2 = B_m^2$, the so-called material buckling of the reactor. This is easily seen when we note that $\overline{P}_{\infty}(k^2)$ is expected to be a monotonically decreasing function of k^2, a fact which will be proved in a later section. Since $(1 + L^2 k^2)^{-1}$ is also

monotonically decreasing, the product can equal unity at most once, and then only if $\eta f \bar{P}_\infty(0) > 1$

13. The Helmholtz Equation and Boundary Conditions

Another important result is that the thermal flux obeys the Helmholtz Equation.

$$\nabla^2 \phi_T(\underline{r}) = -B_m^2 \phi_T(\underline{r}) \tag{1-26}$$

To prove this, we write

$$\phi_T(\underline{r}) = (2\pi)^{-3} \int e^{-i\underline{k}\cdot\underline{r}} \bar{\phi}_T(\underline{k})\, d^3k \tag{1-27a}$$

Then operating with ∇^2:

$$\nabla^2 \phi_T(\underline{r}) = -(2\pi)^{-3} \int k^2 e^{-i\underline{k}\cdot\underline{r}} \bar{\phi}_T(\underline{k})\, d^3k \tag{1-27b}$$

But we have shown in sections 11 and 12 that $\bar{\phi}_T(\underline{k}) = 0$ unless $k^2 = B_m^2$. Therefore we may remove k^2 from the integral, replacing it by B_m^2 and find

$$\nabla^2 \phi_T(\underline{r}) = -B_m^2 (2\pi)^{-3} \int e^{-i\underline{k}\cdot\underline{r}} \bar{\phi}_T(\underline{k})\, d^3k \tag{1-27c}$$

or, comparing with Equation (1-27a):

$$\nabla^2 \phi_T(\underline{r}) = -B_m^2 \phi_T(\underline{r}) \tag{1-27d}$$

QED. This is a general property of a function whose Fourier Transform vanishes everywhere except on a spherical surface of radius B_m in transform space.

Thus, in order to calculate the thermal flux shape in a reactor, we need only solve the critical equation (1-25e) for B_m^2 and then solve the Helmholtz Equation (1-26).

To completely specify the flux shape, boundary conditions must be imposed. Clearly, two conditions on $\phi(\underline{r},E)$ are that it be finite and non-negative everywhere within the reactor. Being a second-order differential equation, the Helmholtz Equation will possess two independent solutions for every B_m. Generally, this condition will suffice to eliminate one of them. Another condition is usually adopted from the solution of the Milne problem.

In solving the problem of a semi-infinite medium bounded by a plane, with a source at infinity it is found that the flux obeys the condition,[10]

$$\frac{1}{\phi}\frac{\partial \phi}{\partial n} = -\frac{\Sigma_{tr}}{.7104} \qquad (1\text{-}28)$$

where n is a coordinate normal to the surface, provided that

$$c = \frac{\nu\Sigma_f + \Sigma_s}{\Sigma_t} = 1$$

a condition which is nearly valid in most reactors. If the radius of curvature of the reactor boundary is large compared with a neutron mean free path, the surface may be considered plane and condition (1-28) applied.

While the condition (1-28) is generally valid for the problem under consideration, it is not the most convenient. A simpler, if somewhat less accurate, condition can be obtained if the radius of curvature of the boundary is large compared even with the root-mean-square-distance a neutron travels in the reactor during its lifetime, which is, of course, greater than the mean free path. Then the boundary may

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[10] Strictly speaking, it is the flux far from the boundary which obeys this condition. This asymptotic flux is shown in Appendix C to be the component with which asymptotic reactor theory deals. See B. Davison, op. cit.

be treated as plane and the flux shape outside the boundary can be taken as a linear extrapolation rather than the analytic continuation of its shape inside the core. The point at which the extrapolated flux goes to zero is easily determined. (This continuation of the internal reactor flux outside the reactor is a mathematical artifice and is not to be confused with the true neutron flux outside the reactor.) From Figure 9 we have:

$$\tan\theta = -\frac{\partial\phi(\underline{r}_s)}{\partial n}$$

$$d = \frac{\phi(\underline{r}_s)}{\tan\theta} = \frac{\phi(\underline{r}_s)}{\partial\phi(\underline{r}_s)/\partial n} = \frac{.7104}{\Sigma_{tr}} \qquad (1\text{-}29)$$

Thus, to a reasonable approximation, we may use the boundary condition that $\phi(\underline{r},E)$ and $\phi_T(\underline{r})$ vanish at a distance $.7104/\Sigma_{tr}$ from the boundary. As the extrapolation distance is usually small compared to reactor dimensions the difference between the points of which the linear extrapolation and the analytic continuation of the flux go to zero will be exceedingly small. If this is not true, then the reactor is probably not large enough to permit use of asymptotic reactor theory at all. As written, the extrapolation distance, d, is a function of energy, since Σ_{tr} is a function of energy. It is of extreme importance, however, to have the flux vanish on the same surface at all energies. Otherwise, the shape of the flux will vary with energy and will not be separable in space and energy. Again, d is usually much smaller than the reactor dimensions to that this effect is rather small unless d varies strongly with energy. For that case Inonu[11] has

[11] Inonu, Proceedings of Internat'l. Conference at Geneva, P/2344 (1958). The result quoted here is not precisely his result, but is easily derived from it.

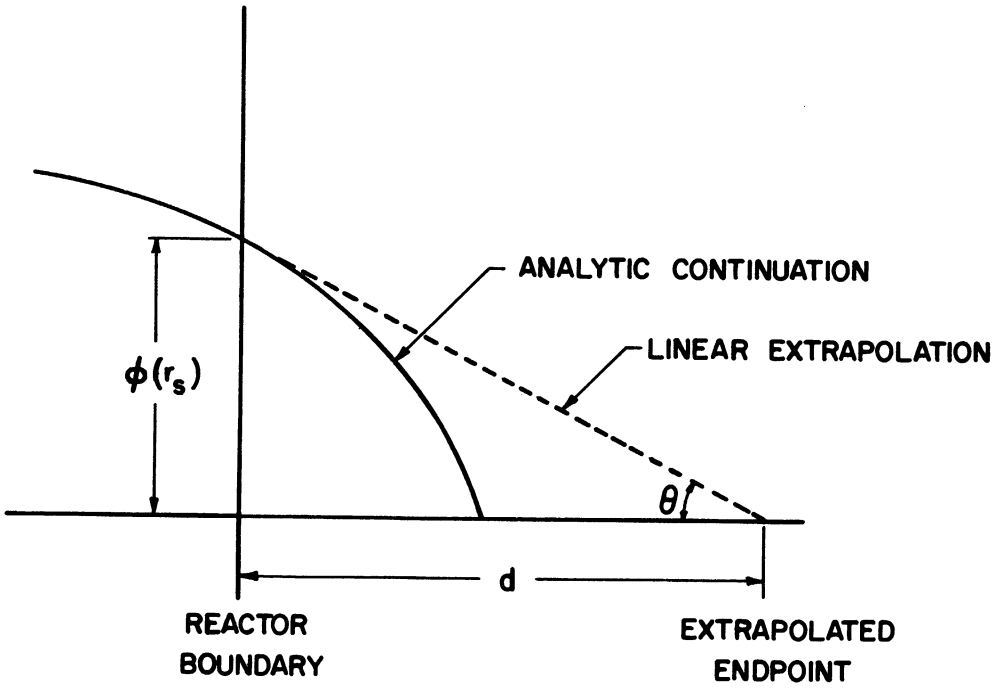

Figure 9

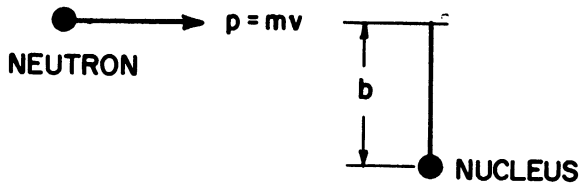

Figure 10

used multigroup methods (see Chapter IV) to define an energy independent average extrapolation length. As his analysis is rather lengthy only his result is quoted:

$$d_{av} = \frac{\int d(E)\phi(E)dE}{\int \phi(E)dE} \qquad (1\text{-}30)$$

14. The Spatial Flux Shape

By virtue of the discussion of the previous section, the problem of finding the spatial flux shape has been reduced to the problem of solving the Helmholtz Equation with the boundary conditions of finiteness, continuity, and non-negativity everywhere within a convex surface on which the flux must vanish. This is a well known problem in mathematical physics and the properties of its solutions have been studied in rather great detail. It is known that the solutions of this problem form an infinite set of eigenfunctions, which may be made orthonormal over the reactor volume (including the small extrapolation distance); all of these eigenvalues are positive ($B_m^2 > 0$) and only the first eigenfunction, which corresponds to the smallest eigenvalue, does not vanish anywhere within the bounding surface.[12] This lowest eigenvalue we call the geometric buckling B_g^2 since it depends only on the geometry of the system.

For a bare reactor, we have seen that the only value of the wave number in the Helmholtz Equation which permits the establishment of a steady state flux is B_m. Obviously, only one of the eigenvalues

[12] A. E. Heins, Private communication. These results can be proved by converting the problem into a Fredholm integral equation on the interior of the volume. The quoted theorems are known to hold for this type of equation. See R. Courant and D. Hilbert, Methods of Mathematical Physics, New York: Interscience, 1950.

of the problem discussed above can be equal to B_m^2; the flux must, therefore, have the spatial behavior of a single eigenfunction of the Helmholtz Equation which must furthermore be the first eigenfunction as a consequence of the physical restriction that $\phi(\underline{r},E)$ be non-negative. Hence

$$B_m^2 = B_g^2 \qquad (1\text{-}31)$$

for criticality. Since B_m^2 is a function of material properties alone and B_g^2 is a function solely of geometry, this is a relation between the material composition and geometry required to achieve criticality.

The eigenfunctions and eigenvalues for infinite slab, spherical, and cylindrical reactors are given in Table I. Note that in each case the dimensions include the extrapolation distance.

TABLE I

Reactor Geometry	Lowest Eigenvalue	First Eigenfunction
Semi-infinite slab, width ℓ	$B_g^2 = (\frac{\pi}{\ell})^2$	$\cos \frac{\pi x}{\ell}$
Sphere of radius R	$B_g^2 = (\frac{\pi}{R})^2$	$\frac{1}{r} \sin \frac{\pi r}{R}$
Cylinder of radius ρ Height H	$B_g^2 = (\frac{\pi}{H})^2 + (\frac{2.405}{R})^2$	$\cos \frac{\pi x}{H} J_o(\frac{2.405\rho}{R})$
Rectangular parallelepiped of dimensions ℓ_1, ℓ_2, ℓ_3	$B_g^2 = (\frac{\pi}{\ell_1})^2 + (\frac{\pi}{\ell_2})^2 + (\frac{\pi}{\ell_3})^2$	$\cos \frac{\pi x}{\ell_1} \cos \frac{\pi y}{\ell_2} \cos \frac{\pi z}{\ell_3}$

All of the other eigenvalues of the Helmholtz Equation are larger than B_g^2. Since k_{eff} is a monotonically decreasing function of k^2 (or B_m^2),

any of these eigenvalues leads to values of k_{eff} less than unity.

It is true the Boltzmann Equation is linear and homogeneous in $\Phi(\underline{r}, E, \underline{\Omega})$ and that the superposition principle may be applied to it. That is to say, the sum of independent solutions (which obey the proper boundary conditions) is also a solution. Hence a sum of solutions of the Helmholtz Equation is a mathematically acceptable solution for the flux, again provided all of the physically imposed restrictions are met. However, only one of these solutions can meet the critical condition; all others have $k_{eff} < 1$, which a study of the time dependent equation will reveal to lead to solutions which decay exponentially in time.[13] Again, it is emphasized that the time independent flux has the shape of the first eigenfunction of the Helmholtz Equation, given in Table I for simple geometries.

It should be pointed out that all of these results depend upon the replacement of the finite medium slowing down kernel by an infinite medium kernel, one which depends on $|\underline{r} - \underline{r}'|$ and extension of the integrals over the reactor volume to infinity. This replacement is approximately valid for a large reactor, i.e., one which is almost infinite. That this replacement is also valid in much more general cases is shown in Appendix E.

15. The Slowing Down Density

A quantity of extreme importance in reactor calculations is the escape probability, defined as the probability that a neutron will not

[13] See for example S. Glasstone and M. C. Edlund, op. cit.

leak out of the reactor or be absorbed before reaching energy E. However, as high energy absorptions may lead to fission, the fast fission factor ϵ must be taken into account. A common definition of ϵ is that it represents the number of neutrons produced by U-238 fission (for which the threshold is about 1 Mev) per neutron produced by U-235 fission. This definition is consistent with the term "fast fission factor" as most fissions induced by neutrons above one Mev are U-238 fissions, for all but very highly enriched systems. When defined in this way the concept of a fast fission factor is most readily applied to intermediate spectrum reactors.

Returning the consideration of the escape probability, we note that it is simply the number of neutrons slowing down past energy E in the core per fission neutron produced at energies above E. The former of these quantities is the slowing down density, now introduced. We define $q(\underline{r}, E)$ such that $q(\underline{r}, E)\, d^3\underline{r}$ is the number of neutrons slowing down past energy $E(> E_T)$ per second in volume element d^3r at $\underline{r}$. To derive an expression for $q(\underline{r}, E)$ we remember that $\Sigma_{S_0}(E' \rightarrow E)$ (where $E' \geq E$) is the macroscopic cross section for neutron scattering from energy E' to E. Then the number of neutrons slowing down past energy E per cm^3 which had their last collision in the enegy range dE' at E' ($> E$) is

$$dq(\underline{r}, E, E') = \left[\int_0^E \Sigma_{S_0}(E' \rightarrow E'')\, \phi(\underline{r}, E')\, dE''\right] dE'$$

where

$$\Sigma_{S_0}(E' \rightarrow E) = \Sigma_S(E')\, F_0(E' \rightarrow E) \qquad (1\text{-}32a)$$

and $F_0(E' \rightarrow E)$ is defined by Equation (1-15e).

The total number of neutrons slowing down past E is therefore

$$q(\underline{r}, E) = \int_E^\infty dE' \int_0^E dE'' \; \Sigma_{s_0}(E' \to E'') \phi(E'') \qquad (1\text{-}32b)$$

16. The Slowing Down Density Kernel

As pointed out in the previous section, the slowing down density is an extremely important quantity in reactor physics. By its very nature it is a much more slowly varying function of energy than the flux and for this reason we will have occasion to employ it frequently in the ensuing chapters. Hence we introduce a slowing down density kernel, $P^*(\underline{r}' \to \underline{r}, E)$ which is the slowing down density per unit volume at $\underline{r}$ at energy E due to a point source of fission neutrons at point $\underline{r}'$. To be consistent with the conventions employed earlier with respect to the slowing down kernel, the slowing down density kernel must include the effects of fast fission, that is, the slowing down density described by the kernel P^* is somewhat enhanced by U-238 fission.

It follows from the definition of the kernel that the slowing down density is given by

$$q(\underline{r}, E) = \int_R S(\underline{r}') P^*(\underline{r}' \to \underline{r}, E) d^3r' \qquad (1\text{-}33a)$$

Following the arguments used earlier, the asymptotic reactor model may be invoked. To do this, one need only replace the kernel P^* in Equation (1-33a) by the infinite medium kernel $P^*_\infty(|\underline{r} - \underline{r}'|, E)$ and extend the integral to all space:

$$q(\underline{r},E) = \int_{\text{All space}} S(\underline{r}')\, P^*_\infty(|\underline{r}-\underline{r}'|, E)\, d^3r' \quad (1\text{-}33b)$$

In a critical reactor, $S(\underline{r}')$ is, of course, the fission source and has the shape of the first eigenfunction of the Helmholtz Equation $\chi(\underline{r})$.

At this point, we must make use of the following lemma: If $\chi(\underline{r})$ is a solution of the Helmholtz Equation with wave number B_n^2, then

$$\int_{\text{all space}} f(|\underline{r}-\underline{r}'|)\, \chi(\underline{r}')\, d^3r' = \chi(\underline{r})\, \bar{f}(B_n^2) \quad (1\text{-}34)$$

The proof is short. Taking the Fourier Transform of the left-hand side of Equation (1-34), we obtain, by virtue of the convolution theorem, $\bar{f}(k^2)\bar{\chi}(\underline{k})$. But, because $\chi(\underline{r})$ obeys the Helmholtz Equation, $\bar{\chi}(\underline{k}) = 0$ unless $k^2 = B_n^2$. Hence the Fourier Transform becomes $\bar{f}(B_n^2)\bar{\chi}(k)$ and inverting, we obtain $\bar{f}(B_n^2)\chi(\underline{r})$, qed. An application of the lemma to Equation (1-33b) quickly yields:

$$q(\underline{r}, E) = S(\underline{r})\, \bar{P}^*_\infty(B_g^2, E')\, dE' \quad (1\text{-}35a)$$

which shows that, within the bounds of asymptotic reactor theory, $q(\underline{r}, E)$ also has the spatial distribution of the first eigenfunction of the Helmholtz Equation and that it is separable in energy and space. This is to be expected from the very close relationship of the slowing down density to the flux. In fact, it can be argued that since Equation (1-32b) relates $q(\underline{r}, E)$ and $\phi(\underline{r}, E)$ by an operator that depends solely on energy, if the flux is separable then the slowing density is also. It should be mentioned in passing that the thermalization kernel $P_T(\underline{r}' \rightarrow \underline{r})$ used earlier is simply the slowing down density kernel evaluated at the thermal cutoff energy E_T, i.e., $P^*(\underline{r}' \rightarrow \underline{r}, E_T)$.

The ratio of the number of neutrons slowing down past energy E to the number of U-235 fission neutrons born at energies above E is:

$$\frac{\int_R q(\underline{r},E)\,d^3r}{\int_E^\infty dE' \int_R S(\underline{r},E')\,d^3r} = \frac{\overline{P}_\infty^*(B_g^2,E)\int_R S(\underline{r})\,d^3r}{\int_E^\infty dE' \int_R S(\underline{r},E')\,d^3r} = \frac{\overline{P}_\infty^*(B_g^2,E)}{\int_E^\infty f(E)\,dE} \qquad (1\text{-}35c)$$

where $S(\underline{r}, E)$ is the source of neutrons due to U-235 fission.* In particular, if E is below the energy region in which the fission spectrum is appreciable, the escape probability $\lambda(B_g^2, E)$ becomes simply $\overline{P}_\infty^*(B_g^2, E)$, a result which is frequently called the "Second Fundamental Theorem of Reactor Theory."[14] Formally, this theorem states that the escape probability in a critical system is the Fourier Transform of the slowing-down density kernel, evaluated at the geometric buckling of the system. This explains the previously used fact that $\overline{P}_\infty(k^2)$ is a monotonically decreasing function of k^2. As a reactor becomes larger, k^2 decreases and the escape probability clearly increases.

For application to mono-energetic neutron diffusion one must extend the definition of the slowing down density kernel. The slowing down density is a collision density (or reaction rate, i.e., $\Sigma\,\phi$) -- the collision density for those neutrons which will have energies below E after a particular collision. Slowing down removes neutrons from energies above E; only once in its lifetime can a neutron experience such a collision. In one-speed diffusion theory the analog is absorption, hence an "absorption density" kernel $\Sigma_a\phi$ should be used.

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* Actually this requires an energy-dependent fast fission factor since U-238 fission neutrons are born with much the same energy spectrum as U-235 fission neutrons. However, most of the fission spectrum is above 0.5 mev, which is an energy region of relatively little interest except in fast systems. Below this level ϵ is energy independent.

[14] A. M. Weinberg and E. P. Wigner The Physical Theory of Neutron Chain Reactions, University of Chicago Press (1959) p. 420.

The lemma just derived can be used to prove that the flux at all energies has the same spatial behavior, i.e., that the flux is separable in space and energy since it is possible to write*

$$\phi(\underline{r}, E) = \int S(\underline{r}') P_\infty(|\underline{r}-\underline{r}'|, E)\, d^3r'$$

$$= S(\underline{r}')\, \overline{P}_\infty(B_g^2, E) \qquad (1\text{-}36)$$

The separability of the flux and slowing-down density, the critical equation, the fact that the flux obeys the Helmholtz Equation, and the expression for the escape probability are the basic results of asymptotic reactor theory.

17. The Six Factor Formula

Frequently, the criticality factor for a thermal reactor is decomposed in a rather arbitrary and intuitive manner. Some of the factors have already been discussed; the formula obtained will be an aid in interpreting other terms in the critical condition for thermal reactors. Imagine fission neutrons starting to slow down from high energies. In the process of slowing down they may induce fast fission, thus increasing their number by the factor ϵ. Alternatively, they may be absorbed without inducing fission before reaching thermal energies. Here we define the resonance escape probability, $p(E' \rightarrow E)$, as the probability that a neutron born at energy E' will not be captured before reaching energy E; p(E) will denote the resonance escape probability averaged over a fission spectrum:

* If E is above the lower limit of the fission spectrum, we must modify the definition of P to include an average only over that portion of the fission spectrum which is about E.

$$p(E) = \int_0^\infty f(E') p(E' \to E) dE' \qquad (1\text{-}37a)$$

Finally, neutrons may leak out of the system before reaching thermal energies. To cover this, the non-leakage probability, $\lambda(B_g^2, E' \to E)$ is defined as the probability that a neutron born at energy E' will not leak out of a system of geometric buckling B_g^2 before reaching energy E. Its fission spectrum average is denoted by:

$$\lambda(B_g^2, E) = \int_0^\infty f(E') p(E' \to E) dE' \qquad (1\text{-}37b)$$

Here B_g^2 has been written explicitly as an argument of λ to call attention to the fact that λ depends very strongly on the geometry of the system. The implication that λ depends only on B_g^2 is accurate only within the limits of asymptotic reactor theory as, of course, are most of the other results of this chapter.

Frequently, ϵ, p, and λ are assumed entirely independent of one another; this is only true within a certain limit. For example p(E) generally depends on the geometry of the system (and hence on B_g^2) while $\lambda(B_g^2, E)$ may depend to a rather great extent on the amount of absorption in the system. If ϵ is defined to include only U-238 fissions, the contribution to ϵ comes entirely from very high energy neutrons and hence from during a small fraction of the slowing down process. Fast fission then occurs before much resonance absorption or leakage has taken place (except in water moderated reactors) and ϵ is effectively independent of p and λ.

A physical description of the situation may make the point clear. The statement that $p(E)$ is independent of geometry is equivalent to saying that it is independent of $\lambda(B_g^2, E)$. This, in turn, says that increasing the leakage has no effect on the fast absorption. But this is clearly untrue, for a neutron which leaks out at energy E has zero probability of being captured at energies below E, and vice versa. Hence, as long as the two processes occur simultaneously, their probabilities cannot be truly independent. If, however, the probabilities are each close to unity, the interaction will be small, and in such a case, for every neutron born due to U-235 fission

$$\epsilon\, p(E_T)\, \lambda\, (B_g^2, E_T)$$

will reach thermal energies. Also, in many systems, such as light water assemblies, resonance absorption sets in at energies below those at which most fast leakage takes place.

After reaching thermal energies the neutrons may either leak or be absorbed. We denote the <u>thermal non-leakage probability</u> by $\lambda_T(B_g^2)$, i.e., $\lambda_T(B_g^2)$ is the fraction of neutrons which are thermalized that get absorbed. Of the neutrons that suffer thermal absorption, a fraction f (the thermal utilization) are absorbed in uranium and each absorption by a uranium atom produces η neutrons on the average. Hence a total of

$$\eta f \epsilon p(E_T) \lambda_T(B_g^2) \lambda(B_g, E_T) \qquad (1\text{-}38a)$$

are produced on the average, for every neutron that started to slow down. This, the famous six factor formula, defines k_{eff}, and must

evidently be unity for criticality. Comparison of Equation (1-38a) with Equation (1-25e) shows that

$$\epsilon p(E_T)\, \lambda(B_g^2, E_T)\, \lambda_T(B_g^2) = \frac{\overline{P}_{T\infty}(B_g^2)}{1 + L_T^2 B_g^2} \qquad (1\text{-}38b)$$

One may note that if neutrons did not diffuse after thermalization there would be no thermal leakage, i.e., λ_T would be unity. This limit also obtains by setting $D_T = 0$ (and hence, $L_T^2 = 0$). Hence

$$\epsilon p(E_T)\, \lambda(B_g^2, E_T) = \overline{P}_{T\infty}(B_g^2) \qquad (1\text{-}38c)$$

Further, in an infinite reactor there can be no leakage, and the geometric buckling, which is related to the inverse square of a dimension (see Table I), goes to zero. Setting $B_g^2 = 0$ in Equation (1-38c) gives, therefore:

$$\epsilon p(E_T) = \overline{P}_T(0) \qquad (1\text{-}38d)$$

Thus, the fast non-leakage probability is the ratio of Equations (1-38c) and (1-38d):

$$\lambda(B_g^2, E) = \frac{\overline{P}_T(B_g^2)}{\overline{P}(0)} \qquad (1\text{-}38e)$$

The arguments leading from Equation (1-38b) to (1-38c) further show that:

$$\lambda_T(B_g^2) = \frac{1}{1 + L_T^2 B_g^2} \qquad (1\text{-}38f)$$

a result which may also be derived from the Second Fundamental Theorem as follows. The Green's Function (the diffusion kernel) for the thermal diffusion equation (Equation (1-21i) with D_T spatially constant) in an infinite medium is

$$\phi_T(\underline{r},\underline{r}') = \frac{e^{-|\underline{r}-\underline{r}'|/L_T}}{4\pi D_T |\underline{r}-\underline{r}'|} \qquad (1\text{-}39)$$

The absorption kernel from which the non-leakage probability may be obtained is $\Sigma_{aT}\phi_T(\underline{r}', \underline{r})$, whose Fourier Transform is indeed the right hand side of Equation (1-39), qed.

18. The Non-Leakage Probability - Non-Critical Systems

The fast non-leakage probability can be interpreted in terms of $\overline{P}(B_g^2, E)$ even for non-critical systems. Consider a subcritical system ($k < 1$); such a system will have a steady neutron population only if a non-fission source is placed in it. This steady flux will obey a thermal diffusion equation of the type:

$$-D_T\nabla^2\phi_T(\underline{r}) + \Sigma_{aT}\phi_T(\underline{r}) = \int d^3r' P_T(|\underline{r}-\underline{r}'|)\left\{\nu\Sigma_{fT}\phi_T(\underline{r}') + S(\underline{r}')\right\} \qquad (1\text{-}40)$$

where it is assumed that this source energy distribution is sufficiently similar to that of the fission spectrum to allow use of the same slowing down kernel for both. The flux $\phi_T(\underline{r})$ of Equation (1-40) must obey the usual boundary condition that it vanish on an extrapolated surface. Now let the flux and source be expanded in terms of the eigenfunctions of the Helmholtz Equation (note that one eigenfunction will not suffice in this case since the criticality condition does not obtain):

$$\phi_T(\underline{r}) = \sum_{n=0}^{\infty} \varphi_n \chi_n(\underline{r})$$

$$S(\underline{r}) = \sum_{n=0}^{\infty} s_n \chi_n(\underline{r}) \qquad (1\text{-}41a)$$

Substituting into (1-40) we have

$$\sum_{n=0}^{\infty}\left[D_T\varphi_n B_n^2\chi_n(\underline{r})+\Sigma_{aT}\varphi_n\chi_n(\underline{r})-\int d^3r'\,P_{T\infty}(|\underline{r}-\underline{r}'|)\cdot\right.$$
$$\left.\cdot\left\{\nu\Sigma_{fT}\varphi_n\chi_n(\underline{r}')+S_n\chi_n(\underline{r}')\right\}\right]=0 \qquad (1\text{-}41b)$$

or

$$\sum_{n=0}^{\infty}\left[D_T\varphi_n B_n^2+\Sigma_{aT}\varphi_n-\overline{P}_{T\infty}(B_n^2)\left\{\nu\Sigma_{fT}\varphi_n+S_n\right\}\right]\chi_n(\underline{r})=0 \qquad (1\text{-}41c)$$

where we have made use of the lemma (1-34). Upon multiplying this equation by $\chi_n(\underline{r})$ and integrating over the reactor volume R, we have, using the orthonormality property of the $\chi_n(\underline{r})$:

$$\left(D_T B_n^2+\Sigma_{aT}\right)\varphi_n-\overline{P}_{T\infty}(B_n^2)\left(\nu\Sigma_{fT}\varphi_n+S_n\right)=0 \qquad (1\text{-}41e)$$

which may be rearranged to yield

$$\varphi_n=\frac{S_n\overline{P}_{T\infty}(B_n^2)}{\nu\Sigma_{fT}\overline{P}_{T\infty}(B_n^2)-(1+L^2B_n^2)}=\frac{S_n\overline{P}_{T\infty}(B_n^2)/\Sigma_{aT}(1+L^2B_n^2)}{1-k_{eff\,n}} \qquad (1\text{-}41f)$$

where, by definition:

$$k_{eff\,n}=\frac{\eta f\,\overline{P}(B_n^2)}{1+L^2B_n^2} \qquad (1\text{-}41g)$$

is the <u>effective multiplication for the n^{th} mode</u>, now shown to be the number of n^{th} mode neutrons (the coefficient of the n^{th} eigenfunction

in the flux expansion) absorbed per n^{th} mode neutron absorbed in the preceding generation.

Physically, it can be argued that if, in a non-multiplying medium ($\Sigma_f = 0$), S_n n^{th} mode neutrons were born per cm^3 per second, the steady thermal flux would be determined by the conservation equation:

$$\Sigma_{aT} \varphi_n = S_n \lambda_T(B_n^2) \lambda(B_n^2, E_T) p(E_T) \epsilon \qquad (1\text{-}41h)$$

where $\lambda_T(B_n^2)$ and $\lambda(B_n^2, E_T)$ are the thermal and fast non-leakage probabilities for n^{th} mode neutrons respectively. This is a simple statement of the fact that all the neutrons that do not leak are absorbed, assuming no mode coupling, i.e., transfer of neutrons from one mode to another. Temporarily ignoring the factor of $1 - k_{eff_n}$, which is the effect of multiple generations, in Equation (1-41f) it is possible to identify

$$\lambda_T(B_n^2) = \frac{1}{1 + L^2 B_n^2} \qquad (1\text{-}41i)$$

since L^2 is the only factor which is specifically introduced by thermal neutron effects. Also

$$\overline{P}_{T\infty}(B_n^2) = \lambda(B_n^2, E_T) p(E_T) \epsilon$$

as these factors arise in the treatment of fast neutrons. Thus $\overline{P}_{T\infty}(B_n^2)$ is the non-leakage probability for n^{th} mode neutrons in sub-critical systems or in fact, in any system.

The factor $(1\text{-}k_{eff_n})$ in the denominator arises from the fact that each neutron absorbed in any mode produces ηf fission neutrons in that mode so that each n^{th} mode neutron produces k_{eff_n} neutrons in the succeeding generation. At steady state the n^{th} mode flux will be:

$$\varphi_n = \varphi_{no}\left\{1 + k_{eff_n} + k_{eff_n}^2 + \cdots\right\} = \frac{\varphi_{no}}{1 - k_{eff_n}} \qquad (1\text{-}42a)$$

where

$$\varphi_{no} = \frac{S_n \bar{P}_{T\infty}(B_n^2)}{\Sigma_a (1 + L^2 B_n^2)} \qquad (1\text{-}42b)$$

is the thermal neutron flux due to neutrons coming directly from the source. This argument verifies that (1-41f) is indeed the effective multiplication constant for n^{th} mode neutrons.

It was shown that $\bar{P}_{T_\infty}(B_g^2)$ is the non-leakage probability for a critical reactor with geometric buckling B_g^2. As the leakage is expected to decrease with increasing size (or decreasing buckling, since B_g^2 is related to reciprocal dimensions squared; see Table I) $\bar{P}_T(B_n^2)$ and the k_{eff_n} must be monotonically decreasing functions of B_n^2, or n. Hence, when a reactor is being fueled, it will first become critical in the first mode and the flux in a critical system will have the first mode shape.

19. Some Results of Asymptotic Reactor Theory

The development of time-independent asymptotic reactor theory is now essentially complete. We have demonstrated that within the limitations of asymptotic reactor theory, the problem of criticality may be formulated in terms of a problem in slowing down theory, namely that of determining the slowing down kernel. In so doing, several assumptions and approximations have been used, the validity of which is, to say the least, open to question.

One of the foremost of these, that of the one group treatment of all thermal neutrons, has not been seriously tested to date. Work in this area[15] is now underway, and has implications not only for reactor theory but also for many areas of physics not specifically related to reactor theory. These calculations will provide better means of describing thermal neutrons but, as they are as yet somewhat incomplete and inconclusive, we shall give no detailed discussion of this work here.

In evaluating the principal results of asymptotic reactor theory, namely the space-energy separability of the flux (often called the "First Fundamental Theorem")[16] and the Second Fundamental Theorem mentioned earlier, one should try to separate the effects of the various assumptions and approximations.

Inonu[17] and Dresner[18] and Yip and Zweifel[19] have investigated the validity of the Second Fundamental Theorem.* Their results indicate that asymptotic reactor theory is applicable even to systems whose linear dimensions are of the order a neutron mean free path. Dresner's results for the non-leakage probability are in better agreement with the rigorous theory than Inonu's due to the fact that he used more appropriate boundary conditions. For systems in which the neutron leakage is very high, $\lambda(B_g^2)$, defined by Equation (1-38e), must also be very large. This, in turn, affects the value of the logarithmic derivative of the flux at the surface.[20]

15 N. Corngold, op. cit.
16 A. M. Weinberg and E. P. Wigner, op. cit.
17 E. Inonu, Nuc. Sci. Eng., 5, 248 (1959).
18 L. Dresner, Nuc. Sci. Eng. 7, 419 (1960)
19 S. Yip and P. F. Zweifel, Nuc. Sci. Eng. 10, 362 (1961).
20 B. Davison, op. cit.

* For a more complete discussion of the validity of asymptotic reactor theory see Appendix C.

These results, which are a little surprising in view of the rather strict assumptions involved in the derivation of asymptotic reactor theory, are explained in Appendix C.

D. Calculation of the Elastic Scattering Frequency

20. Problems Associated with the Calculation of $F(E' \rightarrow E, \mu_o)$

In the previous section, we have derived the various results of asymptotic theory in terms of a "slowing-down kernel" which still remains to be calculated. We have also obtained the basic mechanism for obtaining that kernel, i.e., the Boltzmann Equation. In the remainder of this chapter we begin a discussion of the methods for obtaining the slowing-down kernel from the Boltzmann Equation. The first part of this problem is the derivation of the elastic scattering frequency $F(E' \rightarrow E, \mu_o)$.

A rigorous treatment of slowing down should, of course, include the effects of inelastic scattering. However, it is difficult to arrive at a satisfactory mathematical development of the theory if inelastic scattering effects are to be included. Hence, the discussion of the effect of inelastic scattering on reactor calculations is generally made only in the context of multigroup theory; our discussion of this effect is therefore deferred until Chapter IV.

The problem of low-energy molecular effects is also quite difficult to treat and is a topic which is more properly discussed in connection with the problem of calculating the thermal neutron spectrum.[21] The slowing-down calculations described here will be

[21] See T. J. Krieger and M. S. Nelkin, Phys. Rev., 106, 290 (1957) for a discussion of this problem. These authors give a list of further references for the reader interested in this problem. See also Corngold, op cit.

valid only above the energies associated with the chemical bond in molecules, or approximately 1 ev.[22]

For many purposes it is sufficient to assume that the elastic scattering is spherically symmetric in the center-of-mass system of neutron and scattering nucleus (S-wave scattering), but restriction to this special case is not necessary in general. It is well known that S-wave scattering (zero relative angular momentum) is isotropic in the center of mass while p-wave scattering (angular momentum of one unit) is strongly peaked in the forward direction.[23] Thus, anisotropic corrections are most important at energies at which p-wave scattering comes into prominence. This energy can be estimated by the following simple quasi-classical argument.

Consider a neutron with momentum p, traveling toward a nucleus. It is assumed that scattering will occur when the impact parameter b (see Figure 10) is of the order of the nuclear radius. Then the angular momentum, for collision to occur, must be of the order:

$$pb = \sqrt{\ell(\ell+1)}\,\hbar$$

---

[22] Classically, if the energy that would be gained by a free atom is much greater than the chemical binding energy of the molecule, the atom acts as if it were originally free. At lower energies the effects of binding make it seem that the atom is heavier than it actually is. A useful approximation at very low energies is that the atom behaves as if it had the mass of the entire molecule. Quantum mechanically, however, the atom may act as it were free even if it does not gain enough energy to break the chemical bond. All that is required is that the energy levels of the molecule be sufficiently close together to be representable by a continum. R. E. Marshak, unpublished.

[23] See L. I. Schiff, Quantum Mechanics. New York: McGraw-Hill (1957)

$\sqrt{\ell(\ell+1)}\,\hbar$ being the quantum mechanical angular momentum. For p-wave scattering $\ell=1$, and the nuclear radius is approximately $1.5 \times 10^{-13} A^{1/3}$ cm, so we have $E = 20A^{-2/3}$ Mev. in the center of mass system. Thus, p-wave scattering tends to become important at lower energies for heavy nuclei and is negligible for many moderators. This argument applies only to potential scattering.

21. Kinematics of Elastic Collisions

Since most nuclear data are presented or calculated in the center-of-mass coordinate system, it is necessary to describe the collision of a neutron with a nucleus of mass number A in both the center-of-mass and laboratory coordinate systems. In particular, the relationships among the scattering angle in the laboratory system, $\cos^{-1}\mu_o$, the scattering angle in the center-of-mass system, $\cos^{-1}\mu_c$, and the energy transfer in the collision are to be found. The laboratory system (L) is that in which measurement can be made, that is, the system in which the nucleus may be assumed at rest while the neutron approaches it with a velocity $v_o = \sqrt{2E}$, if the neutron mass is taken to be unity (see Figure 11). After the scattering event, the neutron goes off at an angle $\cos^{-1}\mu_o = \theta_o$ (the scattering angle in L) with speed u_o, after having imparted a speed U_o to the nucleus, which goes off at angle ϕ.

In the center-of-mass system (C), on the other hand, the center of mass of nucleus-neutron system is assumed to be at rest (see Figure 12). Here, the neutron is moving to the right with a speed $v_o - V_M$, where V_M is the speed of the center-of-mass of the neutron-nuclear

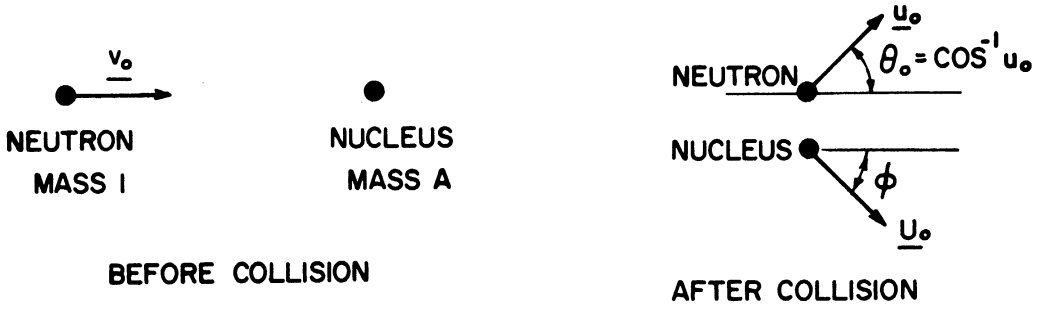

Figure I-11

Kinematics of a Neutron-Nuclear Collision.
(Laboratory System)

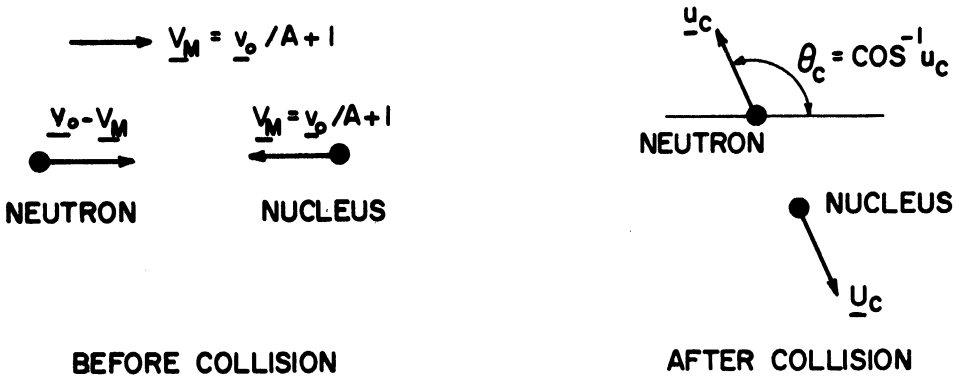

Figure I-12

Kinematics of a Neutron-Nuclear Collision.
(~~System~~ Center of Mass System)

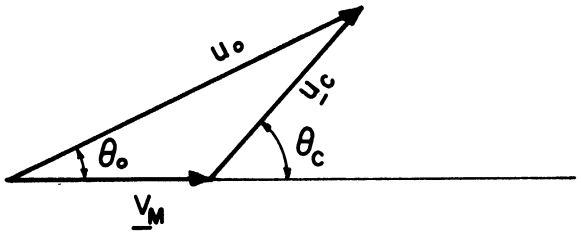

Figure I-13

Relation Between Laboratory and Center
of Mass System Velocities.

system relative to the laboratory system:

$$V_M = \frac{v_0}{A+1} \tag{1-43a}$$

so that the neutron speed is:

$$v_0 - V_M = \frac{A v_0}{A+1} = v_c \tag{1-43b}$$

The nucleus moves to the left with a speed V_M. In the center-of-mass system the neutron and nucleus appear to scatter each other since they are both moving even before the collision. After the collision the neutron has speed u_c and the nucleus speed U_c. The scattering angle in this coordinate system is $\cos^{-1}\mu_c = \theta_c$; the neutron and nucleus come off in opposite directions since the total momentum before the collision in C is

$$1 \cdot (v_0 - V_M) - A V_M = v_0\left[\left(1 - \frac{1}{A+1}\right) - \frac{A}{A+1}\right] = 0 \tag{1-43c}$$

and must, because of momentum conservation, remain zero after the collision. Clearly, this is possible only if the neutron and nucleus are moving in opposite directions after the collision, and furthermore only if

$$u_c = AU_c \tag{1-43d}$$

Energy conservation in C provides another relation between u_c and U_c:

$$\frac{1}{2} A \left(\frac{v_0}{A+1}\right)^2 + \frac{1}{2}\left(\frac{A v_0}{A+1}\right)^2 = \frac{1}{2} u_c^2 + \frac{1}{2} A U_c^2 \tag{1-43e}$$

Upon solving the last two equations for u_c and U_c in terms of v_o one finds that <u>in the center-of-mass system the speeds of neutron and nucleus are unchanged</u> by an elastic collision, that is

$$v_o - V_M = u_c = \frac{A v_o}{A+1} \tag{1-43f}$$

and

$$V_M = U_c = \frac{v_o}{A+1} \tag{1-43g}$$

We are now in a position to derive a relation between μ_o and μ_c. Noting that the velocity of the neutron in L is the vector sum of its velocity in C and the velocity of the center-of-mass in L one can write (see Figure 13),

$$u_o \mu_o = V_M + u_c \mu_c \tag{1-44a}$$

Substituting from Equations (1-43f) and (1-43g) for V_M and u_c:

$$\left(\frac{u_o}{v_o}\right)\mu_o = \frac{1}{A+1} + \frac{A}{A+1}\mu_c \tag{1-44b}$$

The ratio u_o/v_o may be obtained by applying the law of cosines to Figure 13:

$$u_o^2 = u_c^2 + V_M^2 + 2 u_c V_M \mu_c \tag{1-44c}$$

or, using Equations (1-43f) and (1-43g) again:

$$\frac{u_o^2}{v_o^2} = \frac{A^2 + 2A\mu_c + 1}{(A+1)^2} \tag{1-44d}$$

Equations (1-44b) and (1-44d) yield the desired relation between μ_o and μ_c:

$$\mu_0 = \frac{A\mu_c + 1}{\sqrt{A^2 + 2A\mu_c + 1}} \qquad (1\text{-}44e)$$

or, in terms of $\gamma = A^{-1}$

$$\mu_0 = \frac{\mu_c + \gamma}{\sqrt{\gamma^2 + 2\gamma\mu_c + 1}} \qquad (1\text{-}44f)$$

Next, consider the energy change in scattering. In L, the ratio of the energy after collision, E, to that before the collision, E', is just u_o^2/v_o^2, already given by Equation (1-44d):

$$\frac{E}{E'} = \frac{\gamma^2 + 2\gamma\mu_c + 1}{(\gamma+1)^2} \qquad (1\text{-}44g)$$

or, in terms of a more convenient parameter;

$$\alpha \triangleq \left(\frac{1-\gamma}{1+\gamma}\right)^2 = \left(\frac{A-1}{A+1}\right)^2 \qquad (1\text{-}44h)$$

the ratio of the energies is

$$\frac{E}{E'} = \frac{1}{2}\left[(1+\alpha) + (1-\alpha)\mu_c\right] \qquad (1\text{-}44i)$$

Note that Equation (1-44i) implies that $\alpha E' \leq E \leq E'$, since $-1 \leq \mu_c \leq 1$. Thus, a neutron cannot be speeded up and cannot lose more than a fraction $(1 - \alpha)$ of its energy in a single collision of this type. The parameter α is tabulated in Table IV Chapter II.

It is convenient to introduce a new variable, the <u>lethargy</u> (logarithmic energy), u, defined by

$$u = \ln (E_o/E) \; ; \quad E = E_o e^{-u} \qquad (1\text{-}45a)$$

(E_o is some convenient reference energy, generally chosen to be 10 mev.)

for the above results became somewhat simpler. For example, Equation (1-44i) becomes:

$$e^{-U} = \frac{1}{2}\left[(1+\alpha) + (1-\alpha)\mu_c\right] \qquad (1\text{-}45b)$$

where

$$U = u - u' \qquad (1\text{-}45c)$$

is the lethargy gained by the neutron in the collision. Inverting and writing the result in terms of γ, we have

$$\mu_c(U) = 1 - \frac{(1+\gamma)^2}{2\gamma}\left(1 - e^{-U}\right) \qquad (1\text{-}45d)$$

Combining this with Equation (1-44f), one finds

$$\mu_o(U) = \frac{1}{2\gamma}\left[(1+\gamma)e^{-U/2} - (1-\gamma)e^{U/2}\right] \qquad (1\text{-}45e)$$

Here, μ_o and μ_c have been written explicitly as functions of the lethargy change U to call attention to the fact that the angle of scattering is uniquely related to the lethargy change (gain) in a collision. For some purposes later in the development it will be convenient to consider μ_o as the independent variable; while at other times the choice of U will be more convenient. The maximum and minimum possible neutron energy transfer place restrictions on minimum and maximum lethargy change:

$$0 \leq U \leq \ell n \ \ 1/\alpha \qquad (1\text{-}45f)$$

or

$$u - \ell n \ 1/\alpha \ \leq u' \leq u \qquad (1\text{-}45g)$$

22. Transformation of Scattering Cross Sections

In deriving the scattering frequency, it is, of course, highly desirable to express the result in terms of the most basic data available, namely, the differential scattering cross section.* The relationship between the energy transfer in a scattering collision and the scattering angles was derived in the last section; the probability of a scattering angle occurring, which is proportional to the differential cross section, is now needed. However, cross sections are frequently presented in the center-of-mass system, whereas one would like to solve neutron moderation problems in the laboratory system. The conversion from one system to another can be carried out by the following method.[24]

Firstly, we define the $\sigma_s^o(u, \mu_o)d\mu_o$ as the cross section for scattering of neutrons into solid angle $2\pi d\mu_o$ about μ_o in the L system, and $\sigma_s(u, \mu_c)d\mu_c$ as the cross section for scattering into $2\pi d\mu_c$ in the C system. Since, for physical reasons, the number of neutrons cannot depend on the choice of coordinate system:

$$\sigma_s^o(u, \mu_o)d\mu_o = \sigma_s^c(u, \mu_c)d\mu_c \tag{1-46a}$$

where μ_o and μ_c are related by Equation (1-44e). The quantity previously called the microscopic scattering cross section, $\sigma_s(u)$, is the integral of $\sigma_s^c(u', \mu_c)$ over all solid angle or, equivalently, the integral of $\sigma_s^o(u', \mu_o)$ over solid angle:

$$\sigma_s(u) = \int d\mu_c \sigma_s^c(u, \mu_c) = \int d\mu_o \sigma_s^o(u, \mu_o) \tag{1-46b}$$

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* The differential microscopic cross section, defined only for scattering, is the area presented by a nucleus to a neutron for scattering into an element of solid angle $d\underline{\Omega}$ located about $\underline{\Omega}$, i.e., $d\sigma/d\Omega$.

[24] The ensuing development follows P. F. Zweifel and H. Hurwitz, Jr., J. Appl. Phys., 25, 1241 (1954).

Both σ_s^o and σ_s^c may be expanded in terms of Legendre Polynomials of the cosines of the scattering angles. For the L system:

$$\sigma_s^o(u, \mu_o) = \sum_{L=0}^{\infty} \frac{2L+1}{2} B_L^o(u) P_L(\mu_o) \qquad (1\text{-}46c)$$

while for the C system

$$\sigma_s^c(u, \mu_c) = \sum_{L=0}^{\infty} \frac{2L+1}{2} B_L^c(u) P_L(\mu_c) \qquad (1\text{-}46d)$$

The expansion coefficients are readily found from the orthogonality properties of the Legendre Polynomials:

$$\int_{-1}^{1} P_l(\mu) P_{l'}(\mu) d\mu = \frac{2}{2l+1} \delta_{ll'} \qquad (1\text{-}46e)$$

Now, multiplying Equations (1-46c) and (1-46d) by $P_L(\mu)$ and integrating over μ from -1 to 1, we have:

$$B_L^o(u) = \int_{-1}^{1} d\mu_o \sigma_s^o(u, \mu_o) P_L(\mu_o) \qquad (1\text{-}46f)$$

and

$$B_L^c(u) = \int_{-1}^{1} d\mu_c \sigma_s^c(u, \mu_c) P_L(\mu_c) \qquad (1\text{-}46g)$$

Since $P_o(\mu) = 1$, it is also evident that

$$\sigma_s(u) = B_o^o(u) = B_o^c(u)$$

It is possible to interrelate these expansion coefficients by use of the transformation law (1-46a). Insertion of (1-46a) into (1-46f) yields

$$B_L^o(u) = \int_{-1}^{1} d\mu_c \sigma_s^c(u, \mu_c) P_L(\mu_o) \qquad (1\text{-}47a)$$

which, upon insertion of the Legendre Polynomial expansion of $\sigma_s^c(u,\mu_c)$ (1-46d) becomes

$$B_L^o(u) = \int_{-1}^{1} d\mu_c \left[\sum_{L'=0}^{\infty} \frac{2L'+1}{2} B_{L'}^c(u) P_{L'}(\mu_c) \right] P_L(\mu_o) \quad (1\text{-}47b)$$

This equation assumes a simpler form if one defines a matrix $||T||$, with elements $T_{LL'}$:

$$T_{LL'} = \frac{2L'+1}{2} \int_{-1}^{1} d\mu_c P_{L'}(\mu_c) P_L(\mu_o) \quad (1\text{-}47c)$$

for then we have

$$B_L^o(u) = \sum_{L'=0}^{\infty} T_{LL'} B_{L'}^c(u) \quad (1\text{-}47d)$$

That is, the expansion coefficients of the differential cross section in L are the elements of the column vector resulting from multiplication of the matrix $||T||$ and the column vector formed from the expansion coefficients of the differential cross section in C. In an analagous manner, one may obtain the inverse transformation, i.e., the one which gives the $B_L^c(u)$ in terms of the $B_L^o(u)$. To do this one need only substitute (1-46a) and (1-46c) successively into (1-46f) to obtain the results

$$B_L^c(u) = \sum_{L'=0}^{\infty} T_{LL'}^{-1} B_L^o(u) \quad (1\text{-}47e)$$

with the elements of the matrix $||T||^{-1}$ given by*

$$T_{LL'}^{-1} = \frac{2L'+1}{2} \int_{-1}^{1} P_L(\mu_c) P_{L'}(\mu_o) d\mu_o \quad (1\text{-}47f)$$

* The superscript "-1" will always denote "inverse" and is not to be confused with the $T_{LL'}^n$, $(n > 0)$ introduced later.

The matrices $||T||$ and $||T||^{-1}$ are clearly inverse since successive applications of them to a cross section produces the original cross section.* Thus:

$$\sum_{L'=0}^{\infty} T_{LL'} T_{L'M}^{-1} = \delta_{LM} \qquad (1\text{-}47g)$$

It might be noted that these results may be extended from the case of elastic scattering of neutrons from nuclei, discussed here, to the case of any nuclear reaction (including inelastic scattering) redefinition of γ and U:[25]

$$\gamma = \left(\frac{m_1 m_3}{m_2 m_4} \frac{E_c}{E_c + Q} \right)^{1/2}$$

and U is taken to be the logarithm of the ratio of the energy of particle m_3 to the energy it would have if it were ejected in the forward direction. Here, a particle of mass m_1 strikes a particle of mass m_2 yielding products of mass m_3 and m_4 with a reaction energy Q (which may be either positive or negative). E_c, the initial total kinetic energy of the particles in the center-of-mass system, is related to E, the laboratory energy of particle 1 by

$$E = m_1 E/(m_1 + m_2)$$

if particle 2 is initially at rest. Note that for elastic scattering $Q = 0$ and no mass changes occur so γ is the ratio of the neutron mass to the mass of the scattering nucleus.

23. Derivation of the Elastic Scattering Frequency

Having developed the basic materials, we now attempt to exhibit the elastic scattering frequency $F(E' \to E, \underline{\Omega}' \to \underline{\Omega})$ or $F(E' \to E, \mu_o)$

* This result also follows directly from the definitions of T_{LL} and T_{LL}^{-1} and the orthogonality properties of the Legendre Polynomials.

[25] See Schiff, op cit.

explicitly in terms of basic cross sections. A slight extension of the work of the previous section is needed as lethargy changes, which are not described in the formalism just developed, must be taken into account. We have seen in Equation (1-45e) that the variable U is spurious if μ_o is specified since its value is uniquely determined by μ_o. It is, however, convenient to use both U and μ_o as variables (one of them being a dummy) in order to carry out the transformation from μ_o, an observable, to U, the variable required for slowing down calculations.

One can write

$$\sigma_s(\mu' \to \mu, u' \to u) = \sigma_s(\mu_o, u, U) \tag{1-48a}$$

or

$$F(\mu' \to \mu, u' \to u) = \frac{\sum N_i \sigma_s^{oi}(\mu_o, u', U)}{\Sigma_s(u')} \tag{1-48b}$$

where N_i is the number of nuclei of species i per cm^3 and $\sigma_s^{oi}(\mu_o, u', U)$ is the differential scattering cross section in L for the i^{th} species and the spurious variable U has been introduced. Since U is spurious, $\sigma_s^{oi}(\mu_o, u', U)$ may be written

$$\sigma_s^{oi}(\mu_o, u', U) = \sigma_s^{oi}(\mu_o, u')\,\delta(\mu_o(U) - \mu_o)\left(\frac{\partial \mu_o(U)}{\partial U}\right) \tag{1-48c}$$

Here $\delta[\mu_o(U) - \mu_o]$ is the Dirac Delta Function.[26] Equation (1-48c) expresses the fact that $\sigma_s^{oi}(\mu_o, u', U)$ vanishes unless μ_o and U are related by Equation (1-45e). Then the relation:

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[26] For properties of this function see, for example, P. A. M. Dirac, The Principles of Quantum Mechanics, Oxford (1957).

$$\sigma_s^{oi}(\mu_o, u') = \int_0^{\ln\frac{1}{\alpha}} \sigma_s^{oi}(\mu_o, u', U)\,dU \qquad (1\text{-}48d)$$

obtains. The negative sign on the Jacobian $\left|\frac{\partial\mu_o(U)}{\partial U}\right|$ in Equation (1-48c) arises from the fact that the derivative [see Equation (1-45e)] is always negative.

Next, we introduce the Legendre Polynomial expansion of $\sigma_s^o(\mu_o, u, U)$, which is similar to Equation (1-46c) but contains the spurious variable U. For convenience, the superscript 'i' is dropped for the time being, but it is to be remembered that σ^o, σ^c, $B_L^o(u')$, $B_L^o(u',U)$, α, γ, and the $||T||$ matrices are all functions of the species of scattering nucleus being considered.

$$\sigma_s^o(\mu_o, u', U) = \sum_{L'=0}^{\infty} \frac{2L'+1}{2} B_L^o(u', U) P_L(\mu_o) \qquad (1\text{-}49a)$$

where the orthogonality of the $P_L(\mu_o)$ gives, as before:

$$B_L^o(u', U) = \int d\mu_o\, \sigma_s^o(\mu_o, u', U) P_L(\mu_o) \qquad (1\text{-}49b)$$

The above expression for $B_L^o(u,U)$ can be evaluated by use of Equation (1-48c).

$$B_{L'}^o(u', U) = \int_{-1}^{1} d\mu_o\, \sigma_s^o(\mu_o, u') P_{L'}(\mu_o) \delta(\mu_o(U) - \mu_o) \left(-\frac{\partial\mu_o(U)}{\partial U}\right)$$

$$= \sigma_s^o(\mu_o(U), u') P_{L'}(\mu_o(U)) \left(-\frac{\partial\mu_o(U)}{\partial U}\right) \qquad (1\text{-}49c)$$

Finally, the $B_L^o(u',U)$ can be found in terms of the $B_L^c(u')$. First, substitute the expansion (1-46d) into Equation (1-46a) and express μ_o and μ_c in terms of U to obtain

$$\sigma_s^o(\mu_o(U),u') = \sum_{L=0}^{\infty} \frac{2L+1}{2} B_L^c(u') P_L(\mu_c(U)) \left(\frac{\partial \mu_c}{\partial U}\right) \quad (1\text{-}49d)$$

Then substitute Equation (1-49d) into Equation (1-49c) and write the results as

$$B_L^o(u',U) = \sum_{L'=0}^{\infty} T_{LL'}(U) B_{L'}^c(u') \quad (1\text{-}50a)$$

where the $T_{LL'}(U)$ are the elements of a new transformation matrix given by

$$T_{LL'}(U) = \frac{2L'+1}{2} P_L(\mu_o(U)) P_{L'}(\mu_c(U)) \left(-\frac{\partial \mu_c(U)}{\partial u}\right) \quad (1\text{-}50b)$$

Finally, substitution of Equation (1-50a) into Equation (1-49a) gives the desired laboratory system scattering function. Explicitly,

$$\sigma_s^o(\mu_o,u',U) = \sum_{L,L'=0}^{\infty} T_{LL'}(U) \frac{2L+1}{2} P_L(\mu_o) B_{L'}^c(u')$$

$$= \sum_{L,L'=0}^{\infty} \frac{2L+1}{2} P_L(\mu_o) P_L\left[\frac{1}{2\gamma}\left[(1+\gamma)e^{-U/2} - (1-\gamma)e^{U/2}\right]\right] P_{L'}\left[1 - \frac{(1+\gamma)^2}{2\gamma}(1-e^{-U})\right]$$

$$\cdot \left[-\frac{(1+\gamma)^2}{2\gamma} e^{-U}\right] B_{L'}^c(u') \quad (1\text{-}50c)$$

The last square bracket is equal to $\left(\frac{-\partial \mu_c}{\partial U}\right)$ and was obtained by differentiating Equation (1-45d). It is interesting to calculate the angularly

independent scattering function. Integrating Equation (1-50c) over all angles we find:

$$\sigma_s(u' \rightarrow u) = \sum_{L'=0}^{\infty} T_{0L'}(U) B_{L'}^{c}(u') \qquad (1\text{-}50d)$$

The $B_L^c(u')$, it may be remembered, are the Legendre coefficients of the differential cross section in the center-of-mass system. Since in the present section it has been shown that the lethargy change and the scattering angle are uniquely related by the kinematics of the collision, the reader might ask why it was necessary to introduce the angularly dependent cross section at all. The reason is that the angular differential cross section is simpler to measure (and, in cases in which no measurements are available, to calculate) than is the energy or lethargy change differential cross section. But, because the Boltzmann Equation requires that we deal with energy or lethargy variables than in angular variables, the formalism of the present section has been introduced.

As an aside, the relation between the $T_{LL'}(U)$ of this section and the $T_{LL'}$ of the previous section is:

$$T_{LL'} = \int_0^{\ln \frac{1}{\alpha}} T_{LL'}(U)\, dU \qquad (1\text{-}50e)$$

An inverse matrix $||T(U)||^{-1}$ is of little value and has, therefore, not been defined.

24. The Case of Isotropic Scattering

In many cases, elastic scattering is entirely s-wave and is therefore isotropic in the center-of-mass system. For this case,

$\sigma_s^c(u',\mu_c)$ reduces to a single term, namely the coefficient of $P_o(\mu_c) = 1$, i.e.,

$$B_L^c(u') = \sigma_s(u')\delta_{L'0} \tag{1-51a}$$

so that from Equation (1-50a) it is seen that

$$B_L^o(u',U) = T_{Lo}(U)\sigma_s(u') \tag{1-51b}$$

where the $T_{LO}(U)$, as given by Equation (1-50b) are

$$T_{Lo}(U) = \frac{1}{2} P_L(\mu_o(U)) \frac{(1+\gamma)^2}{2\gamma} e^{-U} \tag{1-51c}$$

Combining the last two equations, one obtains

$$B_L^o(u',U) = \frac{(1+\gamma)^2}{4\gamma} e^{-U} P_L\left[\frac{1}{2\gamma}\left[(1+\gamma)e^{-U/2} - (1-\gamma)e^{U/2}\right]\right]\sigma_s(u') \tag{1-51d}$$

and, finally the scattering frequency is:

$$\sigma_s^o(\mu_o,u',U) = \sigma_s(u')\sum_{L=0}^{\infty} \frac{2L+1}{2}\frac{(1+\gamma)^2}{4\gamma} e^{-U} P_L\left[\frac{1}{2\gamma}\left[(1+\gamma)e^{-U/2} - (1-\gamma)e^{U/2}\right]\right] P_L(\mu_o) \tag{1-51e}$$

While the function, $\sigma_s(u' \to u)$ becomes, for isotropic scattering

$$\sigma_s(u' \to u) = \sigma_s(u')\frac{1+\gamma}{4\gamma} e^{-U} = \frac{\sigma_s(u')e^{-U}}{1-\alpha} \tag{1-51f}$$

or, in terms of energy

$$\sigma_s(E' \to E) = \frac{\sigma_s(E')}{(1-\alpha)E'} \tag{1-51g}$$

Note that in this case, and this case only,

$$F(u' \to u) = \frac{\sigma_s(u' \to u)}{\sigma_s(u')} \tag{1-51h}$$

is a function of (u-u') only. Also note that

$$F(E' \rightarrow E) = \frac{\sigma_s(E' \rightarrow E)}{\sigma_s(E')}$$

is independent of E in this case, i.e., the energy distribution is flat in the energy range $\alpha E' < E < E'$.

E. Evaluation and Significance of the Transformation Matrices

25. Evaluation of Some of the Matrix Elements

Before attempting to discuss the physical significance of some of the matrix elements derived in the previous section, some of these elements will be evaluated explicitly so that they will be available when their significance is discussed.

The simplest way to evaluate the integrals for the $T_{LL'}$ and $T^{-1}_{LL'}$ is to substitute the expressions for $\mu_o(U)$ and $\mu_c(U)$, given by Equations (1-45d and c) into Equation (1-47c) or Equation (1-47f) directly, and then perform the integrations over U. This reduces all the integrands to sums of exponential functions, that is,

$$T_{LL'} = \frac{2L'+1}{2} \int_0^{\ln\frac{1}{\alpha}} P_L(\mu_o(U))\, P_{L'}(\mu_c(U)) \frac{\partial \mu_c}{\partial U}\, dU \qquad (1\text{-}52a)$$

$$T^{-1}_{LL'} = \frac{2L'+1}{2} \int_0^{\ln\frac{1}{\alpha}} P_L(\mu_c(U))\, P_{L'}(\mu_o(U)) \frac{\partial \mu_o}{\partial U}\, dU \qquad (1\text{-}52b)$$

where the arguments of the Legendre Polynomials are sums of exponentials from Equations (1-45d) and (1-45e). The results of some of these integrations are given below.[27]

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[27] These results are largely taken from Zweifel and Hurwitz, op cit.

$$T_{0L'} = \delta_{0L'} \qquad T_{20} = \frac{5\gamma^2-3}{8\gamma^2} - \frac{3-6\gamma^2+3\gamma^4}{32\gamma^3}\ln\alpha$$

$$T_{10} = \frac{2\gamma}{3}$$

$$T_{11} = \frac{1}{5}(5-3\gamma^2) \qquad T_{21} = \frac{9-6\gamma^2+9\gamma^4}{16\gamma^3} + \frac{9-9\gamma^2-9\gamma^4+9\gamma^6}{64\gamma^4}\ln\alpha \tag{1-53a}$$

Some of the elements of the inverse matrix $||T||^{-1}$ are

$$T^{-1}_{0L'} = \delta_{0L'}$$

$$T^{-1}_{10} = 2\gamma/3 \tag{1-53b}$$

$$T^{-1}_{11} = \frac{2}{8\gamma^2}(1+\gamma^2) - \frac{3(1+\gamma)^2(1-\gamma)^2}{22\gamma^3}\ln\alpha$$

For small values of γ, i.e., for a heavy scattering nucleus, $T_{LL'}$ and $T^{-1}_{LL'}$, may be represented by the following expansions, correct to order γ:

$$T_{LL'} = \delta_{LL'} - \gamma\left[\frac{L'(L'-1)}{2L'-1}\delta_{L',L+1} - \frac{(L'+1)(L'+2)}{2L'+3}\delta_{L',L-1}\right] \tag{1-54a}$$

and

$$T^{-1}_{LL'} = \delta_{LL'} + \gamma\left[\frac{L'(L'-1)}{2L'-1}\delta_{L',L+1} - \frac{(L'+1)(L'+2)}{2L'+3}\delta_{L',L-1}\right] \tag{1-54b}$$

Amster[28] has derived a general expression for $T_{1L'}$

$$T_{1L'} = \frac{L'}{2L'-1}(-\gamma)^{L'-1} - \frac{L'+2}{2L'+3}(-\gamma)^{L'+1} \tag{1-55a}$$

and a recursion relation:

$$T_{L+1,L'} = (2L'+1)\left(\frac{2L-1}{L+1}\right)\sum_{\lambda=0}^{\infty} T_{1\lambda}\sum_{m=|\lambda-L'|}^{|\lambda+L'|}(\lambda L'00|\lambda L00)\frac{T_{Lm}}{2m+1}\frac{L}{L+1}T_{L+1,L'} \tag{1-55b}$$

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[28] H. Amster, J. Appl. Phys., 27, 307 (1956).

where the $(jL'00|jL00)$ are Clebsch-Gordon coefficients.[29]

For later applications, in Chapter III, it will be convenient to define still another set of matrices,

$$T^{n}_{LL'} = \int_0^{\ln 1/\alpha} U^n T_{LL'}(U)\, dU \tag{1-56}$$

Note that $T^{o}_{LL'} = T_{LL'}$, according to Equation (1-50e). Using straightforward integration with $T_{LL'}(U)$ written in terms of exponentials, Equation (1-50b), one obtains:

$$T^{1}_{00} = -\left(1 - \frac{(1-\gamma)^2}{4\gamma} \ln\alpha\right) \longrightarrow -2\gamma \tag{1-57a}$$

$$T^{1}_{01} = \frac{3+3\gamma^2}{4\gamma} - \frac{3-6\gamma^2+3\gamma^4}{16\gamma^2} \ln\alpha \longrightarrow 2\gamma \tag{1-57b}$$

where the arrows indicate limits valid for small γ. $T^{1}_{OL'}$, for $L' > 1$, vanishes to order γ.

Amster[30] has also derived expansions for $T^{1}_{OL'}$ and $T^{2}_{OL'}$:

$$T^{1}_{OL'} = (-)^{L'+1}(2L'+1) \sum_{P = L' + \delta_{OL'}}^{\infty} A_{PL'}\, \alpha^P \tag{1-58a}$$

$$T^{2}_{OL'} = (-)^{L'}(2L'+1) \sum_{P = L' + \delta_{1L'} + 2\delta_{OL'}} A_{PL'} \left[\sum_{j=1}^{P} \frac{1}{\gamma}\right] \alpha^P$$

where

$$A_{PL'} = \frac{(P!)^2}{P(P-L')!\,(P+L'+1)!} \tag{1-58b}$$

and α is the usual

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29 E. U. Condon and Shortley, Theory of Atomic Spectra, Cambridge Univ. Press.

30 Amster, op cit.

$$\alpha = \left(\frac{1-\gamma}{1+\gamma}\right)^2$$

Furthermore, it was shown by Amster[31] that the T^n_{LL} approach zero as γ goes to zero and $T^n_{LL'}$ is bounded by the lesser of γ^n and $\gamma\,|L-L'|$ for small γ .

26. Moments of the Scattering Frequency

The significance of the matrix elements is readily determined. For example, consider $\xi_i = \bar{U}_i$, the average lethargy gain per collision of a neutron with a nucleus of species i, which is given by

$$\xi_i = \frac{\int d\mu_0 \int d\upsilon\, \sigma_s^{0i}(\mu_0, u', \upsilon)\upsilon}{\int d\mu_0 \int d\upsilon\, \sigma_s^{0i}(\mu_0, u', \upsilon)} \qquad (1\text{-}59a)$$

From the expansion (1-42c) and the orthogonality properties of the Legendre polynomials, this reduces to

$$\xi_i = \frac{\int d\upsilon\, \upsilon\, B_0^0(u', \upsilon)}{\int d\upsilon\, B_0^0(u', \upsilon)}$$

which can, in turn, be written in terms of the expansion coefficients in the center-of-mass system by use of the transformation (1-50a)

$$\xi_i = \frac{\sum_{L=0}^{\infty} B_L^{ci}(u') \int_0^{e^{u'/2}} d\upsilon\, \upsilon\, T_{0L}(\upsilon)}{\sum_{L=0}^{\infty} B_L^{ci}(u') \int_0^{e^{u'/2}} d\upsilon\, T_{0L}(\upsilon)}$$

The integral in the numerator is just $T^1_{0L_i}$ while that in the denominator is $T_{0L_i} = \delta_{0L}$. Remembering that $B_0^c(u) = \sigma_s(u)$ we have finally:

$$\xi_i = \frac{-\sum_{L=0}^{\infty} T^1_{0L_i} B_L^{ci}(u)}{\sigma_s^i(u)} \qquad (1\text{-}59b)$$

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[31] H. Amster, J. Appl. Phys. 29, 623 (1958).

For isotropic scattering in C, an interesting result is that ξ_i is not a function of lethargy. The sum in the numerator of (1-59b) reduces to a single term, $T^1_{00}B^c_0(u')$, so ξ_i becomes simply

$$\xi_{iso\,i} = -T^1_{00\,i} = 1 - \frac{(1-\gamma)^2}{4\gamma}\ln\alpha \to 2\gamma \qquad (1\text{-}59c)$$

which shows that ξ_i is independent of neutron energy in this case. For non-isotropic scattering, however, the average lethargy change generally depends on u. The limit 2γ given above is correct to order γ, while to order γ^2

$$\xi_{iso\,i} = \frac{2\gamma}{1+2/3\gamma} = \frac{2}{A+\frac{2}{3}} \qquad (1\text{-}59d)$$

For hydrogen $\gamma = 1$ and $\alpha = 0$ and in this limit Equation (1-55c) yields $\xi = 1$, a useful result as scattering from hydrogen is isotropic at energies of interest in reactor calculations.

Another useful quantity is the average value of the cosine of the laboratory scattering angle,

$$\langle\mu_0(u')\rangle = \frac{\int d\mu_0 \int dv\ \mu_0 \sigma_s^0(\mu_0, u', v)}{\int d\mu_0 \int dv\ \sigma_s^0(\mu_0, u', v)} \qquad (1\text{-}60a)$$

By following a procedure similar to that above, this can be shown to be

$$\langle\mu_0(u')\rangle_i = \frac{\int dv\ B_1^{0\,i}(u', v)}{\sigma_s^i(u')} \qquad (1\text{-}60b)$$

or, in terms of the expansion coefficients in C:

$$\langle\mu_0(u')\rangle_i = \frac{\sum_{L'=0}^{\infty} T_{1L'i} B_{L'}^{ci}(u')}{\sigma_s^i(u')} \qquad (1\text{-}60c)$$

For isotropic scattering in C, $< \mu >$ is also not a function of neutron energy, and is exactly

$$\langle \mu_0(u) \rangle_i = T_{10i} = \frac{2\gamma}{3} \tag{1-56c}$$

A relation between $\xi(u')$ and $< \mu(u') >$ may be found to some approximation. By expanding Equation (1-41e) in a power series, one has:

$$v = 2\gamma\left[1 - \mu_0 + \frac{\gamma^2}{2}(1-\mu_0^2) + \cdots\right] \tag{1-61a}$$

which, upon averaging, yields:

$$\xi_i = 2\gamma\left[1 - \langle \mu_0 \rangle_i + \frac{\gamma^2}{2}(1-\langle \mu_0^2 \rangle) + \cdots\right] \tag{1-61b}$$

To second order in γ:

$$T'_{0L} = -2\gamma\left[T_{0L} - T_{1L}\right] = -2\gamma\left[\delta_{0L} - T_{1L}\right] \tag{1-61c}$$

Expansions of $\xi_i \sigma_s$ and $< \mu_i > \sigma_s$, to first order in γ, (two quantities which will be very important later),

$$\xi_i \sigma_s^i = \sum_{L'=0}^{\infty} T'_{0L'} B^c_{L'}(u') \approx 2\gamma\left(B^c_0 - B^c_1\right) \tag{1-62a}$$

$$\langle \mu \rangle_i \sigma_s^i = \sum_{L'=0}^{\infty} T_{1L'} B^c_{L'}(u') \approx B^c_1 + \frac{2\gamma}{3}\left(B^c_0 - B^c_2\right) \tag{1-62b}$$

Alternatively, ξ and $< \mu >$ could be expressed in terms of the B^o_L rather than the B^c_L. For example, from Equation (1-60b) and Equation (1-50a) it follows immediately that

$$\langle \mu_0 \rangle_i = \frac{B^{oi}_1(u)}{\sigma_{si}(u)} \tag{1-63a}$$

which, when substituted into Equation (1-61b), yields

$$\xi_i = 2\gamma\left[1 - \frac{B_{1,i}^{0}(u)}{\sigma_s(u)} + \mathcal{O}(\gamma^2)\right] \qquad (1\text{-}63b)$$

By the method employed for ξ and $< \mu >$ above it is possible to find the more general moment:

$$\langle v^n P_L(\mu_0)\rangle_i = \frac{\int d\mu_0 \int dv\, v^n P_L(\mu_0)\sigma_s^{0i}(\mu_0,\mu',v)}{\int d\mu_0 \int dv \quad \sigma_s^{0i}(\mu_0,\mu',v)} \qquad (1\text{-}64a)$$

$$= \sum_{L'=0}^{\infty} T_{LL'}^{n} B_{L'}^{s,i}(u)/\sigma_{s,i}(u)$$

For isotropic scattering this becomes simply

$$\langle v^n P_L(\mu_0)\rangle_i = T_{L0\,i}^{n} \qquad (1\text{-}64b)$$

CHAPTER II

SLOWING DOWN IN AN INFINITE MEDIUM

A. Introductory Remarks

1. Importance of the Infinite Medium Problem

In this chapter, slowing down in an infinite medium is discussed. It was stated in Chapter I, and is proven below, that if sources are uniformly distributed in space and are isotropic, then the neutron angular flux is a function only of energy, $\phi(E)$. Such a case is not as academic as one might at first think. First, many reactors are so large that geometric effects are relatively unimportant; these systems display many of the characteristics of infinite systems. For example, in natural uranium-graphite reactors, which must be large to be critical, leakage is of relatively minor importance and the major problems involve spectral calculations (treated in this chapter) and the effects of inhomogeneities, treated only briefly here.

For other systems, the results derived here will be useful mainly for providing insight into the physical processes occurring. Most systems may be treated accurately only by the numerical methods discussed in Chapter IV. Here, the results obtained are useful as aids in making reasonable first guesses to the flux. Accurate guesses may greatly reduce the numerical work required and thus result in considerable savings in calculational time.

Finally, in some systems, the escape probability separates, to very good approximation, into the product of a non-leakage probability and a non-absorption (resonance escape) probability as was discussed in Chapter I. In such cases, the infinite medium problem is a significant aid in obtaining the resonance escape probability.

2. The Basic Equation

Before actually calculating neutron spectra, we would like to show that the assumptions of uniform and isotropic sources and media do lead to a spatial and angular independent neutron flux. Under these assumptions the Boltzmann Equation can be written

$$\underline{\Omega}\cdot\nabla\Phi(\underline{r},E,\underline{\Omega})+\Sigma_t(E)\Phi(\underline{r},E,\underline{\Omega})=S(E)+\int_E^\infty dE'\int d\underline{\Omega}'\,\Sigma_s(E')\Phi(\underline{r},E',\underline{\Omega}')F(E'\to E,\underline{\Omega}'\to\underline{\Omega}) \qquad (2\text{-}1a)$$

The only boundary conditions are that the flux is everywhere finite and non-negative. To prove that $\Phi(\underline{r},E,\underline{\Omega})$ is independent of E and $\underline{\Omega}$ we first convert Equation (2-1a) into an integral equation with the aid of the Green's Function of the operator on the left-hand side. The result is[1]

$$\Phi(\underline{r},E,\underline{\Omega})=\int_0^\infty dR\,e^{-\Sigma_t(E)R}\left[\int_E^\infty dE'\int d\underline{\Omega}'\,\Sigma_s(E')\Phi(\underline{r}-R\underline{\Omega},E,\underline{\Omega}')\cdot F(E'\to E,\underline{\Omega}'\to\underline{\Omega})+S(E)\right] \qquad (2\text{-}1b)$$

The last term, the one due to the source, immediately reduces to $S(E)/\Sigma_t(E)$. One may solve for $\Phi(\underline{r},E,\underline{\Omega})$ by means of the iteration procedure usually applied to integral equations. For the first iteration one has

$$\Phi^{(1)}(\underline{r},E,\underline{\Omega})=\int_0^\infty e^{-\Sigma_t(E)R}\,dR\left[\int_E^\infty dE'\int d\underline{\Omega}'\,\frac{\Sigma_s(E')}{\Sigma_t(E')}S(E')F(E'\to E,\underline{\Omega}'\to\underline{\Omega})+S(E)\right] \qquad (2\text{-}1c)$$

If rotational invariance is now invoked, one obtains a simple result; the $\underline{\Omega}$ integral then reduces to $F_0(E'\to E)$ and the R integral is again

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[1] The derivation of the Green's Function may be found in Case, Placzek and DeHoffmann, op cit., p. 13.

quite trivial. Equation (2-1c) then reduces to:

$$\Phi^{(\omega)}(\underline{r},E,\underline{\Omega}) = \frac{1}{\Sigma_t(E)}\left[S(E) + \int_E^\infty dE' \frac{\Sigma_s(E')}{\Sigma_t(E')} S(E') F_0(E'\to E)\right] \qquad (2\text{-}1d)$$

Note that the right-hand side is just a function of energy, and plays the role of a modified source. One expects that successive iterations will also be functions only of the energy. This is indeed the case, for upon iterating the result n times one finds

$$\Phi^{(n)}(\underline{r},E,\underline{\Omega}) = \frac{1}{\Sigma_t(E)}\left[S(E) + \int_E^\infty dE' \frac{\Sigma_s(E')}{\Sigma_t(E')} S(E') F_0(E'\to E) + \cdots\right.$$

$$\left. + \cdots + \int_E^\infty dE^{(n)} \frac{\Sigma_s(E^{(n)})}{\Sigma_t(E^{(n)})} F(E^{(n)}\to E) \int_{E^{(n)}}^\infty \cdots\cdots \int_{E''}^\infty dE' \frac{\Sigma_s(E')}{\Sigma_t(E')} S(E') F_0(E'\to E)\right] \qquad (2\text{-}1e)$$

which is still only a function of energy.

But the right hand side of Equation (2-1e) is just the Neumann series obtained if one solves the following equation:

$$\Sigma_t(E)\,\phi(E) = S(E) + \int_E^\infty dE' \Sigma_s(E')\phi(E') F_0(E'\to E) \qquad (2\text{-}2a)$$

This is a Volterra Integral Equation for which it is well known that the series (2-1e) converges provided the kernel

$$\Sigma_s(E') F_0(E'\to E) = \Sigma_{s_0}(E'\to E)$$

is bounded. Physically, it is evident that this kernel is bounded so that the proof that

$$\Phi(\underline{r},E,\underline{\Omega}) = \phi(E)$$

is independent of $\underline{r}$ and $\underline{\Omega}$ is now complete.

In the proof we have obtained a bonus. Equation (2-2a) is the basic equation that we will need to work with in this chapter. In terms

of lethargy it becomes

$$\Sigma_t(u)\phi(u) = S(u) + \int_0^u \Sigma_s(u')\phi(u')F(u'\to u)\,du' \qquad (2\text{-}2b)$$

Equations (2-2) are still quite difficult to solve except for the simplest cases. Generally, solution requires the use of approximate and/or numerical techniques. The difficulties may be circumvented in many cases of interest by noticing that elastic scattering is the dominant means of slowing down neutrons with energies of less than 100 kev. This, however, is precisely the range of energies through which the major part of the slowing down process takes place and it is here that resonance absorption is most important. Then, the elastic scattering frequency developed in Chapter I will be applicable to the solution of Equations (2-2). Specification of individual scattering frequencies will be delayed, however, until such time as they are required.

Equations (2-2) could be derived more easily by the physical argument that the flux be a function only of the energy. By then setting $\Phi(\underline{r},E,\underline{\Omega}) = \phi(E)$ in the Boltzmann Equation, one would obtain Equation (2-2a) immediately. The procedure followed here yields the mathematical basis for this assertion.

B. Slowing-Down in Hydrogeneous Media

3. A Rigorous Solution

A simple rigorous solution for Equation (2-2a) is possible when hydrogen is the only moderating material present. This does not preclude the possibility that absorbing materials which do not moderate ("infinitely heavy absorbers") may be present. This may seem an oversimplification, but is a reasonable approximation to light water-uranium systems. An

important point is that scattering from hydrogen is isotropic in the center-of-mass system up to several Mev, which includes almost all of the energy region of interest in reactors.

Assuming only a single heavy element, which for convenience is assumed to scatter isotropically (these conditions are not essential but simplify the calculations) Equation (2-2b) may be written:

$$\left(\Sigma_a^M + \Sigma_s^M + \Sigma_a^H + \Sigma_s^H\right)_u \phi(u) = \int_0^u \phi(u')\,\Sigma_s^H(u')\,e^{-(u-u')}\,du' + \int_{u-\ln\frac{1}{\alpha_M}}^{u} du'\left[\Sigma_s^M(u')\,\phi(u') \cdot \frac{e^{-(u-u')}}{1-\alpha_M}\right] + S(u) \qquad (2\text{-}3a)$$

where the superscripts H and M refer to hydrogen and the heavy absorbing element respectively. As the atomic weight of the absorber approaches infinity, $\alpha = \left(\frac{A-1}{A+1}\right)^2$ approaches unity and

$$\lim_{\alpha \to 1} \int_{u-\ln\frac{1}{\alpha}}^{u} \Sigma_s^M(u')\,\phi(u')\,\frac{e^{-(u-u')}}{1-\alpha}\,du' = \Sigma_s^M(u)\,\phi(u)$$

Thus for the case of "infinitely heavy absorber" one has

$$\left(\Sigma_a^M + \Sigma_a^H + \Sigma_s^H\right)_u \phi(u) = \int_0^u \Sigma_s(u')\,\phi(u')\,e^{-(u-u')}\,du' + S(u) \qquad (2\text{-}3b)$$

It was shown, by physical arguments, in Section I-15 that the slowing down density $q(\underline{r},E)$ is more slowly varying in energy than the flux. Therefore, most of the development in this and the following will be in terms of the slowing down density rather than the flux. From Equation (1- 32b), remembering that the flux is independent of position, we have for the case of slowing down by hydrogen alone:

$$q(u) = \int_0^u \Sigma_s^H(u')\,\phi(u')\,e^{-(u-u')}\,du' \qquad (2\text{-}4a)$$

which, accidentally, happens also to be the integral term on the right-hand side of Equation (2-3b), the "degradation integral". A useful relation may be obtained by differentiating Equation (2-4a) and adding the result to itself.

$$q(u) + \frac{\partial q}{\partial u} = \Sigma_s^H(u)\,\phi(u) \qquad (2\text{-}4b)$$

Equations (2-4a) and (2-4b), which are peculiar to hydrogen moderation, hold also in the space dependent case, since none of the arguments leading to them need be changed. Eliminating the degradation integral between Equations (2-3b) and (2-4a), one finds

$$q(u) = \Sigma_t(u)\,\phi(u) - S(u) \qquad (2\text{-}4c)$$

where

$$\Sigma_t(u) \triangleq \Sigma_s^H(u) + \Sigma_a^H(u) + \Sigma_a^M(u) \qquad (2\text{-}4d)$$

We next define the collision density, $\chi(u)$, the number of collisons per unit lethargy involving neutrons with lethargies about u per second.

$$\chi(u) \triangleq \Sigma_t(u)\,\phi(u) \qquad (2\text{-}4e)$$

Elimination of $q(u)$ between Equations (2-4b) and (2-4c) yields a differential equation for $\chi(u)$:

$$\frac{d\chi(u)}{du} + C(u)\,\chi(u) = S(u) + \frac{dS}{du} \qquad (2\text{-}5a)$$

where

$$C(u) \triangleq \frac{\Sigma_s^H(u)}{\Sigma_t(u)} \qquad (2\text{-}5b)$$

Let $u = 0$ correspond to some energy above which no neutrons are born, i.e., $S(u) = 0$ for $u < 0$. Then integration of Equation (2-5a) is

straightforward and yields

$$\chi(u) = \int_0^u S(u)C(u')\, e^{-\int_{u'}^{u} C_0(u'')\,du''}\, du' + S(u) \qquad (2\text{-}6a)$$

where

$$C_0(u) \triangleq 1 - C(u) = \frac{\Sigma_a(u)}{\Sigma_t(u)} \qquad (2\text{-}6b)$$

From the definition of the resonance escape probability (see Section 17) $p(u)$ is the ratio of the number of neutrons reaching lethargy u to the total number which would reach it if no absorption took place.

$$p(u) = \frac{q(u)}{\int_0^u S(u')\,du'} = 1 - \frac{\int_0^u \Sigma_a(u')\phi(u')\,du'}{\int_0^u S(u')\,du'} \qquad (2\text{-}7a)$$

Or, for hydrogen

$$p(u) = 1 - \frac{\int_0^u C_0(u')\left[\int_0^{u'} S(u'')\,C(u')\, e^{-\int_{u''}^{u} C_0(u''')\,du'''} + S(u')\right]du'}{\int_0^u S(u')\,du'} \qquad (2\text{-}7b)$$

An often quoted form for p may be obtained if we let $S(u'')$ be $\delta(u''-u')$, a monoenergetic source of one neutron per second. The integral over u'' is then trivial and yields the result:

$$p(u' \rightarrow u) = C(u')\, e^{-\int_{u'}^{u} C_0(u'')\,du''} \qquad (2\text{-}7c)$$

In the limit that $c_0(u)$ vanishes, $p(u' \rightarrow u) = 1$, as expected. For the case of capture only at energies below the source energies, the slowing down density and resonance escape probability are identical

$$\chi(u) = q(u) = p(u) \qquad (2\text{-}8a)$$

assuming a unit source; furthermore

$$\phi(u) = \frac{q(u)}{\Sigma_t(u)} \qquad (2\text{-}8b)$$

The simplicity of the results, e.g., a collision density that is independent of u, is one reason for introducing the lethargy variable. To obtain ϕ in terms of the energy one sets

$$\phi(E)\,dE = \phi(u)\,du \tag{2-9a}$$

so that

$$\phi(E) = \frac{p(E)}{E\,\Sigma_t(E)} \tag{2-9b}$$

In the limit of zero absorption, noting that the scattering cross section of hydrogen is constant between about 0.1 ev. and 100 kev., one has

$$\phi(E) = \frac{1}{E\,\Sigma_s} \tag{2-9c}$$

the well known '1/E' spectrum.

An important equation may be derived by differentiating Equation (2-7a)

$$\frac{dq}{du} = S(u) - \Sigma_a(u)\phi(u) \tag{2-9d}$$

This equation is generally valid in the space-independent case because Equation (2-7a) holds in general, not just for the case of hydrogen moderation. Equation (2-9d) is simply a statement of neutron conservation, i.e., the rate at which neutrons appear in the system is equal to the rate at which they are produced by the source minus the rate at which they are absorbed. For the space-dependent case, by the way, we must also subtract from the right-hand side of Equation (2-9d) the rate at which neutrons leak, which is simply the divergence of the current $\underline{J}$.

$$\frac{\partial q(\underline{r},u)}{\partial u} = S(\underline{r},u) - \Sigma_a(\underline{r},u)\phi(\underline{r},u) - \underline{\nabla}\cdot\underline{J}(\underline{r},u) \tag{2-9e}$$

C. Slowing-Down in Media Containing Heavy Elements:
I. Non Absorbing Media

4. Neutron Slowing Down Spectra

For media containing materials of mass number greater than unity, exact solutions of Equation (2-2b) cannot be obtained in terms of a function which is continuous for all energies. It can, in fact, be shown[2] that the only solution of Equation (2-2b) that is continuous at all energies is a constant in lethargy, which is the asymptotic solution (far from sources) as we shall soon see. Considering only the case of a single non-hydrogenous moderator, we note that a monoenergetic neutron source gives rise to once collided neutrons with energies between αE_o and E_o; neutrons of energy less than αE_o can arise only from multiple collisions. The first collision distribution is indeed continuous for $\alpha E_o < E < E_o$; for isotropic scattering in the center of mass system, it was seen in Chapter I that this distribution is actually constant (in energy) over this energy range and zero elsewhere. Similarly, the twice-collided distribution is continuous and non-zero for $\alpha^2 E_o < E < E_o$ and zero everywhere else. A careful analysis will show that the twice-collided distribution actually goes to zero at $\alpha^2 E_o$ and is therefore continuous there. However, its first derivative is readily shown to be discontinuous there.

From the above argument, we see that the flux at energies just above αE_o will be greater than that at energies just below αE_o by the contribution to the flux of the first collided neutrons reaching energies just above αE_o, i.e., the flux is discontinuous at αE_o. Similarly,

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[2] V. C. Boffi, Annals of Physics, 9, 435 (1960).

the nature of the twice-collided flux creates a discontinuity in the first derivative of the flux at $\alpha^2 E_o$. Continuation of this analysis shows that in general the n-th derivative is discontinuous at $\alpha^{n+1} E_o$. Far from the source, this transient behavior damps out and the flux approaches a smooth asymptotic function (the 1/E spectrum). Hydrogen, of course, displays none of this behavior since a neutron may lose all of its energy in one collision.

A monoenergetic sink, such as might arise from an idealized absorption resonance, will produce analogous results, except, of course, the transient will have to be subtracted from rather than added to the flux due to other sources and/or sinks. Fortunately, in most cases of practical interest, resonance absorption does not set in until some lethargy from the source. In these cases it is sufficient simply to study the effect of capture upon the asymptotic energy distribution arising from the sources. The fact that the rapidity with which the asymptotic distribution is reached decreases sharply with decrease in the mass number of the moderator (except in the anomalous case of hydrogen) makes deuterium moderation problems particularly difficult to treat.

5. Transient Solutions - Placzek Functions[3]

First, we shall derive solutions to Equation (2-2b) near the source, i.e., the transient solutions, which, despite their rigor, have found relatively small practical application. This is largely due to the fact that there are no transients when hydrogen is the only moderator present, and that the transient usually die out before resonance absorption

[3] G. Placzek, Phys. Rev., 69, 423 (1946).

sets in beryllium or carbon moderated reactors. It is possible that these solutions will find increased application if heavy water reactors become more common. One application of these transient solutions, called the "Plazcek Functions", will be given later in this chapter.

Consider the case of pure heavy element moderation. Mixtures of elements may be treated by this method, but it usually suffices to take only the longest lived transient, i.e., that due to the lightest element (other than hydrogen) that may be present. A mono-energetic source is considered, but it is again remarked that the solution for this case is also the Green's Function of the more general problem. Since the functional behavior flux is not continuous to all orders at the points $\alpha^n E_o$, $n = 1, 2, \ldots$, the flux itself must be represented by a different smooth function, which we denote by $\phi_n(E)$ or $\phi_n(u)$, on each energy interval $\alpha^{n+1}E_o < E < \alpha^n E_o$, (or in lethargy $(n+1)\ln 1/\alpha > u > n \ln 1/\alpha$).

On the interval $0 < u < \ln 1/\alpha$ the equation will be slightly different than it is for higher lethargies. Source neutrons collide to give a first collision lethargy distribution $e^{-u}/(1-\alpha)$ for $u < \ln 1/\alpha$; this must be added to the multiple collision contribution so that Equation (2-2b) becomes, on the first collision interval, ignoring absorption,

$$\chi_o(u) = \Sigma_s(u)\phi_o(u) = \frac{e^{-u}}{1-\alpha} + \int_o^u \frac{e^{-(u-u')}}{1-\alpha}\chi_o(u')\,du' \qquad (2\text{-}10a)$$

where $\chi_n(u)$ is to represent the collision density for lethargies in the n-th interval. Equation (2-10a), a linear Volterra Integral Equation of the second kind, can be solved by any of several methods, among them

La Place Transforms and the iteration method used earlier. The simplest attack is probably to multiply Equation (2-10a) by e^u and differentiate, arriving at the differential equation

$$\frac{d\chi_0(u)}{du} - \frac{\alpha}{1-\alpha}\chi_0(u) = 0 \qquad (2\text{-}10b)$$

A suitable boundary condition is obtained by noticing that near the source the multiple collision contribution to $\chi_0(u)$ is small so that

$$\lim_{u\to 0} \chi_0(u) = \frac{1}{1-\alpha} \qquad (2\text{-}10c)$$

the solution of (2-10b) with boundary condition (2-10c) is relatively straightforward and results in

$$\chi_0(u) = \frac{e^{(\alpha/1-\alpha)u}}{1-\alpha} \qquad (2\text{-}10d)$$

while, using the transformation law (2-9a), we have in terms of the energy:

$$\chi_0(E) = \frac{1}{(1-\alpha)E}\left(\frac{E_0}{E}\right)^{\alpha/1-\alpha} \qquad (2\text{-}10e)$$

Note that this reduces to the exact solution for slowing down without absorption in hydrogen. It further shows that the deviation from the '1/E' spectrum in the first collision interval increases with increasing α or A but, of course, the first collision interval does not extend as far for heavy elements.

For the other $\chi_n(u)$ one must separate the contributions from the lethargy intervals $n \ln 1/\alpha < u' < u$ and $u - \ln 1/\alpha < u' < n \ln 1/\alpha$, thus arriving at the integral equation:

$$\chi_n(u) = \int_{n\ln\frac{1}{\alpha}}^{u} \chi_n(u')\frac{e^{-(u-u')}}{1-\alpha}\,du' + \int_{u-\ln\frac{1}{\alpha}}^{n\ln\frac{1}{\alpha}} \chi_{n-1}(u')\frac{e^{-(u-u')}}{1-\alpha}\,du' \qquad (2\text{-}11a)$$

which may be solved by the method used to find $\chi_0(u)$. Again multiplying by e^u and differentiating with respect to u, we have

$$\frac{d\chi_n(u)}{du} - \frac{\alpha}{1-\alpha}\chi_n(u) = -\frac{\chi_{n-1}(u-\ln\frac{1}{\alpha})}{1-\alpha} \qquad (2\text{-}11b)$$

On introducing the integrating factor $e^{-(\alpha/1-\alpha)u}$ one has

$$e^{(\alpha/1-\alpha)u}\frac{d}{du}\left[\chi_n(u)e^{-(\alpha/1-\alpha)u}\right] = -\frac{\chi_{n-1}(u-\ln\frac{1}{\alpha})}{1-\alpha} \qquad (2\text{-}11c)$$

which is readily integrated to yield

$$\chi_n(u) = \chi_n(n\ln\tfrac{1}{\alpha})\, e^{(\alpha/1-\alpha)(u-n\ln\frac{1}{\alpha})} - \int_{n\ln\frac{1}{\alpha}}^{u} \chi_{n-1}(u'-\ln\tfrac{1}{\alpha})\,\frac{e^{(\alpha/1-\alpha)(u-u')}}{1-\alpha}\,du' \qquad (2\text{-}11d)$$

Here we note that except at $u = \ln 1/\alpha$

$$\chi_n(n\ln\tfrac{1}{\alpha}) = \chi_{n-1}(n\ln\tfrac{1}{\alpha}) \qquad (2\text{-}11e)$$

while at $u = \ln 1/\alpha$, the flux is not continuous, but, as was mentioned, the discontinuity is just the direct contribution of the source so that

$$\chi_1(\ln\tfrac{1}{\alpha}) = \chi_0(\ln\tfrac{1}{\alpha}) - \frac{\alpha}{1-\alpha} \qquad (2\text{-}11f)$$

Thus, one has for $\chi_1(u)$:

$$\chi_1(u) = \frac{1-\alpha^{1/1-\alpha}}{1-\alpha}\, e^{(\alpha/1-\alpha)u} - \frac{\alpha^{(\alpha/1-\alpha)}}{(1-\alpha)^2}(u-\ln\tfrac{1}{\alpha})\, e^{(\alpha/1-\alpha)u} \qquad (2\text{-}11g)$$

The functions $\chi_n(u)$ for $n > 1$ are readily obtained by iterating with Equation (2-11d) using the boundary condition (2-11e). They increase rapidly in complexity and are plotted as $(1-\alpha)\,\chi(u)$ in Figure 1 for moderators of $A = 4$ and $A \to \infty$. One notes that this function has almost reached its asymptotic value at $E = \alpha^3 E_0$ which is rather close to the source energy except for deuterium. It is possible to calculate the asymptote using this formulation but another, simpler method can be used, and

will be displayed in the next section. The deviation of $\chi(u)$ from the asymptotic value is shown in Figure 2.

6. Asymptotic Energy Distribution

For a non-absorbing medium the asymptotic energy distribution may be found quite straightforwardly by a method due to Marshak,[4] which has the advantages of greater flexibility and hence, wider applicability. First, the case of a single moderator shall be considered as an illustration of the method and then the physically more interesting case of mixture will be discussed. Later, it will be applied to a simple case that includes capture. The method applies to hydrogen as well as any other moderator.

Again we consider only a non-absorbing medium in which isotropic elastic scattering is the only means of slowing down. Anisotropic scattering is allowed by this method only if the anisotropy is the same at all energies, which is a rather uninteresting problem. Since we will be interested in the behavior of χ far from the source, we let $S(u) = \delta(u)$. Thus the equation:

$$\Sigma_s(u)\phi(u) = \int_{u-\ln\frac{1}{\alpha}}^{u} \Sigma_s(u')\phi(u')F(u'-u)\,du' + \delta(u) \qquad (2\text{-}12a)$$

is the starting point. The fact that $F(u' \to u)$ is a function only of $(u-u')$ has been used explicitly. The Laplace Transform method[5] may be applied when it noted that the lower limit of the integral in Equation (2-12a) could be taken as zero since $F(u'-u)$ is defined as zero outside

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[4] R. E. Marshak, Revs. Mod. Phys., 19, 185 (1947).

[5] For a review of the properties of Laplace Transforms see, for example, R. V. Churchill, Operational Mathematics, New York: McGraw-Hill Book Co., 1958.

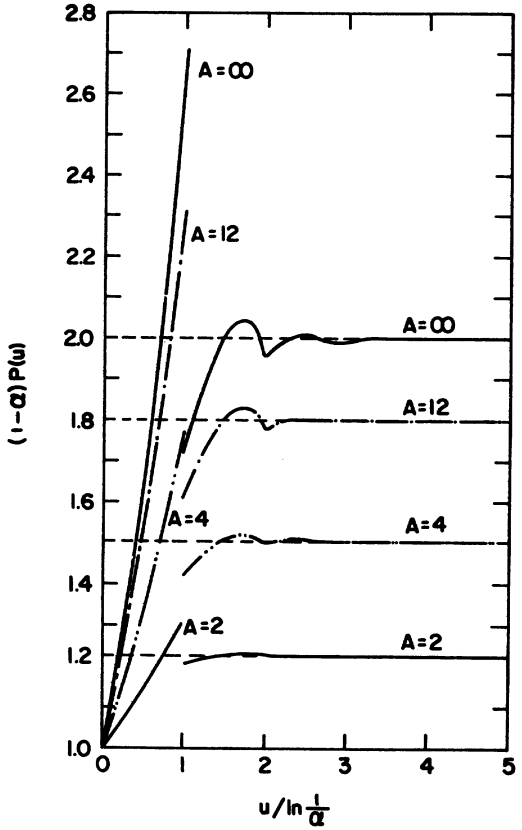

Figure II-1 The Placzek function P(u) as a function of lethargy.

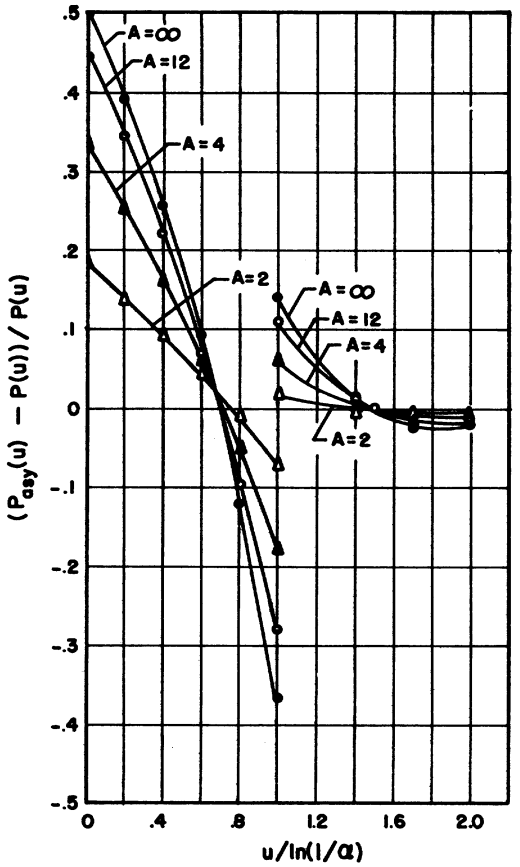

Figure II-2 The deviation of the Placzek function from its asymptotic value.

the interval $u' < u < u' + \ln 1/\alpha$. Then the integral is a Laplace Transform Convolution and the Laplace Transform of Equation (2-12a) is simply:

$$\psi(s) = \psi(s) f(s) + 1 \qquad (2\text{-}12b)$$

where

$$\psi(s) = \mathcal{L}\{\chi(u)\} = \int_0^\infty \chi(u) e^{-su} du \qquad (2\text{-}12c)$$

is the Laplace Transform of $\chi(u)$ and

$$f(s) = \mathcal{L}\{F(u)\} = \int_0^\infty F(u) e^{-su} du \qquad (2\text{-}12d)$$

$$= \int_0^{\ln \frac{1}{\alpha}} \frac{e^{-(s+1)u}}{1-\alpha} du = \frac{1-\alpha^{s+1}}{(1-\alpha)(s+1)} \qquad (2\text{-}12e)$$

is the Laplace Transform of $F(u)$ for elastic scattering, isotropic in the center of mass system. Solving Equation (2-12b) for $\psi(s)$, we have:

$$\psi(s) = \frac{1}{1-f(s)} = 1 + \frac{f(s)}{1-f(s)} = 1 + \frac{1-\alpha^{s+1}}{(1-\alpha)(s+1) - (1-\alpha^{s+1})} \qquad (2\text{-}13a)$$

the unity term has been separated from the remainder of the right hand side of the equation since it is the Laplace Transform of the source term, $\delta(u)$. Applying the inversion theorem for Laplace Transforms to $\psi(s)$, we have:

$$\chi(u) = \delta(u) + \frac{1}{2\pi i} \int_{b-i\infty}^{b+i\infty} \frac{(1-\alpha^{s+1}) e^{su}}{(1-\alpha)(s+1) - (1-\alpha^{s+1})} ds \qquad (2\text{-}13b)$$

where $\delta(u)$ represents the direct source contribution and the line of integration in the complex plane, $\mathrm{Re}(s) = b$, is to the right of all poles of the integrand. These poles are at the zeros of the denominator, i.e., at the roots of

$$(1-\alpha)(s+1) = 1 - \alpha^{s+1} \qquad (2\text{-}13c)$$

since all of the functions appearing in the integrand are, by themselves, analytic everywhere in the finite complex plane. By closing the contour of integration around the left half plane and noting that the integral on the semi circle (see Figure 3) is zero, we can evaluate $\chi(u)$ as a sum of residues:

$$\chi(u) = \delta(u) + \sum_{i=0}^{\infty} \frac{(1-\alpha^{s_i+1})\, e^{s_i u}}{(1-\alpha) + \alpha^{s_i+1} \ln\alpha} \qquad (2\text{-}13c)$$

where the s_i are the roots of Equation (2-13b) and each term represents the contribution of the residue of the pole at s_i. Thus, the flux may be expressed as a sum of exponentials. It may be shown with a little algebraic manipulation that Equation (2-13b) has only one solution with a non-negative real part, for $0 < \alpha < 1$, namely $s_o = 0$. All other terms of the series (2-13c) therefore die out for large u so the asymptotic solution (i.e., the solution at energies from below the source energy) becomes:

$$\chi_{asy}(u) = \Sigma_s(u)\phi_{asy}(u) = \frac{1-\alpha}{1-\alpha+\alpha\ln\alpha} = \frac{1}{1+\frac{\alpha}{1-\alpha}\ln\alpha} = \frac{1}{\xi_{iso}} \qquad (2\text{-}14a)$$

where ξ_{iso} is the average logarithmic energy loss per collision defined by Equation (1-59d). Marshak[6] has determined that the poles with the second largest real part are

$$s = -1.55 \pm 3.37i \quad \text{for deuterium} \quad A = 2 \qquad (2\text{-}14b)$$

$$s = -.52A \pm 1.87Ai \quad \text{for} \quad A >> 1 \qquad (2\text{-}14c)$$

Therefore, terms of order $e^{-1.55u}$ for deuterium and $e^{-.52Au}$ for heavy elements, are neglected in the asymptotic solution (2-14a).

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[6] R.E. Marshak, op. cit.

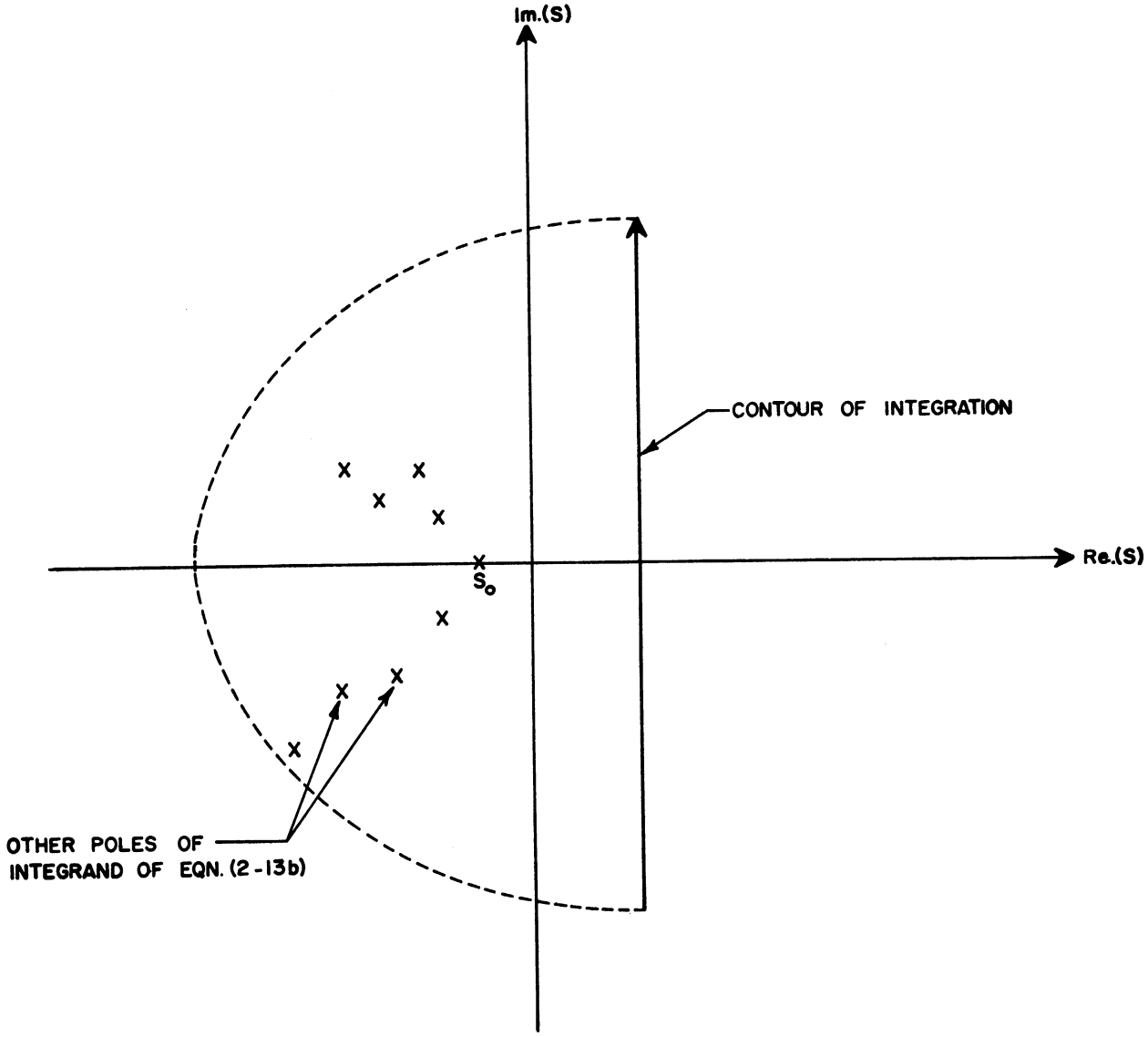

Figure II-3 Contour of integration for Equation (2-13b).

For hydrogen, $\alpha = 0$, and Equation (2-13b) has only a single root, that at $s = 0$, and the rigorous result again follows. Again, deuterium moderation is the worst case, as the series (2-13c) converges most slowly for this case.

For constant Σ_s, the asymptotic flux spectrum is again constant in lethargy, and therefore yields the '1/E' spectrum

$$\phi_{asy}(E) = \frac{1}{E \Sigma_{tot} \Sigma_s} \qquad (2\text{-}14d)$$

Clearly, the series (2-13c) must converge to the Placzek Function. However, the rapid variation of this function near the source (see Figures 1 and 2) would require a large number of terms for reasonable convergence, particularly near the discontinuity at αE_o, where the Gibbs Phenomenon will occur. In this region, the method of Section 5 is more useful.

7. Mixtures of Moderators

A procedure analogous to that of Section 6 may be followed for a mixture of elements, provided the scattering cross sections of all elements vary in the same way with energy (or are constant), and scattering is isotropic. The development will be sketchy as it is essentially the same as the one just given.

Define

$$\beta_j = \frac{\Sigma_s^j}{\Sigma_s} \qquad (2\text{-}15a)$$

the fraction of scattering from nuclei of the j-th type. Then Equation (2-2b) becomes

$$\chi(u) = \sum_j \beta_j \int_{u-\ln\frac{1}{\alpha_j}}^{u} \chi(u') F_j(u'-u)\, du' + \delta(u) \qquad (2\text{-}15b)$$

Proceeding as before, the Laplace Transform of $\chi(u)$ is found to be

$$\psi(s) = \frac{1}{1-\sum_j \beta_j f_j(s)} = 1 + \frac{\sum_j \beta_j f_j(s)}{1-\sum_j \beta_j f_j(s)} \qquad (2\text{-}15c)$$

where $f_j(s)$ is defined exactly as before

$$f_j(s) = \frac{1-\alpha_j^{s+1}}{(1-\alpha_j)(s+1)} \qquad (2\text{-}15d)$$

The inversion integral is:

$$\chi(u) = \delta(u) + \frac{1}{2\pi i}\int_{b-i\infty}^{b+i\infty} \frac{\sum_j \frac{\beta_j(1-\alpha_j^{s+1})}{(1-\alpha_j)(s+1)}}{1-\sum_j \frac{\beta_j(1-\alpha_j^{s+1})}{(1-\alpha_j)(s+1)}} e^{su}\, ds \qquad (2\text{-}16a)$$

and the poles of the integrand are at the zeros of:

$$\sum_j \frac{\beta_j(1-\alpha_j^{s+1})}{(1-\alpha_j)(s+1)} = 1 \qquad (2\text{-}16b)$$

Thus

$$\chi(u) = \delta(u) + \sum_{i=0}^{\infty}\left[\frac{\sum_j \frac{\beta_j(1-\alpha^{s_i+1})}{(1-\alpha_j)(s_i+1)} e^{s_i u}}{\sum_j\left[\frac{\beta_j \alpha_j^{s_i+1}\ln\alpha_j}{(1-\alpha_j)(s_i+1)} + \frac{\beta_j(1-\alpha^{s_i+1})}{(1-\alpha_j)(s_i+1)^2}\right]}\right] \qquad (2\text{-}16c)$$

Again, the only root of Equation (2-22a) with non-negative real part is $s_o = 0$ so that the asymptotic flux becomes

$$\chi_{asy}(u) = \Sigma_s(u)\phi_{asy}(u) = \frac{1}{1+\sum_j \frac{\beta_j \alpha_j \ln\alpha_j}{(1-\alpha_j)}} = \frac{1}{\bar{\xi}_{1s_o}} \qquad (2\text{-}16d)$$

where the definition

$$\bar{\xi}_{iso} = \sum_j \beta_j \xi_{j iso} \tag{2-16e}$$

has been invoked. As one would expect, $\bar{\xi}_{iso}$ is the average lethargy gain per collision in the mixture. This is readily shown. Since β_j is the fraction of neutrons which scatter off j type nuclei, the scattering frequency must be written

$$F(u'-u) = \sum_j \beta_j F_j(u'-u)$$

and upon averaging $(u-u')$ over this scattering frequency one finds that $\langle u-u' \rangle = \bar{\xi}_{iso}$.

In the limit of vanishingly small capture, one might assert that the effect of capture on the neutron energy spectrum would be negligible. The resonance escape probability for this limit could then be written:

$$p(u) = 1 - \int_0^u \Sigma_a(u')\phi(u')\,du' = 1 - \int_0^u \frac{\Sigma_a(u')}{\bar{\xi}_{iso}\,\Sigma_s(u')}\,du' \tag{2-17a}$$

assuming that capture takes place at lethargies far from the source. Since the integral is, by assumption, small, we may write

$$p(u) \approx \exp\left\{-\int_0^u \frac{C_0(u')}{\bar{\xi}_{iso}}\,du'\right\} \tag{2-17b}$$

8. Scattering Resonances

The case just treated is a useful first approximation; it does not, however, successfully account for scattering resonances. In heavy elements, such as the common reactor fuels, absorption resonances are

almost always accompanied by scattering resonances.* Furthermore, other materials, for example moderators, structural materials and coolants, generally display strong scattering resonances in the energy region traversed by a neutron in slowing down. Thus a more detailed treatment of the problem must be made. This problem is of very great significance in fast reactors, in which most neutron absorption takes place in the resonance region.

Qualitatively, a change in the scattering cross section one element changes $\bar{\xi}$, sometimes by quite a significant amount. For the sake of argument, let us say that the resonance occurs in a light element and that the resonance width is of the order of at least some of the $\ln 1/\alpha$, a not unreasonable case. Now, most of the neutrons arriving at energies near the high-energy end of the resonance, will come from energies at which the effect of the resonance is unimportant. Hence the collision density $\Sigma_s(u)\phi(u)$ will still behave like $1/\bar{\xi}_o$, where $\bar{\xi}_o$ is the non-resonance value of $\bar{\xi}$. In the resonance, a greater proportion of the neutrons will be scattered by the light nucleus displaying the resonance and on the average they will lose more energy in a collision than they would outside the resonance. As a result the collision density at the low-energy end of the resonance will be less than $1/\bar{\xi}_o$. Still later, at energies just below the resonance, the collision density will tend to return to its $1/\bar{\xi}_o$ behavior. However, some of the neutrons scattered in the resonance may reach these energies and the collisions density may

* Generally speaking, resonances at low energies tend to absorb more heavily (i.e., σ_a/σ_s is higher) than high energy resonances. This is due to the behavior of the Breit-Wigner parameters Γ_n and Γ_γ discussed later.

be greater than $1/\bar{\xi}_o$. Eventually, of course, $\Sigma_s(u)\phi(u)$ does resume its asymptotic value, assuming that no other resonances are found below the resonance in question. The important point is that the behavior of the collision density is not at all like $1/\bar{\xi}(u)$, as might be inferred from the previous section.

A complete description of these processes can only be done numerically and the results of such a calculation,[7] which displays the features described above, is given in Figure 4.

D. Slowing-Down in Media Containing Heavy Elements: II-Absorbing Media

9. The Case of Constant Capture*

Now consider the more general case in which the effects of neutron absorption are no longer necessarily small. The effects of absorption act primarily on the asymptotic spectrum, since absorption usually does not become important until after the asymptotic distribution has set in. A solution for the case in which absorption takes place close to the source is possible but will be delayed until the more important case of the effect on the asymptotic flux has been presented.

For a single moderating element, with isotropic scattering, and monoenergetic source, Equation (2-2b) becomes:

$$\chi(u) = \Sigma_t(u)\phi(u) = \int_{u-\ln\frac{1}{\alpha}}^{u} c(u')\chi(u')\frac{e^{-(u-u')}}{1-\alpha}\,du' + \delta(u) \qquad (2\text{-}18a)$$

with

$$c(u) \triangleq \frac{\Sigma_s(u)}{\Sigma_t(u)} \qquad (2\text{-}18b)$$

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* As the scattering cross section is usually nearly constant, this amounts to constant capture in most cases.

[7] R. Nicholson, P.F. Zweifel and J. H. Ferziger, Trans. Amer. Nuc. Soc., 4, 1 (June, 1961) Paper 2-5.

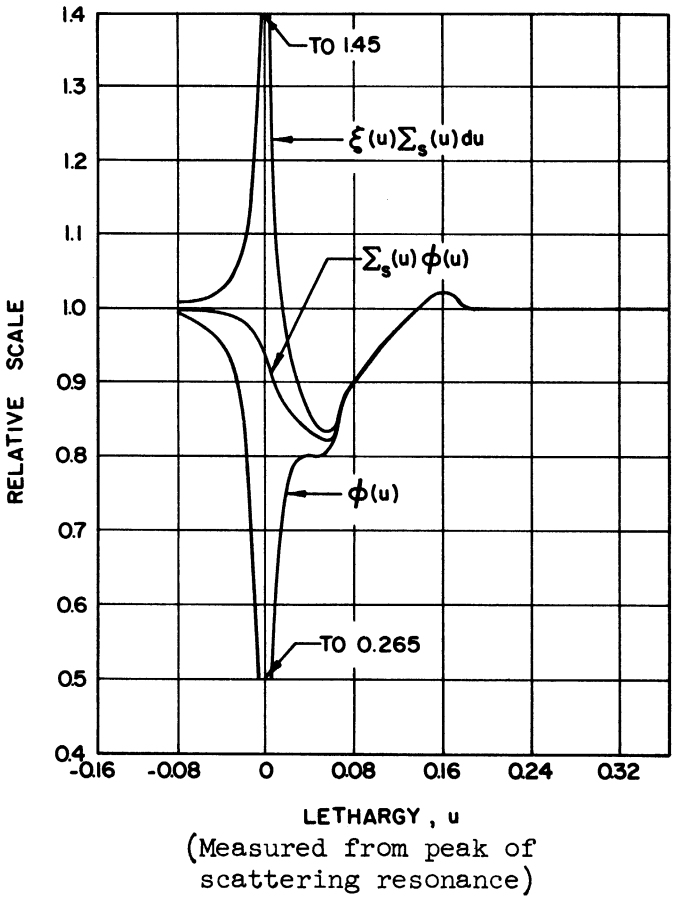

Figure 4. The flux and collision density through a sodium resonance in a sodium-iron mixture. The resonance is assumed at $u = 0$ with a lethargy width $\Delta u = .01$ (Breit Wigner width) and the parameters were

$$\Sigma_p^{Na} = 1, \quad \Sigma_p^{Fe} = 3,$$

$$\Sigma_o \text{ (resonance height)} = 10.$$

This equation is not amenable to solution by the previous method as it stands. If, however, $c(u)$ is constant, i.e., the ratio of capture and scattering cross sections is independent of energy,* the mathematical solution is the same as in the no capture case but with $f(s)$ replaced by $cf(s)$. The case of a single element will be illustrated for simplicity; mixtures are, in principle, no more difficult to treat but lead to more complicated expressions.

In analogy to Equation (2-13c) one obtains:

$$\chi(u) = \delta(u) + \sum_i \frac{c\,(1-\alpha^{\nu_i+1})\,e^{\nu_i u}}{(1-\alpha) + c\,\alpha^{\nu_i+1}\ln\alpha} \qquad (2\text{-}19a)$$

where the ν_i are the roots of the transcendental equation:

$$(1-\alpha)(\nu_i+1) = c\,(1-\alpha^{\nu_i+1}) \qquad (2\text{-}19b)$$

Again it may be shown (by separating the real and imaginary parts of the equation) that there are no ν_i with real parts greater than zero. For $c = 1$, it is clear that the ν_i are identically the roots of Equation (2-13b). For c slightly less than unity one expects that the roots will change only slightly. In particular, the root at zero for $c = 1$ is a single root and can be expected to remain real since complex roots must occur in conjugate pairs. The single root can be expected to move to the left along the real axis in the complex plane, but should still be the root with largest real part for c near unity. The asymptotic distribution will then be that due to the first term of the series (2-19a):

$$\chi_{asy}(u) = \chi_t(u)\,\phi_{asy}(u) = \frac{c\,(1-\alpha^{\nu_0+1})\,e^{\nu_0 u}}{(1-\alpha) + c\,\alpha^{\nu_0+1}\ln\alpha} \qquad (2\text{-}20a)$$

---

* As the scattering cross section is usually nearly constant, this amounts to constant capture in most cases.

For c near unity, and therefore small ν_0, the expansion

$$\alpha^{\nu_0} \approx 1 + \nu_0 \ln \alpha \tag{2-20b}$$

is valid and

$$\nu_0 \approx \frac{1-c}{1+\frac{c\alpha}{1-\alpha}\ln\alpha} \approx \frac{c_0}{\xi_{1s0}} \tag{2-20c}$$

So that the asymptotic flux is approximately

$$\phi_{asy}(u) = \frac{1}{\Sigma_t(u)}\left[\frac{c\,(1-\nu_0(\xi_{1s0}-1))}{1+c(1+\nu_0\ln\alpha)(\xi_{1s0}-1)}\right] e^{-c_0 u/\xi_{1s0}} \tag{2-20d}$$

$$\approx \frac{e^{-c_0 u/\xi_{1s0}}}{\xi_{1s0}\,\Sigma_t(u)}$$

The asymptotic flux is only roughly proportional to 1/E. The resonance escape probability for this situation is approximately given by:

$$p(u) = 1 - \int_0^u \Sigma_a(u')\,\phi_{asy}(u')\,du'$$

$$= 1 - \int_0^u \frac{c_0}{\xi_{1s0}}\, e^{-c_0 u'/\xi_{1s0}}\, du' = e^{-c_0 u/\xi_{1s0}} \tag{2-20e}$$

10. Slowly Varying Capture[8]

If c is not a constant, but is a function of lethargy, the Laplace Transform method breaks down. Of most practical interest is the case in which absorption is negligible until a considerable distance from the source. Then as we have seen in Section 5 source transients will have died out and only the effect of absorption on the asymptotic flux need be considered. This requires solution of Equation (2-18a) subject

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[8] This treatment follows G. Placzek, op. cit.

to the conditions:

$$C(u) = 1 \qquad u < u_o$$
$$\chi(u_o) = \frac{1}{\xi} \qquad \text{(2-21a)}$$

where u_o is the smallest lethargy at which Σ_a is non-zero.

To facilitate solution for this case, a transformation will be applied to Equation (2-18a). First it is rewritten (noting that sources are absent):

$$e^u \chi(u) = \int_{u-\ln\frac{1}{\alpha}}^{u} \frac{C(u')\,\chi(u')}{1-\alpha} e^{u'} du' \qquad \text{(2-21b)}$$

Differentiation with respect to u and subsequent integration over u (changed to u' for convenience) from u_o to u gives the result

$$\int_{u_o}^{u} \chi(u')\,du' + \chi(u) - \chi(u_o) = \int_{u_o}^{u} \frac{C(u')\chi(u')}{1-\alpha}\,du' - \frac{\alpha}{1-\alpha}\int_{u_o}^{u} C(u'-\ln\tfrac{1}{\alpha})\,\chi(u'-\ln\tfrac{1}{\alpha})\,du' \qquad \text{(2-21c)}$$

Now change variables in the last term on the right side of this equation to $w = u' - \ln 1/\alpha$. The resulting integral, which runs between the limits of $u_o - \ln 1/\alpha$ to $u - \ln 1/\alpha$, can be broken into three integrals, symbolically:

$$\int_{u_o-\ln\frac{1}{\alpha}}^{u-\ln\frac{1}{\alpha}} = \int_{u_o-\ln\frac{1}{\alpha}}^{u_o} + \int_{u_o}^{u} - \int_{u-\ln\frac{1}{\alpha}}^{u} \qquad \text{(2-21d)}$$

Now, noting that the boundary conditions (2-21a) state that $c = 1$ for $u < u_o$ and further assuming that $\chi(u) = 1/\xi$ for $u > u_o - \ln 1/\alpha$, we can evaluate the integral from $u_o - \ln 1/\alpha$ to u_o. Combining the resulting terms leads to

$$\chi(u) = 1 - \int_{u_o}^{u} C_o(u')\,\chi(u')\,du' + \frac{\alpha}{1-\alpha}\int_{u-\ln\frac{1}{\alpha}}^{u} C(u')\,\chi(u')\,du' \qquad \text{(2-21e)}$$

If $(\xi-1)\chi(u)$ is now added to both sides of this equation, and it is noted that $(\xi-1)\chi(u)$ can be written as

$$(\xi-1)\chi(u) = -\frac{\alpha}{1-\alpha}\int_{u-\ln\frac{1}{\alpha}}^{u}\chi(u)\,du' \qquad (2\text{-}21f)$$

we obtain finally the following equation, equivalent to Equation (2-18), under the assumptions made:

$$\Sigma\chi(u) = 1 - \int_{u_0}^{u} C_0(u')\,\chi(u')\,du' + \frac{\alpha}{1-\alpha}\int_{u-\ln\frac{1}{\alpha}}^{u} du' \left[\qquad \right] \qquad (2\text{-}21g)$$

or, defining $\xi\chi(u) = q_0(u)$

$$q_0(u) = 1 - \frac{1}{\xi}\int_{u_0}^{u} C_0(u')\,q_0(u')\,du' + \frac{\alpha}{1-\alpha}\,\frac{1}{\xi}\int_{u-\ln\frac{1}{\alpha}}^{u} du' \left[\qquad \right] \qquad (2\text{-}21h)$$

Note the restriction implicit in the above derivation, that the asymptotic distribution be attained at least one collision interval before the absorption sets in (i.e., the absorption is assumed to set in at u_0 but the asymptotic flux is assumed to exist from $u_0 - \ln 1/\alpha$ on).

For hydrogen moderation, $\alpha = 0$, and the last term on the right hand side of Equation (2-21h) drops out. Thus, this term distinguishes between hydrogen and heavy element slowing down. Note that $\frac{\alpha}{1-\alpha} = \frac{(A-1)^2}{4A}$ is proportional to A and $\xi \approx 2/3A$ for large A so that the coefficient of the last term of Equation (2-21h) is proportional to A^2 and is important for heavy moderators.

For slowly varying capture, the effect of changes of c(u) in one collision interval may be neglected. Then, if we try a function of

the form[9] $q_o(u) = e^{s(u)}$ in Equation (2-21h) and approximate $s(u - \ln 1/\alpha)$ by a Taylor series expansion about u we find that, on keeping only the first two terms, s'(u) satisfies a relation exactly like (2-20b):

$$(1-\alpha)(s'(u)+1) = c(u)\left(1-\alpha^{s'(u)+1}\right) \qquad (2\text{-}22a)$$

where

$$s'(u) = ds/du$$

In analogy to our previous notation we denote the solution of Equation (2-22a) with largest real part by $\nu_o(u)$, so that to a good approximation

$$s_o'(u) = \nu_o(u) \qquad (2\text{-}22b)$$

$$s(u) = \int_{u_o}^{u} \nu(u')\,du' \qquad (2\text{-}22c)$$

Thus we arrive at the result

$$q_o(u) = \xi \Sigma_t(u) \phi(u) = e^{\int_{u_o}^{u} \nu_o(u')\,du'} \qquad (2\text{-}22d)$$

which is analogous to Equation (2-20d) except that ν_o is now a function of lethargy. This result can be generalized to mixtures but it would be necessary to derive an equation similar to (2-21h) for this case and it probably is not worthwhile to carry out the procedure here. It is perhaps intuitively obvious, and can be shown[10] that the results of such a calculation are that $\nu_o(u)$ is the root of

$$1 = \sum_j \frac{\beta_j(u)\left(1-\alpha_j^{\nu_o(u)-1}\right)}{(1-\alpha_j)(1+\nu_o(u))} \qquad (2\text{-}23)$$

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[9] This is essentially the well known WKB approximation of quantum mechanics. See any text in quantum mechanics, e.g., Schiff, op. cit.

[10] R. E. Marshak, op. cit.

with largest real part. Here β_j is the fraction of neutrons of lethargy u that collide with j type nuclei [see Equation (2-15a)]. In the limit of small $c_o(u)$ an approximation to $\nu_o(u)$ similar to Equation (2-20c) can be obtained, yielding for the resonance escape probability:

$$p(u) = \exp\left\{ - \int_{u_o}^{u} \frac{c_o(u')}{\bar{\xi}(u')} du' \right\} \qquad (2\text{-}24a)$$

where $\bar{\xi}(u)$ is a function of lethargy by virtue of the fact that $\beta_j(u)$ is a function of lethargy.

In terms of energy, the flux can be written

$$\phi(E) = \frac{1}{\bar{\xi}\, \Sigma_t(E)\, E} \exp\left\{ - \int_{E_o}^{E} \frac{c_o(E')}{\bar{\xi}(E')} \frac{dE'}{E'} \right\} \qquad (2\text{-}24b)$$

E_o here is the energy corresponding to lethargy u_o. In this case, the flux drops off somewhat slower than $1/E$. These formulae may be applied to non-resonance capture and, in particular, they could be used to determine the resonance escape probability in a medium with '1/v' absorption, i.e., a material whose absorption cross section varies with the reciprocal of the neutron velocity, a situation which obtains in many cases of interest.

11. Rapidly Varying Capture - Strong Resonances[11]

The problem with $c_o(u)$ varying rapidly with energy is important as it covers the case of large absorption resonances. A rigorous solution, by a method similar to that used in deriving the Placzek Function, is possible but the calculations reach high orders of complexity

[11] This treatment closely follows G. Placzek, op. cit.

very rapidly. One might imagine a situation in which there are sharp resonances which are widely separated from each other. Such a problem is not unreasonable from a physical point of view and since resonance absorption in sharp resonances does not disturb the flux distribution far from the resonances very greatly, the problem posed is considerably simpler.

Again it is assumed that the asymptotic flux is established one collision interval prior to the onset of absorption, so that we may solve Equation (2-18a) subject to the conditions that $\chi(u) = 1/\xi$ and $c(u) = 1$ for $u < u_o$. For $u_o + \ln 1/\alpha > u > u_o$, Equation (2-21h) may then be written

$$\chi(u) = \int_{u-\ln\frac{1}{\alpha}}^{u_o} c(u')\chi(u')\frac{e^{-(u-u')}}{1-\alpha}du' + \int_{u_o}^{u} c(u')\chi(u')\frac{e^{-(u-u')}}{1-\alpha}du'$$

$$= \frac{e^{u_o-u} - \alpha}{\xi(1-\alpha)} + \int_{u_o}^{u} c(u')\chi(u')\frac{e^{-(u-u')}}{1-\alpha}du' \qquad (2\text{-}25a)$$

which is of the same form as some of the integral equations we have met previously. Differentiation of Equation (2-25a) yields a simple linear first-order differential equation whose solution is readily found to be:

$$\xi\chi(u) = q_o(u) = e^{\gamma(u)}\left[1 - \frac{\alpha}{1-\alpha}\int_{u_o}^{u} e^{-\gamma(u')}du'\right] \qquad (2\text{-}25b)$$

where the exponent of the integrating factor, $\gamma(u)$, is

$$\gamma(u) = \int_{u_o}^{u}\left[\frac{c(u')}{1-\alpha} - 1\right]du' \qquad (2\text{-}25c)$$

Following the derivation of the Placzek Function, this process may be repeated iteratively on the intervals $u_o - n \ln 1/\alpha < u < u_o - (n+1)\ln 1/\alpha$ to obtain the complete energy spectrum. The formulae

thus obtained grow in complexity even more rapidly than the Placzek Functions but they are rarely used even when resonances are closely spaced.

A very useful formula for the calculation of the resonance escape probability for the case of isolated sharp resonances is now obtainable. A few collision intervals after the resonance the flux again attains its asymptotic $1/E$ form if there is no absorption other than the isolated resonance present ($c_o = 0$), but its intensity is reduced by the absorption in the resonance. In this region the last term of Equation (2-21h) vanishes and the flux can be calculated quite simply:

$$q_o(u) = \xi \Sigma_t(u) \phi(u) = 1 - \int_{u_o}^{u} c_o(u') \chi(u') du' \qquad (2\text{-}26a)$$

For a very sharp resonance, in which practically all of the absorption takes place in a lethargy interval much smaller than $\ln 1/\alpha$, the collision density in the resonance will be nearly that of the asymptotic distribution so that $\chi(u')$ in the integrand of Equation (2-26a) may be replaced by $1/\xi$.* Furthermore, most of the contribution to the integral will come from the resonance. Thus:

$$q_o(u) \approx 1 - \frac{1}{\xi} \int_{Res} c_o(u') du' \qquad (2\text{-}26b)$$

where the subscript 'Res' on the integral denotes integration only over the lethargy region for which Σ_a is large. If the integral is small:

$$q_o(u) \approx \exp\left\{ - \frac{1}{\xi} \int_{Res} c_o(u') du' \right\} \qquad (2\text{-}26c)$$

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* i.e., a scattering collision within the resonance is assumed to remove the neutron from the resonance energy.

The calculation of the resonance escape probability for this case is simple, when the fact that most of the absorption takes place in the resonance is noted.

$$p(u) = 1 - \int_0^u \Sigma_a(u')\phi(u')du'$$

$$\simeq \exp\left\{-\frac{1}{\xi}\int_{Res} C_0(u')du'\right\} \qquad (2\text{-}26d)$$

which is the well known "narrow resonance" (NR) formula. In Section E absorption by individual resonances will be considered in more detail.

12. Anisotropic Scattering

These results are readily generalized to non-isotropic scattering by means of the formalism of Chapter I. For non-isotropic scattering, it is necessary to employ the more general scattering frequency (1-50d) which, when substituted into Equation (2-18a) yields

$$\Sigma_t(u)\phi(u) = \sum_i N_i \int_{u-\ln\frac{1}{\alpha_i}}^{u} \phi(u') \sum_{L'=0}^{\infty} B^c_{L'}(u') T_{oL'}(u-u')du' + S(u) \qquad (2\text{-}27a)$$

where it is again understood that α, $B^c_L(u')$ and $T_{LL'}(U)$ are properties of particular nuclear types. Unfortunately, Equation (2-27a) cannot be solved in general, firstly, because the $T_{OL'}(U)$ are rather complex functions of their argument, and secondly because the $B^c_L(u)$ are generally supplied as empirical data. To simplify matters, one frequently expands the function $B^c_{L'}(u')\,\phi(u')$ in a Taylor Series about u. Doing so, and noting that the necessary convergence for interchanging the sum and integral exists, we can write

$$\Sigma_t(u)\phi(u) = \sum_i N_i \sum_{L'=0}^{\infty}\sum_{\nu=0}^{\infty} \int_{u-\ln\frac{1}{\alpha}}^{u} \frac{(u-u')^\nu}{\partial u^\nu}\left[B^c_{L'}(u)\,\phi(u)\right] T_{oL'}(U)du' + S(u) \qquad (2\text{-}27b)$$

The derivative terms may be taken outside outside the integral and the remaining integral is just the definition of $T^{\nu}_{OL'}$ [see Equation (1-56)

Thus

$$\Sigma_t(u)\phi(u) = \sum_i N_i \sum_{\nu=0}^{\infty}\sum_{L'=0}^{\infty} T^{\nu}_{OL'} \frac{\partial^{\nu}}{\partial u^{\nu}}\left[B^c_{L'i}(u)\phi(u)\right] + S(u) \qquad (2\text{-}27c)$$

But if consideration is restricted to terms of order γ or greater only,* from (1-53b) and (1-57a,b) we have

$$\Sigma_t(u)\phi(u) = \sum_i N_i\left[B^c_0(u)\phi(u) + 2\gamma \frac{\partial}{\partial u}\left[\left(B^c_1(u) - \bar{\xi}(u)B^c_0(u)\right)\phi(u)\right]\right] + S(u) \qquad (2\text{-}27d)$$

or, since $B^c_0(u) = \sigma_s(u)$ and

$$\Sigma_s(u) = \sum_i N_i \sigma^i_s(u) \qquad (2\text{-}27e)$$

Equation (2-27d) becomes

$$\Sigma_a(u)\phi(u) = \sum_i \frac{\partial}{\partial u}\left[2\gamma_i\left(N_i B^{c\,i}_1(u) - \Sigma_s(u)\right)\phi(u)\right] + S(u) \qquad (2\text{-}27f)$$

But, from Equation (1-62a)

$$\sum_i 2\gamma_i\left(\frac{N_i B^{c\,i}_1(u)}{\Sigma_s(u)} - 1\right) = \bar{\xi}(u) \qquad (2\text{-}27g)$$

is seen to be the mean lethargy change per collision. Thus we arrive at the differential equation:

$$\frac{\partial}{\partial u}\left(\bar{\xi}(u)\Sigma_s(u)\phi(u)\right) + \frac{\Sigma_a(u)}{\bar{\xi}(u)\Sigma_s(u)}\left[\bar{\xi}(u)\Sigma_s(u)\phi(u)\right] = S(u) \qquad (2\text{-}28a)$$

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* This is closely related to the Age Diffusion Approximation of Chapter III and in fact the results derived here are the Age Diffusion results.

for which the solution, found by methods used previously in this chapter, is:

$$\bar{\xi}(u)\,\Sigma_s(u)\,\phi(u) = \int_0^u S(u')\, e^{-\int_{u'}^{u} \frac{\Sigma_a(u'')}{\xi(u'')\,\Sigma_s(u'')}\,du''}\,du' \qquad (2\text{-}28a)$$

The resonance escape probability is easily extracted and is [setting $S(u) = \delta(u)$ again]:

$$P(u' \to u) = e^{-\int_{u'}^{u} \frac{\Sigma_a(u'')}{\xi(u'')\,\Sigma_s(u'')}\,du''} \qquad (2\text{-}28b)$$

which is the extension of Equation (2-26d) to a more general case, subject to the approximations made above.

13. Resonance Escape Probability in the Goertzel Greuling Approximation

Another slightly more accurate formula for the resonance escape probability can be developed from an approximation due to Goertzel and Greuling.[12] In Chapter III we shall derive an approximation to the Boltzmann Equation which reduces to

$$\left[\Sigma_a(u) + \frac{\xi}{\lambda}\Sigma_s(u)\right]\phi(u) = S(u) + \frac{\xi}{\lambda^2}\int_0^u e^{-(u-u')/\lambda}\,\Sigma_s(u')\,\phi(u')\,du' \qquad (2\text{-}29a)$$

for an infinite medium. Here,

$$\lambda = \frac{\langle U^2 \rangle}{2\xi} = 1 - \frac{\alpha\left[1 + \ln\frac{1}{\alpha} + 2\ln^2\frac{1}{\alpha}\right]}{1 - \alpha\left(1 + \ln\frac{1}{\alpha}\right)} \qquad (2\text{-}29b)$$

for isotropic scattering.

Let the function on the left hand side of Equation (2-29a) be defined as $\chi(u)$. The solution is similar to those of previous cases;

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[12] G. Goertzel and E. Greuling, Nuc. Sci. Eng., 7, 69 (1960).

differentiation of Equation (2-29a) yields

$$\frac{\partial \chi}{\partial u} + \frac{\Sigma_a(u)}{\lambda \Sigma_a(u) + \xi \Sigma_s(u)} \chi(u) = \frac{S(u)}{\lambda} + \frac{\partial S}{\partial u} \qquad (2\text{-}29c)$$

which may be solved to yield a solution analogous to Equation (2-6a)

$$\chi(u) = \frac{\lambda \Sigma_a(u) + \xi \Sigma_s(u)}{\lambda} \phi(u) = S(u) +$$

$$\frac{1}{\lambda} \int_0^u \frac{\xi \Sigma_s(u')}{\lambda \Sigma_a(u') + \xi \Sigma_s(u')} S(u') \exp\left\{ - \int_{u'}^u \frac{\Sigma_a(u'')\, du''}{\lambda \Sigma_a(u'') + \xi \Sigma_s(u'')} \right\} du'$$

(2-29d)

The resonance escape probability, for this case is given by

$$p = 1 - \int_0^u du' \frac{\Sigma_a(u')}{\lambda \Sigma_a(u') + \xi \Sigma_s(u')} \left\{ S(u') + \right.$$

$$\left. \frac{1}{\lambda} \int_0^{u'} S(u'') \frac{\xi \Sigma_s(u'')}{\lambda \Sigma_a(u'') + \xi \Sigma_s(u'')} \exp\left\{ - \int_{u''}^{u'} \frac{\Sigma_a(u''')\, du'''}{\lambda \Sigma_a(u''') + \xi \Sigma_s(u''')} \right\} du'' \right\}$$

(2-30a)

which, for a monoenergetic source, becomes:

$$p = \frac{\xi \Sigma_s(0)}{\lambda \Sigma_a(0) + \xi \Sigma_s(0)} \exp\left\{ - \int_0^u \frac{\Sigma_a(u'')\, du''}{\lambda \Sigma_a(u'') + \xi \Sigma_s(u'')} \right\} \qquad (2\text{-}30b)$$

Values of ξ, λ, and α for common moderators are given in Table I. Since ξ and λ are not greatly different, it will usually suffice to use Equation (2-24a) if absorption is not too large.

TABLE I

Element	ξ	λ	α
Hydrogen	1.000	1.000	0
Deuterium	0.725	0.583	.111
Beryllium	0.209	0.149	.640
Carbon	0.158	0.116	.716

E. Capture By Individual Resonances

14. The Narrow Resonance Approximations

We now turn our interest to some approximation methods which are frequently used to calculate the resonance escape probability for individual resonances. Consider first a homogeneous mixture of moderator and a heavy absorbing element. Most heavy-element cross sections are a superposition of resonances and a constant potential scattering base. If, in addition, a background of slowly varying capture is present, it might be possible to apply resonance corrections to the slowly varying capture formula, previously derived (Section 10), essentially by combining the slowly varying and narrow resonance approximations. Another derivation of the narrow resonance formula is first given in order to clarify the meaning of the term "narrow resonance." The so-called "narrow resonance infinitely heavy absorber" (NRIA) approximation will also be introduced.

A quantity which can be used as a yardstick for describing resonances, the practical width,[13] is defined as that energy (or lethargy) interval for which the resonance portion of the capture cross section is greater than the non-resonance total cross section. For resonances encountered in reactors, the practical width is generally much smaller than the average energy a neutron at the resonance energy would lose in a collision with a moderator atom. There is, however, another distinguishing feature of resonances. Some resonances are so narrow that even the energy loss in an elastic collision with an absorber nucleus (e.g. U-238) removes most of the neutrons from the resonance; other resonances are so broad that a single collision between a neutron with an energy near the resonance peak and a heavy absorber nucleus could not possibly remove the neutron from the resonance. Whether the quantity $E_R(1 - \alpha_u)$, where E_R is the energy at the resonance peak and $\alpha_u = (\frac{A_u-1}{A_u+1})^2 (\approx .98$ for U-238), is greater or less than the practical width of the resonance is conventionally[14] taken as a means of distinguishing the first case from the second.[15] The quantity $E_R(1 - \alpha_u)$ is, of course, the maximum energy loss in an elastic collision with a heavy nucleus. Thus, to a reasonable approximation, if the maximum energy loss in a collision with a uranium nucleus is greater than the width of the resonance, elastic scattering in uranium must be considered as a means of slowing down; this is the narrow resonance (NR) approximation. Similarly, if the inequality is reversed, elastic

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[13] The notion of "practical width" is due to E. P. Wigner.

[14] K. T. Spinney in BNL 433, p. 103; L. Dresner, ORNL 2659.

[15] Some resonances fall into neither category; see W. Rothenstein and J. Chernick, Nuc. Sci. Eng., 7, 454 (1960).

scattering with uranium atoms cannot remove the neutron from the resonance in a single collision; this is the narrow resonance-infinitely heavy absorber (NRIA) approximation. If, in a particular resonance, $\Sigma_{a_u} >> \Sigma_{s_u}$, the effect of scattering from uranium may be ignored entirely. It may be noted that in uranium and thorium most of the resonances are of the NR type. However, as the NRIA resonances are broader and tend to occur at lower energies,[16] where the flux is highest, it is this type of resonance which is responsible for most of the resonance absorption (see Table II).

A simple way to derive the NR formula is to note that N(u), the number of neutrons slowing into lethargy interval du, within the resonance is given by

$$N(u) = \sum_i N_i \int_{u-\ln\frac{1}{\alpha_i}}^{u} \Sigma_s^i(u') \phi(u') F(u' \to u) du' \qquad (2\text{-}31a)$$

Since the resonance is assumed to be narrow we can neglect the difference between the contribution to the integral (2-31a) due to those neutrons which scatter in the resonance and that obtained by replacing $\Sigma_s \phi$ by its value outside the resonance, $1/\xi$. It is assumed that the non-resonance or potential scattering is constant, and that the resonance under consideration far enough removed in energy from any neutron sources or other resonances so that ϕ has attained its asymptotic value. In this case, Equation (2-16d) applies.

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16 This is a direct result of the fact that resonance widths vary as $E^{1/2}$ while the energy loss in a collision is directly proportional to E. For a discussion of resonance widths see J. M. Blatt and V. Weiskopf, Theoretical Nuclear Physics, Wiley, 1952.

TABLE II*

1 Resonance energy E_R	2 Natural width Γ	3 Practical width kT = 0.025	4 Maximum energy loss in collision with U-238	5 Resonance Escape probability
418	0.105	2.56	7.00	0.001950
278	0.065	1.87	4.65	0.003495
212	0.085	2.63	3.55	0.005021
192	0.165	5.66	3.21	0.007119
117.5	0.040	1.32	1.97	0.009170
90	0.0251	0.13	1.51	0.001104
81.3	0.0271	0.76	1.36	0.009596
36.9	0.0575	3.65	0.62	0.05820
21.0	0.0339	1.95	0.35	0.06755

* From Spinney, BNL 433, p. 105. The practical width includes the effect of Doppler Broadening (see Sec. 19). These are only a few (typical) U-238 resonances.

Under these assumptions, Equation (2-31a) becomes

$$N(u) = q/\bar{\xi} \qquad (2\text{-}31b)$$

Since, by definition,

$$\int F(u' \rightarrow u)\, du = 1$$

Here, q is the total source strength.

The number of neutrons absorbed in du will be equal to $N(u)\,\frac{\Sigma_a(u)}{\Sigma_t(u)}\,du$ since every scattering event is assumed to degrade the neutron to below the resonance energy. Then, the total number of neutrons absorbed in the resonance will be

$$q \int \frac{\Sigma_a(u)}{\bar{\xi}\,\Sigma_t(u)}\, du \qquad (2\text{-}31c)$$

and p, the resonance escape probability, is simply

$$P_{NR} = 1 - \int \frac{\Sigma_a(u)}{\bar{\xi}\,\Sigma_t(u)}\, du \approx e^{-\int \frac{\Sigma_a(u)}{\bar{\xi}\,\Sigma_t(u)}\, du} \qquad (2\text{-}31d)$$

In the NRIA approximation it is assumed that a scattering event with an absorber atom does not change the neutron energy. Thus Equation (2-31c) clearly must be modified by subtracting $\Sigma_s^u(u)$, the absorber scattering cross section, from $\Sigma_t(u)$. In this approximation we find:

$$P_{NRIA} = 1 - \int \frac{\Sigma_a(u)}{\bar{\xi}\,(\Sigma_t(u) - \Sigma_s^u(u))}\, du \approx e^{-\int \frac{\Sigma_a(u)}{\bar{\xi}\,(\Sigma_t(u) - \Sigma_s^u(u))}\, du} \qquad (2\text{-}31e)$$

Note that here $\bar{\xi}$ is defined only in terms of potential scattering cross sections

$$\bar{\xi} = \frac{\sum_{i \neq u} \Sigma_{pi}\,\xi_i}{\sum_{i \neq u} \Sigma_{pi}} \qquad (2\text{-}31f)$$

15. Resonance Integrals

Equations (2-31d) and (2-31e) are frequently written in the form

$$p = \exp\left\{-\frac{N_u}{\xi \Sigma_p} I_{eff}\right\} \tag{2-32a}$$

where N_u is the number density of absorber atoms, Σ_p is the potential scattering cross section, and I_{eff} is called the "effective resonance integral". For the NR case, we have

$$I_{eff}^{NR} = \Sigma_p \int \frac{\sigma_a^u(u)}{\Sigma_t(u)} du \tag{2-32b}$$

while in the NRIA case, I_{eff} is given by

$$I_{eff}^{NRIA} = \Sigma_p \int \frac{\sigma_a^u(u)}{\Sigma_t(u) - \Sigma_s^u(u)} du \tag{2-32c}$$

If the absorber concentration is very small, $\Sigma_t(u) \approx \Sigma_p(u)$ and both (2-32b) and (2-32c) approach the "infinitely dilute resonance integral"

$$I_\infty = \int \sigma_a(u) du \tag{2-32d}$$

which is larger than either the NR or NRIA effective resonance integrals. The effect which causes the resonance integrals (2-32b) and (2-32c) to be smaller than the infinitely dilute value is sometimes called "energy self-shielding."[17] The reduction is simply due to the depletion of the resonance flux by absorption.

Resonance integrals are often given in terms of $\sigma_p' = \frac{\Sigma_p}{N_u}$, the total potential scattering cross section per absorber atom and

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[17] G. Goertzel, H. Feshback, and J. Yamanchi, Nuc. Sci. Eng., 1, 4 (1956).

$\sigma_s(u)$, the resonance scattering cross section. In this notation Equations (2-32b and 2-32c) become*

$$I_{eff}^{NR} = \int \frac{\sigma_a(u)}{1 + \frac{\sigma_a(u) + \sigma_s(u)}{\sigma_p'}} du \qquad (2\text{-}32e)$$

$$I_{eff}^{NRIA} = \int \frac{\sigma_a(u)}{1 + \frac{\sigma_a(u)}{\sigma_p' - \sigma_p}} du \qquad (2\text{-}32f)$$

The distinction between NR and NRIA resonances can be quite important as scattering and absorption resonances almost always occur together. If the scattering cross section of the absorber in the resonance is comparable to or larger than the absorption cross section, it is also likely to be a large part of total scattering cross section. Then it is extremely important to choose the correct approximation, a point clearly illustrated by the results given for (1-p) in uranium resonances given in columns 3 and 4 of Table III.

Spinney[18] and others have done calculations for resonances which fit neither the NR nor the NRIA description. In addition, Spinney has compared the results predicted by the formulae just given, his modified narrow resonance formula, and an exact result obtained by numerical integration of the slowing down equations for the case of a uranium-hydrogen mixture; this comparison is shown in Table III. Figure 5, also taken from Spinney's work, compares the NR and NRIA calculations.

In some resonances, interference between the resonance scattering and potential cross sections reduces the absorber scattering cross section very sharply just below the resonance. Neumann[19] has made some

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[18] K. T. Spinney, op. cit.; Rothenstein and Chernick, op. cit.

[19] H. Neumann, BNL-433, p. 110.

* In the NRIA case scattering by uranium is to be ignored in computing σ_p'.

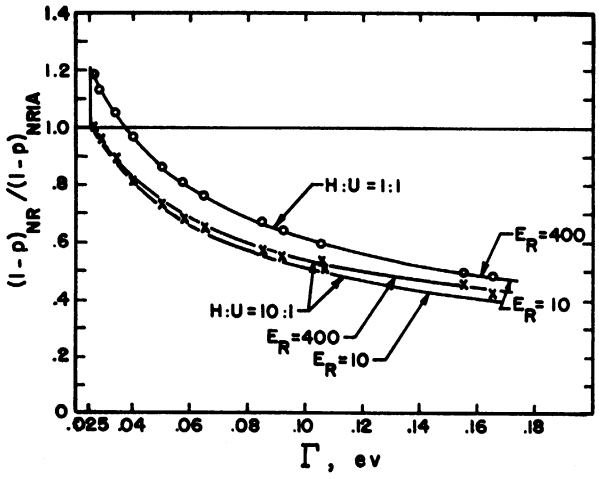

Figure II-5 Comparison of narrow resonance approximation with narrow resonance with infinitely heavy absorber approximation for mixtures of hydrogen and uranium. After K. Spinney, BNL 433, p. 107.

TABLE III*

1	Values of (1-p) 2	3	4
Resonance energy E_R	Exact	NR	NRIA
418	0.001950	0.001816(- 6.9%)	0.003855(+97.7%)
278	0.003495	0.003318(- 5.1%)	0.004936(+41.2%)
212	0.005021	0.004440(-11.6%)	0.007689(+53.1%)
192	0.007119	0.005086(-28.6%)	0.01228 (+73.0%)
117.5	0.009170	0.009035(- 1.5%)	0.009500(+ 3.6%)
90	0.001104	0.001114(+ 0.9%)	0.000998(- 9.6%)
81.3	0.009596	0.010163(+ 5.9%)	0.008109(-15.5%)
36.9	0.05820	0.04739 (-18.6%)	0.06110 (+ 5.0%)
21.0	0.06755	0.07455 (+10.4%)	0.07059 (+ 4.5%)

*From Spinney, BNL-433, p. 105. These resonances are the ones for which resonance parameters are given in Table II.

calculations of the effect of this phenomenon on resonance absorption, but the reader is referred to the original work for greater detail.

16. Corrections to the Six Factor Formula

The methods described in this section are strictly applicable only to isolated, narrow resonances. If absorption in a single resonance is small, however, resonances do not interfere with each other to any strong degree. Then the resonance escape probabilities for the individual resonances are independent and the total resonance escape probability is simply the product of the resonance escape probabilities for the individual resonances.

This method has the advantage of being readily adaptable to multi-group procedures, as will be seen in Chapter IV. As a simple example, suppose one wishes to obtain a better estimate of k_{eff} without greatly increasing the complexity of the formulae obtained in Chapter I. One procedure might be to break the fast group arbitrarily into two smaller groups and assign to each a resonance escape probability, say

$$P_1 = p(E')$$
$$P_2 = p(E' \rightarrow E_T) \qquad (2\text{-}33a)$$

where p_1 is averaged over a fission spectrum. In a similar fashion one could break up the non-leakage probability into $\lambda_1(E')$ and $\lambda_2(E' \rightarrow E_T)$. The fast effect is, as we have seen, often independent of both p and λ. Using the resonance formulae just developed, it is a relatively simple matter (in principle) to calculate p_1 and p_2; the calculation of λ_1 and λ_2 will be indicated in Chapter III. Then, one could write for

the multiplication factor

$$k = \frac{\eta f p_1 p_2 \lambda_1 \lambda_2 \epsilon}{1 + L^2 B^2} \qquad (2\text{-}33b)$$

which is presumably more accurate than the formulae of Chapter I as it allows for an interaction between the resonance escape and non-leakage probabilities neglected in the simple six factor formula. By further breaking up the fast group one could obtain still more accurate expressions for k_{eff}, which in the limit of infinite subdivision must yield the exact result.

17. Closely Spaced Resonances

The assumption of wide separation of resonances is frequently not valid, e.g., U-238 has at least 20 strong resonances below 200 ev. However, the method just described is usually sufficiently accurate since even the strongest resonances capture only a small fraction of the neutrons passing through them. Thus the transients they introduced into the neutron spectrum cannot be more than a few per cent of the asymptotic flux in amplitude and may be ignored to good approximation.

The resonance escape probability for closely spaced resonances can be calculated more rigorously by using the rapidly-varying capture solution already obtained in Section 11. The solution is, however, not readily adaptable to simple calculations. Another method of calculating the interference effect in resonance capture is due to Weinberg and Wigner.[20]

Absorption in a sharp resonance may be considered a monoenergetic neutron sink, or at worst a superposition of such sinks. The effect of

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[20] A. M. Weinberg and E. P. Wigner, BNL 433, p. 125. See also N. Corngold, Proc. Phys. Soc. (London) (1958).

such sinks on the neutron flux is the introduction of transients of the Placzek Function type. These transients must, of course, be subtracted from the asymptotic flux that would exist if the resonance were not present. One can write

$$\chi(u) = \frac{1}{\xi} - \int_0^u C_0(u')\chi(u')\phi_p(u',u)du' \qquad (2\text{-}34a)$$

where $\phi_p(u, u')$ is the Placzek Function, the collision density, χ, at lethargy u due to a unit source of neutrons at u'. The Placzek Function may be decomposed into an asymptotic (1/E) part and a difference term:

$$\phi_p(u', u) = \frac{1 - \varphi_p(u', u)}{\xi} \qquad (2\text{-}34b)$$

When this is substituted into Equation (2-34a) one finds

$$\xi\chi(u) = 1 - \int_0^u C_0(u')\chi(u')du' + \int_0^u C_0(u')\chi(u')\varphi_p(u,u')du' \qquad (2\text{-}34c)$$

In Equation (2-34c), the last term represents the correction sought; omission of it leads once again to the narrow resonance formula. However, if the correction is small, as expected, the narrow resonance formula may be used to evaluate the last term of Equation (2-34c). That is, we set

$$\chi(u') = \chi(u)e^{\int_{u'}^{u} C(u'')du''} \qquad (2\text{-}34d)$$

where the positive exponent is chosen because $u' < u$.

If one further defines

$$\int_0^u C_0(u')\varphi_p(u,u')e^{\int_{u'}^{u} C_0(u'')du''} = \xi_1(u) \qquad (2\text{-}34e)$$

the integral equation for $\chi(u)$ simplifies to:

$$\left[\xi - \xi_1(u)\right] \chi(u) = 1 - \int_0^u C_0(u')\chi(u')\,du' \qquad (2\text{-}34f)$$

This equation is exactly that involved in the narrow resonance problem except that ξ has been replaced by $[\xi - \xi_1(u)]$. Proceeding in the same manner as that previously followed, we obtain:

$$\chi(u) = \frac{1}{\xi - \xi_1(u)} \exp\left\{ - \int_0^u \frac{C_0(u'')}{\xi - \xi_1(u'')}\,du'' \right\} \qquad (2\text{-}35a)$$

which yields the resonance escape probability:

$$p(u) = \exp\left\{ - \int_0^u \frac{C_0(u')}{\xi - \xi_1(u')}\,du' \right\} \qquad (2\text{-}35b)$$

This procedure is successful in obtaining the correction in a relatively simple form. However, the difficulty is calculating $\xi_1(u)$ and in evaluating Equation (2-34b) has rendered this method relatively inutilitarian.

F. Calculation of Resonance Integrals

18. Natural Line Shape

For a single isolated resonance, the Breit-Wigner Formulae give good approximations to the line shape. Within an absorption resonance, the resonance portion of cross section is well fitted by[21]

$$\sigma_a(E) = \sigma_0 \frac{\Gamma_\gamma}{\Gamma} \frac{\Gamma^2/4}{(E - E_0)^2 + (\Gamma/2)^2} \qquad (2\text{-}36a)$$

where σ_0 is the maximum total cross section (at energy E_0), Γ_γ is the level width for gamma emission and Γ is the total level width.

[21] J. M. Blatt and V. S. Weisskopf, op. cit.

In terms of

$$x = \frac{E - E_0}{\Gamma/2} \qquad (2\text{-}36b)$$

Equation (2-36a) becomes:

$$\sigma_a(E) = \frac{\sigma_0 \, \Gamma_\gamma/\Gamma}{1 + x^2} \qquad (2\text{-}36c)$$

Ignoring the effects of non-resonance absorption and overlap of resonances, the infinitely dilute resonance integral for a single resonance of this type [see Equation (2-32d)] is:

$$I_\infty = \int_{-\infty}^{\infty} \frac{\sigma_0 \, \Gamma_\gamma/\Gamma}{1 + x^2} \, \frac{\Gamma}{2E} \, dx \qquad (2\text{-}37a)$$

The extension of the limits on the integral from $-\infty$ to $+\infty$ is only a device for making the integral easier to handle; most of the contribution to the integral comes from energies near E_0. If the resonance line is very sharp, as are most resonances, E may be approximated by its value at the resonance peak, E_0. Also, Γ_γ can be taken out of the integral as it is essentially constant in energy. Thus,

$$I_\infty = \int_{Res} \sigma_a(E) \frac{dE}{E} = \frac{\sigma_0 \, \Gamma_\gamma}{2E_0} \int_{-\infty}^{\infty} \frac{dx}{1 + x^2} \qquad (2\text{-}37b)$$

The integration is straight forward, and yields:

$$I_\infty = \frac{\pi}{2} \, \frac{\sigma_0 \, \Gamma_\gamma}{E_0} \qquad (2\text{-}37c)$$

This is the contribution to I_∞ from a single resonance line and can be evaluated if Γ_γ, σ_0, and E_0 are known. Since these quantities have to be determined experimentally, Equation (2-37c) can be applied only to

those resonances which have been resolved.

Resonance integrals for the self-shielded case are also readily calculated. If we ignore interference between resonance and potential scattering the resonance scattering cross section is given by

$$\sigma_s(u) = \frac{\sigma_0 \Gamma_n/\Gamma}{1+x^2} \qquad (2\text{-}37d)$$

where Γ_n is the netron width and

$$\Gamma = \Gamma_n + \Gamma_\gamma$$

Inserting Equations (2-36c) and (2-37d) into Equation (2-32e) we find

$$I_{eff}^{NR} = \frac{\sigma_0 \Gamma_\gamma}{2E_0} \int_{-\infty}^{\infty} \frac{dx}{1+x^2+\frac{\sigma_0}{\sigma_p'}} \qquad (2\text{-}37e)$$

Or defining

$$\beta = \frac{\sigma_p'}{\sigma_0} \qquad (2\text{-}37f)$$

we have

$$I_{eff}^{NR} = \frac{\pi}{2} \frac{\sigma_p' \Gamma_\gamma}{E_0} \frac{1}{\sqrt{\beta(1+\beta)}} \qquad (2\text{-}37g)$$

This formula also applies to the NRIA case if Γ_γ is replaced by Γ and if uranium potential scattering is neglected in computing σ_p'.

The resonance integral cannot be evaluated using Equations (2-37c) or (2-37d) alone. At low energies the absorption cross section

is approximately "1/v" and its contribution must be included

$$\int_{E_T}^{\infty} \sigma_{a\,1/v}(E)\frac{dE}{E} = \sigma_{aT}\,(.025)^{1/2}\int_{E_T}^{\infty}\frac{dE}{E^{3/2}} = \frac{\sigma_{aT}}{2} \qquad (2\text{-}37h)$$

where E_T is taken as .4 ev, the cadmium cutoff energy, which is convenient for experimental work; σ_{aT} is actually $\sigma_a(.025\text{ ev})$ and not an averaged thermal value.

Finally, at high energies the resonances can no longer be resolved. Here one has to make some guess, on statistical grounds, as to the resonance parameters. Hence, this energy range is called the statistical region. Rather than enter into the details of these calculations, which are rather involved, we shall quote only the results. They are given in Tables IV and V for U-238 and Th-232 and include the effects of temperature on resonances, discussed in the next section,[22] but neglect the 1/v portion of the resonance integral.

19. Doppler Broadening

The foregoing has been based on the assumption that the absorber nuclei are stationary, which is generally a rather good approximation if cross sections are slowly varying. As we shall soon see, the thermal motion of nuclei results in an apparent broadening of resonance lines

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[22] For a discussion of this and other fine points not fully discussed here see L. Dresner, Resonance Absorption of Neutrons in Nuclear Reactors, Pergamon Press, 1960.

TABLE IV

DRESNER'S CALCULATIONS OF THE EFFECTIVE RESONANCE INTEGRAL OF HOMOGENEOUS MIXTURES OF URANIUM

Temperature	σ_p (barns)	Contribution of resolved resonances (barns)	Contribution of unresolved resonances (barns)	Total (barns)
0°K	20	7.9	1.7	9.6
	200	24	4.8	28.8
	2000	74	11	85
300°K	20	8.1	3.0	11.1
	80	17	6.6	23.6
	200	27	9.4	36.4
	2000	86	12	98

TABLE V

DRESNER'S CALCULATIONS OF THE EFFECTIVE RESONANCE INTEGRAL OF HOMOGENEOUS MIXTURES OF THORIUM

Temperature	σ_p (barns)	Contribution of resolved resonances (barns)	Contribution of unresolved resonances (barns)	Total (barns)
0°K	20	3.7	2.2	5.9
	200	12	6.3	18.3
	2000	33	14	47
300°K	20	4.0	4.0	8.0
	80	8.9	8.6	17.5
	200	15	12	27
	2000	42	20	62

TABLE VI

MEASURED RESONANCE INTEGRALS I_∞

$(10^{-24}\ CM^2)$

NUCLIDE	ACTIVATION	ABSORPTION
$_{24}Cr$		1.9
$_{26}Fe$		2.1
$_{40}Zr$		3
$_{47}Ag^{107}$	74	
$_{47}Ag^{109}$	1160	
$_{49}In^{113}$	1050	
$_{49}In^{115}$	2640	
$_{62}Sm^{152}$	>1750	
$_{63}Eu^{153}$	950	
$_{79}Au^{197}$*	1558	
$_{90}Th^{232}$	69.8	
$_{92}U^{238}$	282	

*Adopted as standard, using σ_{th}=98 barns.

and an accompanying increase in absorption; omission of the "Doppler Broadening" may lead to underestimating of the effective resonance integral by a large amount.

Clearly, the cross section can depend only on the relative velocity of the nucleus and neutron. Therefore, to take into account the fact that nuclei are in motion one must average the cross section over the velocity distribution of the nuclei. One can thus write:

$$v\,\sigma_{a\,eff}(v) = \int |\underline{v} - \underline{V}|\,\sigma_a(|\underline{v}-\underline{V}|)\,P(\underline{V})\,d^3V \qquad (2\text{-}3$$

where $\underline{v}$ and $\underline{V}$ are the laboratory system velocities of the neutron and the absorber respectively, and $P(\underline{V})$ is the distribution of absorber velocities. Note that

$$\frac{V}{v} \approx \left(\frac{kT/A}{E}\right)^{1/2} \ll 1 \qquad (2\text{-}38b$$

at normal temperatures.* Here T is the absolute absorber temperature, A the mass of the absorber, and E the energy of neutron. Then, except for a few very high energy nuclei:

$$|\underline{v} - \underline{V}| \approx v \qquad (2\text{-}38c)$$

Under this approximation Equation (2-38a) becomes:

$$\sigma_{a\,eff}(v) = \int \sigma_a(|\underline{v}-\underline{V}|)\,P(\underline{V})\,d^3V \qquad (2\text{-}38d$$

The relative kinetic energy is

$$E' = \frac{1}{2}\,m\,|\underline{v}-\underline{V}|^2 \qquad (2\text{-}38e)$$

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* For U-238 at 300°K, V/v is about .004 at the (first) 6.7 ev resonance. At higher energy resonances, the ratio is even smaller.

where m is the mass of the neutron. Choosing the direction of $\underline{v}$ as the z-axis, we observe that for $V/v \ll 1$ (see Figure):

$$|\underline{v} - \underline{V}|^2 = v^2 + V^2 - 2vV\cos\theta \approx v^2 - 2vV_z \qquad (2\text{-}38f)$$

so that the relative kinetic energy is

$$E' = \frac{1}{2}mv^2 - mvV_z = E - (2mE)^{1/2}V_z \qquad (2\text{-}38g)$$

under the approximations made here, the relative energy E' is therefore a function only of the component of $\underline{V}$ in the direction of $\underline{v}$. The integration of Equation (2-38e) over V_x and V_y is therefore trivial and we have

$$\sigma_{a\,eff}(v) = \int \sigma_a(|\underline{v} - \underline{V}|)\,P(V_z)\,dV_z \qquad (2\text{-}39a)$$

where $P(V_z)$ is the one-dimensional velocity distribution of the absorber nuclei.

Using Equation (2-38g), we have

$$\sigma_{a\,eff}(E) \approx \int \sigma_a(E')\,P\left(\frac{E-E'}{\sqrt{2mE}}\right)\frac{dE'}{\sqrt{2mE}} \qquad (2\text{-}39b)$$

The appropriate distribution of nuclear velocities is the Maxwell-Boltzmann Distribution,* mentioned in Chapter I, Section 1,

$$P(V_z)\,dV_z = \left(\frac{M}{2\pi kT}\right)^{1/2}\exp\left\{-\frac{MV_z^2}{2kT}\right\}dV_z \qquad (2\text{-}39c)$$

where M is the mass of the nucleus. Using the Breit-Wigner line shape (2-36a) for $\sigma_a(E')$ and Equation (2-39c) for $P(V_z)$, the integral

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* This distribution is not quite correct in some crystals, but is a sufficient good approximation for the current application.

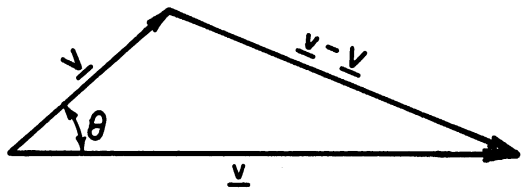

Figure II-6 Kinematics for Computation of the Doppler Effect.

Equation (2-39b) may be explicitly exhibited as

$$\sigma_{aeff}(E) = \int \sigma_0 \frac{\Gamma_\gamma}{\Gamma} \frac{\Gamma^2/4}{(E'-E_0)^2+(\Gamma/2)^2} \left(\frac{M}{2\pi kT}\right)^{1/2} \exp\left\{\frac{-M(E-E')^2}{2mE\,kT}\right\} \frac{dE'}{2mE} \qquad (2\text{-}40a)$$

Use of the substitutions

$$y = \frac{E'-E_0}{\Gamma/2} \qquad (2\text{-}40b)$$

$$\xi = \Gamma/\Delta = \left(\frac{\Gamma^2 A}{4kTE}\right)^{1/2} \qquad (2\text{-}40c)$$

$$\Delta = \left(\frac{4kTE}{A}\right) \qquad A = \frac{M}{m} \qquad (2\text{-}40d)$$

and the previous definition of x Equation (2-36b), reduces Equation (2-40a) to

$$\sigma_{aeff}(E) = \sigma_0 \frac{\Gamma_\gamma}{\Gamma} \frac{\xi}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\exp\left\{-\frac{\xi^2}{4}(x-y)^2\right\}}{1+y^2}\, dy \qquad (2\text{-}40e)$$

which gives the temperature dependence of the effective absorption cross section in a resonance. The quantity Δ, which has the dimensions of energy, is known as the Doppler Width of the resonance, as it plays a role similar to that of Γ in the Breit Wigner Formula. As T increases, the Doppler Width increases; i.e., the resonance broadens.

$$\psi(\xi, x) = \frac{\xi}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\exp\left\{-\frac{\xi^2}{4}(x-y)^2\right\}}{1+y^2}\, dy \qquad (2\text{-}40f)$$

is called the Doppler broadened line shape, and is the temperature-dependent counterpart of the natural line shape $(1+x^2)^{-1}$ previously considered.

Some properties of the function $\psi(\xi,x)$ may be briefly noted. Firstly,

$$\lim_{\xi\to\infty} \psi(\xi,x) = \int_{-\infty}^{\infty} \frac{\delta(x-y)}{1+y^2}\,dy = (1+x^2)^{-1} \qquad (2\text{-}41a)$$

since

$$\lim_{\xi\to\infty} \left[\frac{\xi}{2\sqrt{\pi}} \exp\left\{ -\frac{\xi^2}{4}(x-y)^2 \right\} \right] = \delta(x-y) \qquad (2\text{-}41b)$$

The significance of Equation (2-41a) is somewhat obvious; $\xi \to \infty$ implies $kT \to 0$. Thus, in the limit of stationary absorber nuclei, the Doppler broadened line shape reduces to the natural line shape, as expected. Another property is that

$$\int_{-\infty}^{\infty} \psi(\xi,x)\,dx = \pi \qquad (2\text{-}41c)$$

which is readily shown by integrating first over x and then over y, and is independent of ξ, i.e., the area under the absorption cross section curve is independent of temperature, but the curve is broader, and not as high at the peak. This is the key to understanding of the phenomenon of the Doppler Effect. Absorption resonances are generally strong enough to cause a lump to be "black", i.e., impenetrable, to neutrons with energies near the resonance peak. The Doppler effect does not lower the peak sufficiently to make the lump significantly less "black", but it does increase the energy range over which the lump absorbs. Hence, Doppler broadening increases the neutron absorption in a given resonance.

The Doppler broadened line shape may be substituted into the formulae for I_{NR} and I_{NRIA} to yield the temperature dependent

resonance escape probabilities for single resonances.* The results of these calculations give:

$$I_{NR} = \frac{\sigma_p \Gamma_\gamma}{E_0} J(\xi, \beta) \qquad (2\text{-}41d)$$

where

$$J(\xi, \beta) = \int_{-\infty}^{\infty} \frac{\psi(\xi, x)}{\psi(\xi, x) + \beta} dx \qquad \beta = \frac{\sigma_p}{\sigma_0}$$

is a tabulated function (see Reference in Footnote 22).

G. Resonance Integrals in Heterogeneous Systems

20. Effects of Heterogeneities

Heretofore, it has been assumed that the reactor under consideration is homogeneous, but it was also mentioned that most reactors are, in the strictly physical sense, heterogeneous. We have indicated that a hetergeneous system might be replaced by a fictitious homogeneous system, if it is composed of repeating substructures or cells. In this section, we will briefly describe some of these cell calculations but great detail will not be given. The reader is once again reffered to Dresner's work or to Nordheim's[23] excellent review article.

In the early days of reactor analysis, it was realized that a heterogeneous system could have a higher k_∞ than the same materials in homogeneous form. This results from several phenomena. Firstly, neutrons born in a lump have higher probabilities of hitting fuel nuclei on their first few collisions and thus increase the fast effect. Then they leave the lump and slow down in the moderator. At resonance energies few

* Note that as a result of Equation (2-41c), I_∞ is not temperature dependent.

[23] L. W. Nordheim, Report GA-638 (General Atomics, 1960).

neutrons are able to penetrate to the center of the lumps so that the absorber in the center of the lump absorbs fewer neutrons than it would in a homogeneous medium. Thus fewer resonance neutrons are captured and the resonance escape probability increases. This effect also works to reduce the thermal utilization f but the overall effect can be an increase in the infinite multiplication constant k_∞ if the reactor is properly designed. The effect on the fast effect and the resonance escape probability will be briefly indicated here.

21. Effect on Resonance Escape Probability

In order to compute resonance escape probabilities in heterogeneous systems, we shall consider a binary lattice of absorber (region "0") and moderator (region "1"). It has been shown[24] that the flux in such a system is spatially constant at energies far enough removed from neutron sources or sinks. (Close to sources or sinks, spatial oscillations, similar in nature to the Placzek oscillations in energy, Section 5, occur.)

Assuming, then, a spatially constant flux above the resonance energy, we may break the resonance absorption into two parts.

(a) Those neutrons which, before absorption, suffered their last collisions in the absorber (defined as n_0). The volume of the absorber will be denoted by V_0.

(b) Those neutrons which, before absorption, suffered their last collision in the moderator (defined as n_1). The moderator volume is V_1.

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[24] W. T. Hays, M. Luming and P. F. Zweifel, Trans. Amer. Nuc. Soc., 3, 2 (1960), Paper 8-4.

Making use of the assumed flat distribution of the flux above the resonance, one can write:

$$n_0 = V_0 \int_{Res} \frac{\Sigma_a^0(u)}{\Sigma_t^0(u)} P_{00}(u)\,du \int_{u-\ln\frac{1}{\alpha_0}}^{u} \Sigma_p^0\, \phi(u')\, F_0(u' \to u)\,du' \qquad (2\text{-}42a)$$

Here $\phi(u)$ is the flux at lethargy u, and $P_{ij}(u)$ is the probability that a neutron, born isotropically and uniformly in region i at lethargy u, will suffer its first collision in region j (i and j being either 0 or 1). The subscript 'Res' indicates that the integral is to be taken only over the lethargy range for which the resonance absorption is strong, i.e., approximately over the practical width. Similarly:

$$n_1 = V_1 \int_{Res} \frac{\Sigma_a^0(u)}{\Sigma_t^0(u)} P_{10}(u)\,du \int_{u-\ln\frac{1}{\alpha_1}}^{u} \Sigma_p^1\, \phi(u')\, F_1(u' \to u)\,du' \qquad (2\text{-}42b)$$

The asymptotic flux in this case is given by:

$$\phi(u) = \frac{q}{\bar{\xi}\,\Sigma_p} \qquad (2\text{-}42c)$$

where

$$V\,\bar{\xi}\,\Sigma_p = V_0\,\xi_0\,\Sigma_p^0 + V_1\,\xi_1\,\Sigma_p^1 \qquad V = V_1 + V_0 \qquad (2\text{-}42d)$$

and q is the slowing down density in the cell above the resonance. Now, noting that Σ_p is constant (or nearly so) in energy, and neglecting the resonance width compared to both $\ln 1/\alpha_i$ as in Section 14, we have

$$n_0 = \frac{q\,\Sigma_p^0}{\bar{\xi}\,\Sigma_p} V_0 \int_{Res} \frac{\Sigma_a^0(u)}{\Sigma_t^0(u)} P_{00}(u)\,du \qquad (2\text{-}43a)$$

and

$$n_1 = \frac{q\,\Sigma_p^1}{\bar{\xi}\,\Sigma_p} V_1 \int_{Res} \frac{\Sigma_a^0(u)}{\Sigma_t^0(u)} P_{10}(u)\,du \qquad (2\text{-}43b)$$

and defining the resonance escape probability as the ratio of the number of neutrons absorbed to the number slowing down, we have

$$1-p = \frac{n_0+n_1}{q_0 V} = \frac{N^0}{\bar{\xi}\Sigma_p} I_{eff} \qquad (2\text{-}43c)$$

Thus

$$I_{eff}^{NR} = \frac{V_0 \Sigma_p^0}{V} \int_{Res} \frac{\sigma_a^0(u)}{\Sigma_t^0(u)} P_{00}(u)\,du + \frac{V_1 \Sigma_p^1}{V} \int_{Res} \frac{\sigma_a^0(u)}{\Sigma_t^0(u)} P_{10}(u)\,du \qquad (2\text{-}43d)$$

Now, it follows from the definitions of the quantities that

$$P_{01}(u) = 1 - P_{00}(u) \qquad (2\text{-}44a)$$

and under the assumption of flat flux above the resonance, $P_{01}(u)$, the probability that a neutron born at lethargy u in the absorber suffers its first collision in the moderator is formally identical with the one-velocity escape probability, E, for purely absorbing media defined by Case, DeHoffmann, and Placzek.[25] (Only the first collisions need be considered when the NR approximation is being invoked.) Furthermore, $P_{01}(u)$ is related to $P_{10}(u)$ through the reciprocity relation for one velocity neutron transport:[26]

$$V_0 \Sigma_t^0(u) P_{01}(u) = V_1 \Sigma_p^1 P_{10}(u) \qquad (2\text{-}44b)$$

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[25] Case, Placzek, DeHoffmann, op. cit. For the single pin case or cases in which interactions with neighboring cells may be ignored, one may use the escape probabilities as tabulated in this reference. In the more practical case, escape probabilities for the entire lattice must be computed. See the section on Dancoff corrections.

[26] This result follows quite simply from the more general one velocity reciprocity relation given in Reference 25. One should also note that Equation (2-44b) is always true, not only for the single pin case.

Thus, the effective resonance integral reduces to

$$I_{eff}^{NR} = \frac{V_o}{V}\left\{\int_{Res} L(u)\,\sigma_a^o(u)\,\frac{(\Sigma_t^o(u)-\Sigma_p^o)}{\Sigma_t^o(u)}\,du + \Sigma_p^o\int\frac{\sigma_a^o(u)}{\Sigma_t^o(u)}\,du\right\} \qquad (2\text{-}44c)$$

In the development above, we have assumed some sort of unit cell of volume for which we are computing the resonance escape probability. For a single pin in the midst of an infinite homogeneous medium (a situation roughly approximated in measurements of I_{eff}) note that I_{eff} as we have defined it goes to zero because $V_1 \to \infty$. Such a situation is reasonable physically since we begin with an infinite number of neutrons and only a finite number are captured. Thus p must equal unity.

For this reason, some authors lump the volume factor V_o/V into the coefficient of I_{eff}, i.e.,

$$1 - p = \frac{N}{\bar{\xi}\,\Sigma_p\,V}\,R_{eff}$$

where $N = N_o V_o$ = the total number of absorber atoms (in a cell), and $\bar{\xi}\,\Sigma_p\,V$ is the cellular slowing down power, if we may coin a term (or perhaps we should say "borrow"). $R_{eff} = I_{eff}\,V/V_o$, and does not vanish as $V \to \infty$. Note that for a homogeneous medium $R_{eff} = I_{eff}$. In addition, Equation (2-44c) can be written in terms of the microscopic cross sections rather than macroscopic cross sections so long as we employ the artifice of using $\sigma_p^{o\prime}$, the potential scattering cross section (in the lump) per absorber atom. The reason for this artifice is obscure, but it must be historical as it is certainly not logical.

In the above equations, Σ_p^o must include the scattering cross section, per absorber atom, of any moderating element mixed with the absorber, e.g., oxygen in uranium oxide fuel elements.

For the NRIA approximation, the situation is somewhat more complicated than in the NR case because collisions with absorber atoms are assumed not to degrade the neutron energy. Such collisions do, however, affect the P_{ij} since they change the direction of the neutrons. Thus, the P_{ij} which are required in the NRIA approximation, cannot be given in terms of the one velocity escape probability E but are, in fact, related to the escape probabilities for absorbing and scattering bodies calculated for slabs by Stewart et al.[27] and for cylinders by Stuart[28] and Stuart and Woodruff.[29] These works calculate the escape probability for bodies which are surrounded by scattering media. To obtain the result required here, we must set

$$\text{"}\Sigma_a^o(u)\text{"} = \Sigma_{au}^o(u) + \Sigma_{pm}^o(u) \qquad (2\text{-}45a)$$

where $\Sigma_{au}^o(u)$ is the fuel absorption cross section and $\Sigma_{pm}^o(u)$ is the scattering (potential) cross section of any moderator mixed with the fuel. Also

$$\text{"}\Sigma_s^o(u)\text{"} = \Sigma_{su}^o(u) \qquad (2\text{-}45b)$$

is the "absorber scattering cross section" and

$$\Sigma_s'(u) = 0 \qquad (2\text{-}45c)$$

since a collision with the surrounding moderator will degrade the neutron

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[27] N. C. Francis, J. C. Stewart, L. S. Bohl and T. J. Krieger, PIGG P/627 (1958).

[28] G. W. Stuart, Nuc. Sci. Eng., 2, 617 (1957).

[29] G. W. Stuart and R. W. Woodruff, Nuc. Sci. Eng., 3, 339 (1958).

energy to below the resonance. A first order correction to E for this case is given by

$$P_{01}(u) = \frac{E(u)}{1 - \frac{\text{"}\Sigma_s^0(u)\text{"}}{\Sigma_t^0(u)} E(u)} \qquad (2\text{-}45d)$$

a result first derived by Stuart.[30] In addition, $\Sigma_t^0(u)$ must be replaced by $\Sigma_t^0(u) - \Sigma_{su}^0(u)$ in the factor $\sigma_a^0(u)/\Sigma_t^0(u)$ that appears in Equations (2-43a, b). (The reciprocity relation (2-44b) may, however, be retained intact.) The resonance integral in the NRIA approximation thus becomes:

$$I_{eff}^{NRIA} = \frac{\Sigma_p^0 V_0}{V} \int_{Res} \frac{\sigma_a^0(u)}{\Sigma_t^0(u) - \Sigma_{su}^0(u)} du + \frac{V_0}{V} \int_{Res} \sigma_a^0(u) \left[\frac{\Sigma_a^0(u)}{\Sigma_t^0(u) - \Sigma_{su}^0(u)} \right] \cdot \frac{E(u)}{1 - \frac{\text{"}\Sigma_{su}^0(u)\text{"}}{\Sigma_t^0(u)} E(u)} du \qquad (2\text{-}45e)$$

These equations have been integrated numerically by Adler, Hinman, and Nordheim,[31] who also considered the effects of Doppler Broadening.* Their results display very good agreement with the experimental results of Hellstrand. (See Table VI.)

It should be noted, however, that Adler's calculations omitted the interference between resonance and potential scattering, an effect studied by Neumann, op. cit. (Neumann also applied the work of Stuart

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* To take Doppler Broadening into account, one merely uses the Doppler line shape for σ_a. Otherwise, the formulae given above remain intact.

30 G. W. Stuart, op. cit.

31 F. T. Adler, G. W. Hinman, and L. W. Nordheim, PICG P/1988 (1958). Geneva

32 E. Hellstrand, J. Appl. Phys., 28, 1493 (1957).

TABLE VI

RESONANCE ESCAPE PROBABILITIES FOR CYLINDRICAL RODS OF U^{238}

Radius	Calculated (Ref. 31)	Experimental (Ref. 32)
0.422 cm	15.2	15.21
0.845 cm	11.4	11.26
1.68 cm	8.7	8.72
3.38 cm	7.0	7.21

and Woodruff to the resonance absorption case.) Adler also found that the factor $(1-\Xi(u)\ "\Sigma_s^o(u)"/\ \Sigma_t^o(u)\ )^{-1}$ did not appreciably aid agreement between theory and experiment, i.e., by completely ignoring the effect of multiple collisions in the NRIA case good values for I_{eff} were obtained. This may be due to cancellation of errors introduced by the two neglects, one of interference between resonance and potential scattering, and the other of multiple scattering.

To apply Adler's results to calculations of R_{eff}, it is necessary to first determine for each resonance whether it falls into the NR or NRIA category. He then writes

$$R_{eff} = R_V + R_S$$

where R_V, the "volume term", is the first term of Equation (2-44d) and R_S, the "surface term", is the second. (The reason for this notation is discussed in the next section.) For the NR case,

$$R_V^{NR} = \frac{\sigma_p^o \Gamma_\gamma}{E_o} J(\xi,\beta) \qquad (2\text{-}46a)$$

$$R_S^{NR} = \frac{\sigma_o \Gamma_\gamma}{E_o} \int_{-\infty}^{\infty} dx\, P_o\left[t\left(\frac{\psi}{\beta}+1\right)\right] \frac{\psi^2}{\psi+\beta} = \frac{\sigma_o \Gamma_\gamma}{E_o} L(t,\xi,\beta) \qquad (2\text{-}46b)$$

where σ_o , Γ_γ, β, and E_o are resonance parameters previously defined and $t = 4V_o\Sigma_p^o/S_o$ where S_o is the surface area of the lump. Since $4V_o/S_o$ is the mean chord length of a lump, t is its thickness in units of $(\Sigma_p^o)^{-1}$. The function $J(\xi, \beta)$ was defined by Equation (2-41d) and Equation (2-46b) defines $L(t, \xi, \beta)$. Extensive tables of these functions are given by Adler and Nordheim.[33]

A similar treatment is possible for the NRIA case with some redefinitions. Thus

$$R_V^{NRIA} = \frac{\sigma_{pm}\Gamma}{E_o} J(\xi, \beta') \tag{2-47a}$$

$$R_S^{NRIA} = \frac{\sigma_{pm}\Gamma}{\beta' E_o} L(t', \xi, \beta') \tag{2-47b}$$

where σ_{pm} is the scattering cross section per absorber atom of any moderator contained in the lump and

$$\beta' = \frac{\sigma_{pm}\Gamma}{\sigma_o \Gamma_\gamma} \tag{2-47c}$$

$$t' = \frac{4V_o\Sigma_{pm}}{S_o} \tag{2-47e}$$

For the case in which no moderator is mixed with the absorber, $\beta' = 0$ and R_V^{NRIA} becomes zero. However, this is clearly incorrect as some neutrons will always be slowed down into the resonance. We can

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[33] F. T. Adler and L. W. Nordheim, "Tables for the Computation of Resonance Integrals," GA-377 (1958).

make an approximate correction for this by saying that all neutrons slowed down into the resonance are captured. Then R_V^{NRIA} becomes simply the slowing down density and the number of neutrons captured per absorber nucleus will be

$$R_v^{NRIA} = \xi_U \sigma_{pu} \approx \frac{2}{A} \sigma_{pu} \tag{2-48a}$$

The surface term may, however, be correctly computed by setting $\sigma_{pm} = 0$ in Equation (2-47b). Equation (2-47b) then reduces to

$$R_S^{NRIA} = \frac{\sigma_0 \Gamma_\gamma}{E_0} \quad L'(t'', \xi) \tag{2-48b}$$

where

$$L'(t'', \xi) = \int_{-\infty}^{\infty} dx \, E(t'' \psi(\xi, x)) \psi(\xi, x) \tag{2-48c}$$

$$t'' = \frac{4 V_0 \Sigma_{a0}}{S_0} \tag{2-48d}$$

and

$$\Sigma_{a0} = \frac{N_u \sigma_0 \Gamma_\gamma}{\Gamma} \tag{2-48e}$$

is the macroscopic absorption cross section at the peak of resonance.

22. The Rational Approximation

Wigner noted that for small bodies $E \approx 1$, and for large bodies,

$$E \approx S/4V\Sigma$$

where S is the surface area and V the volume and so devised the well-known rational approximation

$$P_{01} = E = \frac{S_o/4V_o\Sigma_t}{1 + S_o/4V_o\Sigma_t} \tag{2-49a}$$

which gives both limits correctly. Fortunately, by using the Wigner rational approximation, much of the hard work described above can be avoided if extremely accurate answers are not required.

When this approximation is applied to the NR formula (2-44c) one obtains

$$I^{NR} = \frac{S_o}{4V} \int_{Res} \frac{\sigma_a^o(u)\left[\Sigma_t^o(u) - \Sigma_p^o(u)\right]}{\left[\Sigma_t^o(u)\right]^2 \left(1 + \frac{S_o}{4V_o\Sigma_t^o(u)}\right)} du \tag{2-49b}$$

$$+ \frac{V_o\Sigma_p^o}{V} \int_{Res} \frac{\sigma_a^o(u)}{\Sigma_t^o(u)} du$$

I_{NRA}

An interesting result can be arrived at by rearranging Equation (2-49b) and writing the result in terms of R_{eff}:

$$R_{eff}^{NR} = \int \frac{\sigma_a(u)\left[\Sigma_p + \frac{S_o}{4V_o}\right]}{\Sigma_t(u) + \frac{S_o}{4V_o}} du \qquad (2\text{-}49c)$$

On comparing this result with Equation (2-32b), we see that R_{eff}^{NR} is identical to I_{eff}^{NR}, the resonance integral for a homogeneous system, if Σ_p is replaced by $\Sigma_p + S_o/4V_o$. A similar analysis with respect to the NRIA approximation reveals that R_{eff}^{NRIA} becomes identical to the resonance integral I_{eff}^{NRIA} for a homogeneous system when the same substitution is made.

The consequences of this result are many-fold. Firstly it gives rise to the equivalence theorem that any two systems with the same $(\Sigma_p + S_o/4V_o)$ have the same resonance integral regardless of what the individual quantities Σ_p and $S_o/4V_o$ may be. This result may be used whenever results are desired only to the accuracy of the rational approximation. Since the rational approximation is always valid to within 10%, the results obtained by using this equivalence theorem are generally quite satisfactory. This theorem was first pointed out

by Chernick and Vernon.[34] This result also leads to the interpretation of $S_o/4V_o$ as an "escape cross section," i.e., a cross section for removal of a neutron from the lump. In this fashion, the rational approximation may be interpreted as stating that the escape probability, E, is the ratio of the escape cross section to the total (escape plus actual) cross section.[35]

This result also allows one to write an analytical expression for the resonance integral in the absence of Doppler Broadening. For, by redefining

$$\beta = \frac{\Sigma_p + \frac{S_o}{4V_o}}{N_u \sigma_o} \tag{2-50a}$$

Equation (2-37g) may be used. Thus

$$R_{eff}^{NR} = \frac{\pi}{2} \frac{(\sigma_p' + S_o/4V_o N_u)\Gamma_\gamma}{E_o \sqrt{\beta(1+\beta)}} \tag{2-50b}$$

Some of the limits of this equation are interesting. When $\sigma_p' + S_o/4V_o N_u$ is small compared to σ_o (i.e., for large lumps containing little moderator) β may be neglected compared to unity. Then

$$R_{eff}^{NR} = \frac{\pi}{2} \frac{\Gamma_\gamma}{E_o} \left(\sigma_o \left(\sigma_p' + \frac{S_o}{4V_o N_u}\right)\right)^{1/2} \tag{2-51a}$$

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[34] J. Chernick and E. Vernon, Nuc. Sci. Eng., 4, 649 (1958).

[35] L. W. Nordheim, GA-638 (1959).

Hence it has been suggested by Levine[36] that empirical fits to resonance integral data should be given in the form

$$I_o = f\left(\sigma_p + \frac{S_{eff}}{4VN_u}\right) \qquad (2\text{-}51b)$$

where S^{eff} is an effective surface area which includes a correction for interaction between lumps as discussed in the next section. As shown in Figures 7 and 8, this representation is a rather good one. If σ_p is small compared with $S_o/4V_oN_u$, as is the case for lumps of pure absorber, Equation (2-51a) becomes

$$I = \frac{\pi}{2}\frac{\Gamma_\gamma}{E_o}\sigma_o^{1/2}\left(\frac{S}{4VN_u}\right)^{1/2} = C\left(\frac{S}{M}\right)^{1/2} \qquad (2\text{-}51c)$$

or

$$I \simeq I_V + I_S(S/M)^{1/2} \quad (I_V \approx 0)$$

a form which has frequently been used.[37]

On the other hand, if $(\sigma_p + S_o/4V_oN_u)$ is still small compared with σ_o, but σ_p is large compared to $S_o/4V_oN_u$, Equation (2-51a) can be expanded to give

$$R_{eff}^{NR} \approx \frac{\pi}{2}\frac{\Gamma_\gamma}{E_o}\sigma_o^{1/2}\sigma_p^{1/2}\left[1 + \frac{S_o}{4V_oN_u\sigma_p}\right] \qquad (2\text{-}52a)$$

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36 M. M. Levine, Nuc. Sci. Eng., 8, 363 (1960).

37 This form was first suggested by I. I. Gurevich and I. Y. Pomeranchouck, PICG 5, 466 (1955).

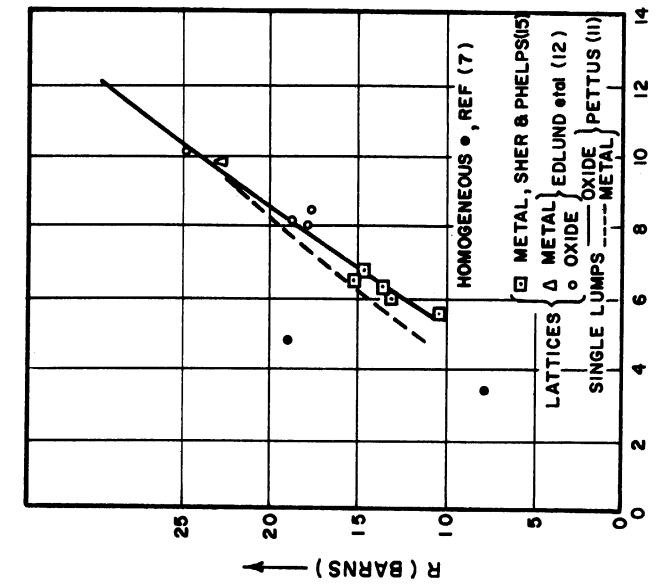

Figure II-8 Thorium resonance integral.

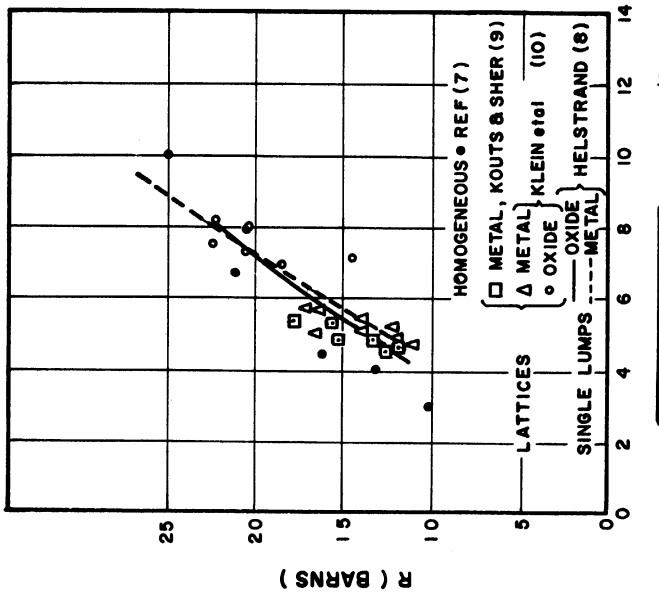

Figure II-7 U-238 resonance integral.

which is similar to the form given originally by Wigner.[38]

$$R_{eff}^{NR} = I_v' + I_s' \left(\frac{S}{M}\right) \qquad (2\text{-}52b)$$

and which was frequently used before Equation (2-51c) was suggested. It is found that Equation (2-51c) is generally more applicable.

Finally, if

$$\sigma_p + \frac{S_o}{4V_o N_u}$$

is large compared with σ_0, R_{eff}^{NR} correctly becomes the infinite dilution resonance integral I_∞.

23. Dancoff Corrections; Interactions of Cells

All of the numerical calculations discussed so far have been for the single pin case, i.e., for lattices in which adjacent absorber lumps do not interfere appreciably with each other's resonance absorption. To correct for this effect, it is necessary only to use the generalized escape probability in the equations for I_{eff}, i.e., to use the probability that a neutrons born uniformly and isotropically in the lump will suffer its first collision neither in that lump nor in any other lump.

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38 A. M. Weinberg and E. P. Wigner, op. cit.

Unfortunately, this quantity is quite difficult to calculate so that Monte Carlo calculations are frequently used.[39] Some analytical approaches have also been attempted.[40]

The historical approach[41] is based on the following argument. Insofar as absorption is concerned, the effect of a neighboring lump is to reduce the number of neutrons incident on a particular lump from the direction of the neighbor. Thus, not as many neutrons will be incident on the part of the surface that faces another lump as on the part that faces pure moderator. Hence not all of the surface is equally effective in capturing neutrons. To account for this an effective surface area S_{eff} is introduced and defined as:

$$S_{eff} = S(1 - c) \qquad (2\text{-}53a)$$

where (1 - c) is the "Dancoff Correction." This approach was mentioned in the previous section with regard to Equation (2-51b) and Figures 7 and 8.

The calculation of c (or of S_{eff}) is of course the most difficult portion of this calculation. Many authors[42] have considered this problem in various approximations and for various geometries but space does not permit inclusion of even a summary of this work here. Rather

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[39] A short discussion of the Monte Carlo method is given in Chapter III. Examples of its application to the problem of calculating resonance integrals may be found in R. D. Richtmyer, BNL 433, p. 82 (1957).

[40] J. Stewart and P. F. Zweifel, PICG P/631 (1958).

[41] S. M. Dancoff and M. Ginsburg CP-2157 (1944).

[42] To quote a few: J. A. Thie, Nuc. Sci. Eng., 5, 75 (1959); H. Takahashi, J. Nuc. Ener., 12, 1 (1960); Y. Fuaki, Trans. Amer. Nuc. Soc., 2, Paper 8-5 (1960); W. Rothenstein, Nuc. Sci. Eng., 7, 162 (1960).

we shall quote only a very simple result which is quite analogous to the rational approximation[43]:

$$S_{eff} = \frac{S\,\Sigma_p'}{\Sigma_p' + S\left(\frac{V_o}{V_1}\right)} \qquad (2\text{-}53b)$$

The approximation gives the correct result in the limits $(V_o/V_1) \to 0$ and $(V_o/V_1) \to \infty$ and is sometimes used. Unfortunately, it is not as accurate as the rational approximation.[44]

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[43] G. I. Bell, Nuc. Sci. Eng. 5, 75 (1959).

[44] L. W. Nordheim, GA 638.

CHAPTER III

SLOWING DOWN IN FINITE MEDIA

A. The Slowing Down Kernels

1. Introductory Remarks - Green's Function

In this chapter an attempt will be made to obtain approximations which are applicable to reactors in general. Much of the development is made in the context of asymptotic theory but a more general exposition of the theory, particularly of that portion which is usually applied in reactor calculations, is also given. In the previous chapter it was shown, rather briefly it must be admitted, how the resonance escape probability and fast fission factor could be obtained for non-homogeneous systems. These results can be used to define a set of fictitious cross sections, which depend on both the material composition and on the geometry and which yield the same resonance escape probability and fast effect when applied to calculations in a homogeneous medium of the same gross dimensions as the actual system.*

In a similar manner, values of other pertinent parameters can be obtained by insisting that the homogenized system have the same overall properties as the actual system. To simplify matters, it will be assumed that this homogenization has been carried out and hence we shall deal only with homogeneous systems in this chapter, except for one method designed specifically for calculations of heterogeneous systems

* Generally speaking, this homogenization is carried out by regions. Thus, a fuel-moderator region might be homogenized, while a region containing control rods might be homogenized separately.

which is discussed near the end of the chapter.

It may be worthwhile at this point to review the development of asymptotic reactor theory as presented in Chapter I. It was shown that by treating thermal neutrons by one group theory, the calculation of the effective multiplication constant may be reformulated in terms of the calculation of certain slowing down kernels. In this manner all of the details of slowing down were put aside and hidden within these slowing down kernels which must still be calculated; this chapter will be devoted largely to the calculation of the required slowing down kernels. Before attacking this problem directly, several results which will make the task simpler will be introduced.

First, we shall return to the mono-energetic source infinite medium slowing down kernel* $P(|\underline{r}' - \underline{r}|, E' \to E)$, and treat it as a Green's Function for the fission-averaged kernel $P(|\underline{r}' - \underline{r}|, E)$ discussed in Chapter I. This has the double advantage that:

1. monoenergetic sources are simpler to deal with than are distributed energy sources, and
2. such a slowing down kernel can be applied to sources other than U-235 fission.

Thus, such a kernel can be used in the design of reactors using fuels other than U-235 (e.g., U-233 or Pu-239); it can accurately account

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* Angular dependence of this kernel, i.e., of the kernel $P(\underline{r}' \to \underline{r}, E' \to E, \underline{\Omega})$, may be described by some of the methods presented.

for delayed neutrons or neutrons arising from (n, 2n) reactions, which generally do not have the same energy spectrum as fission neutrons.

From the definition of the slowing down kernel it is seen that in order to obtain the infinite-medium slowing down kernel $P_\infty(|\underline{r} - \underline{r}'|, E' \to E)$ it is necessary to solve the Boltzmann Equation for an infinite medium with a unit monoenergetic isotropic point source of neutrons at $\underline{r}'$. In practice, we will solve the Fourier Transform of the Boltzmann equation (or, what is the same thing, the Boltzmann equation with a "sinusoidal" source, $e^{-i\underline{k}\cdot\underline{r}}$). The transform may then be inverted to obtain the spatial distribution or, as we have seen in Chapter I, the transform itself may be used directly in critically calculations.

2. The One Dimensional Problem

Another important property of the slowing-down kernel is that the Fourier Transform of the infinite medium point source slowing-down kernel, namely the one employed up to now, is precisely the Fourier Transform of the kernel defined with respect to the plane source problem. This last kernel, $P(|z' - z|, E' \to E)$, or $P(z, E' \to E)$, is the neutron flux at distance z from the source due to a unit isotropic plane source of neutrons (one neutron per cm^2 per sec.) of energy E' at $z = 0$.

To prove this, let $P_{pt}(r)$ be the neutron flux* due to a unit

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* The energy variables are temporarily dropped for this argument.

point source at $\underline{r} = 0$. Then for any source distribution $S(\underline{r})$, the flux distribution $\phi(\underline{r})$ is:

$$\phi(\underline{r}) = \int S(\underline{r}') P(|\underline{r}-\underline{r}'|) d^3r' \qquad (3\text{-}1a)$$

If, in particular $S(\underline{r}) = \delta(z)$, we have, using cylindrical coordinates (see Figure 1):

$$P_{pl}(z) = \int_0^{2\pi} d\varphi \int_0^{\infty} \rho\, d\rho \int_{-\infty}^{\infty} dz' \, \delta(z') P_{pt}\left(\sqrt{(z-z')^2+\rho^2}\right) \qquad (3\text{-}1b)$$

The integration over z' is trivial, as is the azimuthal integration.

$$P_{pl}(z) = 2\pi \int_0^{\infty} P_{pt}\left(\sqrt{z^2+\rho^2}\right) \rho\, d\rho \qquad (3\text{-}1c)$$

Now, changing the variable of integration from ρ to $r = \sqrt{z^2 + r^2}$, we have

$$P_{pl}(z) = 2\pi \int_{|z|}^{\infty} r\, P_{pt}(r) dr \qquad (3\text{-}1d)$$

which may be differentiated to give

$$P_{pt}(r) = -\frac{1}{2\pi r} \left.\frac{dP_{pl}(z)}{dz}\right|_{z=r} \qquad (3\text{-}1e)$$

That is, the point source kernel may be found by differentiating the plane source kernel.

It is now possible to show that the Fourier Transforms of both kernels are identical. First, $P_{pl}(z)$ is written as the inverse

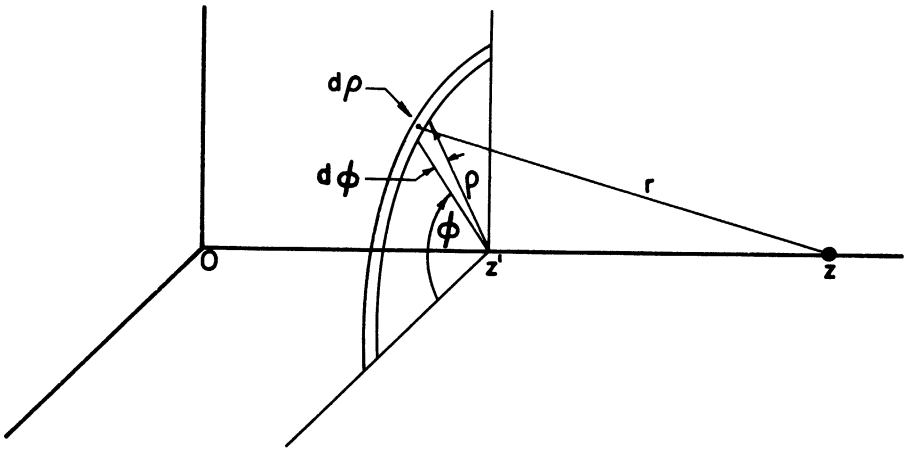

Figure 1

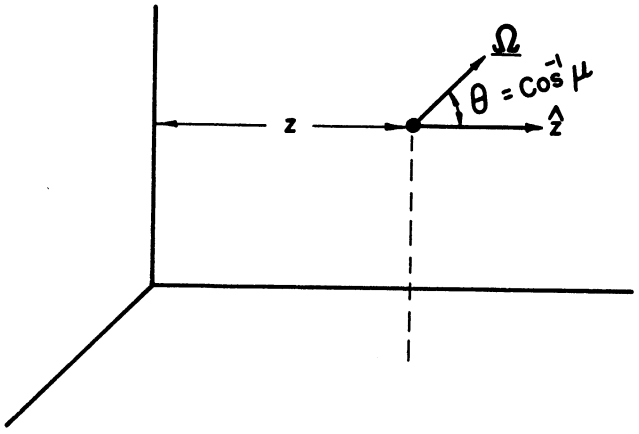

Figure 2

of its Fourier Transform, $\bar{P}_{pl}(k^2)$:

$$P_{pl}(z) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikz}\,\bar{P}_{pl}(k^2)\,dk = \frac{1}{\pi}\int_0^{\infty}\cos kz\,\bar{P}_{pl}(k^2)\,dk \qquad (3\text{-}2a)$$

since $\bar{P}_{pl}(k)$, like $\bar{P}_{pt}(k)$, can depend only on the magnitude of k (or on k^2) and is therefore an even function of k . Now, substituting into Equation (3-1e)

$$P_{pt}(r) = \frac{1}{2\pi^2}\int_0^{\infty} k\,\frac{\sin kr}{r}\,\bar{P}_{pt}(k^2)\,dk \qquad (3\text{-}2b)$$

Alternatively, $P_{pt}(r)$ may be written as the inverse of its Fourier Transform $\bar{P}_{pt}(k)$:

$$P_{pt}(r) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} e^{i\underline{k}\cdot\underline{r}}\,\bar{P}_{pt}(k)\,d^3k \qquad (3\text{-}2c)$$

The angular integrals are easily carried out and since $\bar{P}_{pt}(k)$ depends only on the magnitude of $\underline{k}$

$$P_{pt}(r) = \frac{1}{2\pi^2}\int_0^{\infty} k\,\frac{\sin kr}{r}\,\bar{P}_{pt}(k)\,dk \qquad (3\text{-}2d)$$

Comparing (3-2b) with (3-2d) we have

$$\bar{P}_{pt}(k^2) = \bar{P}_{pl}(k^2)$$

The import of this is that the entire problem of finding the slowing down kernels required in asymptotic reactor theory can be formulated and solved in plane geometry. The one dimensional problem can be solved, Fourier Transformed, and inverted to yield the point source

kernel, or Equation (3-1e) may be used to effect the conversion directly. The three dimensional problem is thus reduced to a simpler one dimensional problem. Furthermore, the one dimensional problem allows the approximations used to take a simpler form.

Having justified the use of the one dimensional form of the Boltzmann Equation, we will use this form whenever asymptotic reactor theory is to be applied. The one dimensional Boltzmann Equation, obtained by using the coordinate system shown in Figure 2 and noting the azimuthal symmetry in the problem, is

$$\mu \frac{\partial \Phi(z,E,\mu)}{\partial z} + \Sigma_t(E)\,\Phi(z,E,\mu) = \int d\mu' \int dE' \Phi(z,E',\mu') \Sigma_s(\mu_0, E' \to E) + S(z,E,\mu) \qquad (3\text{-}3a)$$

while its Fourier Transform is:

$$(\Sigma_t(E) - ik\mu)\,\bar{\Phi}(k,E,\mu) = \int d\mu' \int dE' \,\bar{\Phi}(k,E',\mu') \Sigma_s(\mu_0, E' \to E) + \bar{S}(k,E,\mu) \qquad (3\text{-}3b)$$

This is the basic equation on which much of this chapter will be based. Sources will be assumed isotropic so as to permit transformation to the point source problem, but the restriction is not a serious one for the class of problems under consideration.

3. Non-Leakage Probabilities

Since we obtained expressions for the fast effect and resonance escape probability in the previous chapter, the main concern here will be non-leakage probabilities. Under the as-

sumptions of asymptotic reactor theory the non-leakage probability λ is equal to the Fourier Transform of the slowing-down kernel $\bar{P}(B_g^2)$ divided by $\bar{P}(0)$.

Let us now expand $\bar{P}(B_g^2)$ in a Maclaurin series in B^2_g:

$$\bar{P}(B_g^2) \approx \bar{P}(0) + B_g \left.\frac{d\bar{P}}{dB_g}\right|_{B_g=0} + \frac{1}{2}\left.\frac{d^2\bar{P}}{dB_g^2}\right|_{B_g=0} \qquad (3\text{-}4a)$$

But from the definition of the Fourier Transform one has, for the one dimensional case:

$$\left.\frac{\partial^n}{\partial B_g^n}\right|_{B_g=0} = \int_{-\infty}^{\infty} (iz)^n P(z)\,dz \qquad (3\text{-}4b)$$

which is, except for normalization, the n^{th} spatial moment of the slowing-down kernel. But we are dealing with the problem of a unit plane isotropic source in an infinite homogeneous medium so that one would physically expect $P(z)$ to be an even function of z,* in which case the odd moments vanish. Frequently, one half the second moment is defined as the neutron age or simple the age, $\tau(E)$,

$$\frac{1}{2}\langle z^2(E)\rangle = \tau(E) = \frac{\int_{-\infty}^{\infty} z^2 P(z)\,dz}{\int_{-\infty}^{\infty} P(z)\,dz} \qquad (3\text{-}4c)$$

and is an extremly important quantity in reactor calculations. For large reactors, B_g^2 is small, and the non-leakage probability is

* Mathematically this can be shown by noting that the one dimensional Boltzmann Equation is unchanged under the transformation $z \to -z$ and $\mu \to -\mu$. Therefore $\Phi(z,\mu) = \Phi(-z, -\mu)$. On integrating over angle we have $\phi(z) = \phi(-z)$ which is the above statement.

approximately

$$\lambda(B_g^2) = 1 - B_g^2 \tau \qquad (3\text{-}4d)$$

In the limit of small reactors, one also frequently encounters the formulae:

$$\lambda(B_g^2) = e^{-B_g^2 \tau} \qquad (3\text{-}4e)$$

and

$$\lambda(B_g^2) = \frac{1}{1 + B_g^2 \tau} \qquad (3\text{-}4f)$$

which are equivalent to (3-4d) for small B_g^2.

From the identity of the Fourier Transform of the point and plane source kernels these results hold in general. However, the second spatial moment for slowing down from a point source $\langle r^2 \rangle$, is three times that from a plane source, $\langle z^2 \rangle$. To prove this, we write

$$\langle r^2 \rangle = \frac{\int_0^\infty r^2 P_{pt}(r) d^3r}{\int_0^\infty P_{pt}(r) d^3r} \qquad (3\text{-}5a)$$

or, using Equation (3-1e):

$$\langle r^2 \rangle = \frac{-\frac{4\pi}{2\pi} \int_0^\infty r \frac{dP_{pl}}{dr} dr^3}{-\frac{4\pi}{2\pi} \int_0^\infty \frac{1}{r} \frac{dP_{pl}}{dr} dr^3} \qquad (3\text{-}5b)$$

Now, using spherical coordinates, the angular integrations can be performed to yield:

$$\langle r^2 \rangle = \frac{\int_0^\infty r^3 \frac{dP_{pl}}{dr} dr}{\int_0^\infty r \frac{dP_{pl}}{dr} dr} \qquad (3\text{-}5c)$$

On integrating by parts, this becomes:

$$\langle r^2 \rangle = 3 \frac{\int_0^\infty r^2 P_{pl}(r)\,dr}{\int_0^\infty P_{pl}(r)\,dr} \qquad (3\text{-}5a)$$

since $P_{pl}(r)$ may be expected to go to zero exponentially at infinity. Hence:

$$\langle r^2 \rangle_{pt} = 3 \langle z^2 \rangle_{pl} \qquad (3\text{-}5e)$$

Thus, in general, the age is one sixth the mean square slowing down length, the generalization of the diffusion area L^2 to slowing down.

B. The Spherical Harmonics Method

4. Reduction of the Boltzmann Equation

In attempting to solve the Boltzmann Equation one soon discovers that most of the difficulty is introduced by the degradation term:

$$J(k,u,\mu) = \sum_i N_i \int d\Omega' \int du' \, \sigma_s(u', U, \mu_0)\, \Phi(k,u',\mu') = \sum_i N_i J_i \qquad (3\text{-}6)$$

where N_i is the number density of nuclei of species i. One would like a simple approximation with which to handle this term. One such approximation might be the estimation of this integral by a quadrature formula and indeed such procedures are frequently used and will be applied later. Another scheme that comes to mind is a series

expansion of the integrand in terms of a set of orthogonal functions, followed by a truncation of the series, yielding, it is hoped, a useful low order approximation.

If the flux and scattering cross section (or scattering frequency) are to be expanded separately, it is seen that it would be very valuable to choose a set of functions for which one is able to express functions of the angle between two vectors ($\underline{\Omega} \cdot \underline{\Omega}'$) in terms of functions of the individual vectors. Because of their relationship to the two dimensional Laplace Equation, the spherical harmonics provide a simple addition theorem and for this reason are the most convenient set of functions for this purpose.

For expanding the flux, one need only use the Legendre Polynomials since azimuthal symmetry has already been assumed:

$$\Phi(k,u,\mu) = \sum_{L=0}^{\infty} \frac{2L+1}{2} \phi_L(k,u) P_L(\mu) \qquad (3\text{-}7a)$$

where the expansion coefficients are:

$$\phi_L(k,u) = \int_{-1}^{1} d\mu \, \Phi(k,u,\mu) \qquad (3\text{-}7b)$$

The same expansions are, of course, possible in ordinary configuration ($\underline{r}$) space; these expansion coefficients are designated by $\phi_L(z, u)$ and are simply the inverse Fourier Transforms of the $\phi_L(k, u)$. For the (elastic) scattering cross section we already

have the expansion (1-49a):

$$\sigma_S(\mu_0, u', v) = \sum_{L=0}^{\infty} \frac{2L+1}{4\pi} B_L^\circ(u', v) P_L(\mu_0) \qquad (3\text{-}7c)$$

Using these expansions, the $J_i(k, u, u)$ of Equation (3-6) can be written:

$$J_i(k,u,\mu) = \int d\Omega' \int_{u-\ln\frac{1}{\alpha}}^{u} du' \sum_{L,L'=0}^{\infty} \frac{2L'+1}{4\pi} \frac{2L+1}{2} \phi_L(k,u) B_{L'}^\circ(u;v) \cdot P_L(\mu) P_{L'}(\mu_0) \qquad (3\text{-}7d)$$

It is here that the choice of Legendre Polynomials as the orthogonal set bears fruit. $P_{L'}(\mu_0)$ may be expanded by means of the addition theorem for Legendre Polynomials and the integration over $d\Omega'$ becomes rather trivial. This theorem may be stated as:

$$P_{L'}(\mu_0) = P_{L'}(\mu) P_{L'}(\mu') + 2\sum_{m=1}^{L'} (-)^m \frac{(L'-m)!}{(L'+m)!} P_L^m(\mu) P_L^m(\mu') \cdot \cos m(\varphi-\varphi') \qquad (3\text{-}7e)$$

where the $P_L^m(\mu)$ are the associated Legendre Polynomials.[1] The angles ϕ and ϕ' are the azimuthal angles associated with Ω and Ω' respectively. Upon inserting this expansion into Equation (3-7d), one observes that the only ϕ dependence appearing is that arising from the summation in the addition theorem (due to the assumed azimuthal symmetry of the flux) and that each of these terms integrates to zero because of the periodicity properties of the cosine functions.

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[1] For definitions of these functions as well as a proof of this theorem, see E. T. Whittaker and G. N. Watson, Modern Analysis, Oxford (1953).

Then

$$J_i(k,u,\mu) = \int_{u-\ell n\frac{1}{\alpha_i}}^{u} du' \int_{-1}^{1} d\mu' \sum_{L,L'=0}^{\infty} \frac{2L+1}{2} \frac{2L'+1}{2} \phi_L(k,u) B_L(u',U) P_L(\mu') \cdot P_{L'}(\mu') P_{L'}(\mu) \qquad (3\text{-}8a)$$

Application of the orthogonality property of the Legendre polynomials (1- 46e) reduces Equation (3-8a) to

$$J_i(k,u,\mu) = \sum_{L=0}^{\infty} \frac{2L+1}{2} J_{iL}(k,u) P_L(\mu) \qquad (3\text{-}8b)$$

where the $J_{iL}(k,u)$ may be interpreted as the Legendre expansion coefficients of the degradation integral and are related to the flux expansion coefficients by

$$J_{iL}(k,u) = \int_{u-\ell n\frac{1}{\alpha_i}}^{u} du' \phi_L(k,u') B^0_{iL}(u',U)$$

$$= \int_{u-\ell n\frac{1}{\alpha_i}}^{u} du' \phi_L(k,u') \sum_{L'=0}^{\infty} B^c_{L'}(u') T_{LL'}(U) \qquad (3\text{-}8c)$$

where the $T_{LL'}(U)$ are defined by Equation (1- 50b).

From the definition of the Fourier Transform it may be seen that $\phi_0(0, u)$, hereafter abbreviated to $\varphi(u)$,corresponds to the value of $\Phi(\underline{r}, \mu, u)$ integrated over all space and angle and is the total neutron flux in the reactor. Setting $k = 0$ in the Fourier Transformed Boltzmann Equation (3-3b) (this corresponds to an infinite medium), integrating over angle, and again using the orthogonality properties of the Legendre polynomials, we find

$$\Sigma_t(u)\varphi(u) = \sum_i N_i J_{0i}(k,u) + S(u) \qquad (3\text{-}8d)$$

with $J_{oi}(u)$ given by

$$J_{oi}(u) = \int_{u-\ln\frac{1}{\alpha_i}}^{u} du' \varphi(u') \sum_{L'=0}^{\infty} B_{L'}^{C}(u') T_{LL'}(U) \qquad (3\text{-}8e)$$

which are the basic equations that were treated in Chapter II. This is, therefore, an alternative derivation of Equations (2- 2a) and (2- 2b).

Using the above expansions, the Fourier Transformed Boltzmann Equation may be written:

$$\left(\Sigma_t(u) - \lambda k\mu\right)\sum_{L=0}^{\infty}\phi_L(k,u)P_L(\mu) = \sum_i N_i \sum_{L=0}^{\infty} J_{iL}(k,u)P_L(\mu) + \sum_{L=0}^{N} S_L(u)P_L(\mu) \qquad (3\text{-}9)$$

5. The PL Approximation

The most straightforward procedure for solving Equation (3-9) is to multiply the entire equation by $P_j(\mu)$ and integrate over all μ, which leads to the coupled set of integral equations

$$\Sigma_t(u)\phi_j(k,u) - \frac{\lambda k}{2j+1}\left[j\,\phi_{j-1}(k,u) + (j+1)\phi_{j+1}(k,u)\right]$$
$$= N_H J_j^H(k,u) + N_D J_j^D(k,u) + \sum_{i\neq H,D} N_i J_{ij}(k,u) + S_j(u) \qquad (3\text{-}10a)$$

where $\phi_{-1}(k, u)$ is zero by convention and the recursion relation for Legendre Polynomials[2]

$$\mu P_L(\mu) = \frac{1}{2L+1}\left[(L+1)P_{L+1}(M) + L P_{L-1}(M)\right] \qquad (3\text{-}10b)$$

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[2] Ibid.

has been employed in the evaluation of the second term. For an isotropic (fission) source, $S_j(u) = 0$ for $j \neq 0$ as a result of the orthogonality of the Legendre polynomials. The first two terms of the right-hand side of Equation (3-10a) represent neutron degradation (slowing down) due to hydrogen and deuterium, respectively, while the third term represents the degradation due to heavier elements, which may frequently be treated as a group.

For hydrogen, which scatters isotropically at neutron energies relevant to reactor calculations, $B_L^C(u) = 0$ for $L'>0$, so that $J_j^H(k, u)$ reduces to a single term:

$$J_j^H(k,u) = \int_0^u \phi_j(k,u') \Sigma_s^H(u') e^{-(u-u')} P_j\left(e^{-(u-u')/2}\right) du' \qquad (3\text{-}11)$$

If deuterium is present, the $J_j^D(k, u)$ term will also appear in Equation (3-10), but scattering from deuterium is not isotropic so that the degradation integral does not reduce to a single term. Again, deuterium moderation will be the most difficult one to handle.

The technique employed here is often called the "Spherical Harmonics Method"[3] because the orthogonal set of expanding functions used are the spherical harmonics (although in the case of azimuthal symmetry they are only to the ordinary Legendre polynomials necessary).*

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[3] P.M. Morse & H. Feshbach, Methods of Theoretical Physics. New York: McGraw Hill (1950) Vol I.

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* This procedure was used Chapter I to derive the Diffusion Equation.

This technique succeeds in converting the integro-differential Boltzmann Equation into an infinite set of simpler, but coupled, integro-differential equations, essentially by a variable transformation from the continuous variable μ to the discrete variable j. This, in and of itself, represents no real simplification and possibly an increase in complexity; the advantages of the method are realized only when it is noted that the neutron flux in a large reactor is not very anisotropic and hence a few Legendre components might suffice to describe its angular variation accurately. This, plus the fact that the j-th of Equations (3-10) is coupled only above and below it $(j - 1, j + 1)$, suggests setting $\phi_j(k, u) = 0$ for some j, say $j = L + 1$, thus uncoupling the first $L + 1$ equations from all others and leaving a set involving only $\phi_0, \ldots, \phi_L$. The truncated set so obtained can then be solved to yield an approximate flux. The accuracy of the method may be tested by using higher-order approximations (increasing L) until the fluxes (or multiplication constant) predicted are the same, within a predetermined limit, for two successive approximations. This is called the P_L approximation.

The simplest of the P_L approximations is, of course, the P_0. However, it is based on the assumption of isotropic flux and hence can predict no neutron transport; Equations (3-10) then reduces to (2-2a). The next simplest is the P_1 approximation, which is probably the most frequently used reactor calculation technique.

Methods of solving the P_1 equations, under various assumptions, will be discussed in the next few sections. The P_2 and other even L P_L approximations are of little value, for reasons to be discovered later. Higher P_L approximations are applied mainly to special problems, especially where great accuracy is required or where the flux is highly anisotropic, as in regions near heavily absorbing rods.

6. The Spherical Harmonics Method in Other Geometries.[4]

In plane geometry, we have just seen that the Spherical Harmonics method leads to an extremely simple set of equations for an approximate flux. This, unfortunately, is in great measure due to the unusual amount of symmetry found in problems of this type. Since the angular dependence of the flux was a function of only one angular variable, an expansion of the flux in ordinary Legendre Polynomial was possible. In the more general case, not only will the angular dependence be a function of two angular variables but the flux itself will depend on more than a single spatial coordinate. In this situation, the flux must be expanded in terms of the full set of spherical harmonics.

The equivalent of the P_1 approximation for general geometry was given in Chapter I when an expansion of the type

$$\Phi(\underline{\Omega}) = \phi_0 + \sum_i \phi_{1i}\,\Omega_i$$

where Ω_i is the i-th component of $\underline{\Omega}$, was made.

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[4] J. C. Mark, The Spherical Harmonics Method, Reports MT92, MT97 National Research Council of Canada.

7. Boundary Conditions for the Spherical Harmonics Method.

Some of the conditions that must be imposed on the components of the flux $\left(\text{the } \phi_L(r, u)\right)$ are probably quite clear; each of them must be finite and non-negative everywhere within the reactor volume. Furthermore, the fact that $\Phi(\underline{r}, u, \underline{\Omega})$ must be continuous everywhere within the reactor volume requires that each of its components be continuous at any internal point of the system. The conditions to be imposed on the spherical harmonics equations are then completely specified except for those which must be applied at the outer boundary of the system, i.e., at a material-vacuum interface.

First we recollect that the rigorous condition to be imposed at a "free" interface is that no neutrons enter the system from outside, that is

$$\Phi(\underline{r}, u, \underline{\Omega}) = 0 \quad \cdot \underline{\Omega} \cdot \underline{n} < 0 \qquad (3\text{-}12a)$$

for $\underline{r}$ on a surface. It is, however, impossible to make any finite series of the form

$$\sum \phi_L P_L(\mu) \qquad (3\text{-}12b)$$

fit a function of the form (3-12a), except in the trivial (and unphysical) case for which $\Phi(\underline{r}, u, \mu)$ is also zero for $\mu > 0$. This then implies 1) that another set of approximate conditions will have to be found and 2) that this approximate set of conditions is not

unambigouosly defined. Furthermore in an odd L approximation one can in general apply only (L+1)/2 boundary conditions at an interface, or in an even approximation L/2. The reason for this lies in the fact that in plane geometry there will always be two free surfaces in a finite system and that in any other geometry half of the solutions will blow up at some point in the system.[5] Since the boundary conditions are ambiguous, we are free to choose any conditions we like, provided that they are consistent with the rigorous condition (this implies, for one thing, that they approach the correct condition in the limit $L \to \infty$). The most frequently applied boundary condition are those which were proposed by Mark[6] and Marshak[7].

Mark pointed out that the problem of a slab imbedded in an absorbing, but non-scattering, medium is completely equivalent to that of the same medium in a vacuum. Then one can use the

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[5] See Davison, op. cit., Chapter 10, for a more complete discussion. For an odd L approximation this follows from the fact (shown by Davison) that the PL equation can always be recast (for L odd) into the form

$$\sum_{n=0}^{L} a_n \nabla^{2n} \phi_o = S$$

where the a_n are in general energy dependent operators. This can then be factored into L equations of the type $(\nabla^2 + b^2_n)\phi_o = 0$ which always has one irregular solution (except in slab-geometry)

[6] J.C. Mark op. cit.

[7] R.E. Marshak, Revs. Mod. Phys., 19, 185 (1947).

continuity boundary conditions at the interface together with finiteness conditions in the surrounding medium at infinity to solve the problem. He could then show that the conditions were equivalent to the requirement that

$$\Phi(z,\mu,\mu_j) = 0 \qquad j = 1,2\cdots\frac{L}{2} \tag{3-12c}$$

when the μ_j are the positive roots of

$$P_L(\mu) = 0 \tag{3-12d}$$

This provides just the correct number of conditions. Alternatively one could apply condition (3-12c) at any $(L+1)/2$ points μ_j provided that they are uniformly spread in the interval $0 \geq \mu \geq -1$ as $L \to \infty$. The set given by Mark (3-12d) do however give the best results of any condition of this type.

Marshak, on the other hand, pointed out that it follows from (3-12a) that

$$\int_{-1}^{0} f(\mu)\,\phi(z,\mu)\,d\mu = 0 \tag{3-12e}$$

for any regular function $f(\mu)$ in the interval $-1<\mu<0$. Then by choosing $(L+1)/2$ such functions (for L odd, again), a set of applicable conditions will result. Clearly, if the $P_j(\mu)$ are chosen Equation (3-12e) will result in a set of relations among the $\phi_j(\mu)$. Hence, one should choose $(L+1)/2$ of the $P_j(\mu)$, $j<L$.

But, on the interval $-1<\mu<0$ the set $\left\{ P_{2k}(\mu) \right\}$ is complete as is the set $\left\{ P_{2k+1}(\mu) \right\}$, $k = 0, 1, 2, \ldots$. Condition (3-12a) is thus met in the limit $L \to \infty$ if either of these sets of boundary conditions is chosen. The first conditions of each of these sets are

$$\int_{-1}^{0} \Phi(z,u,\mu)\, d\mu = 0 \qquad (3\text{-}12f)$$

and

$$\int_{-1}^{1} \mu\, \Phi(z,u,\mu)\, d\mu = 0 \qquad (3\text{-}12g)$$

Calculations have shown[8] that the Marshak conditions yield more accurate results in the P1 approximation but that the Mark conditions become superior for higher order approximations. In general, however, the Marshak ~~conditions are somewhat~~ simpler to apply and are therefore more frequently used.

8. Heavy Elements Approximations

The degradation integral $J_j(k, u)$ is relatively difficult to handle. First, if more than one moderator is present, J_j consists of a sum of integrals over different lethargy ranges. Secondly, if the cross sections are grossly anisotropic a large number of $B_L^c(u)$ are required to describe J_j accurately. An approximation valid for the general case of mixtures would be useful, but as we have seen in Chapter II the flux may vary rapidly in energy if resonances

8 Davison op.cit.

in the cross sections exist. From this standpoint the slowing down density is therefore a better quantity with which to work, since, in general, it is more slowly varying than the flux. From Equation (2-14a) we have, for the infinite medium without capture $\phi(u) = \frac{S}{\xi \Sigma_t(u)}$ at lethargies far from the sources, S being the integrated source density. Physically, the slowing-down density in this case must be equal to S (all neutrons slow down all the way to thermal) so that

$$q \approx \xi \Sigma_t(u) \phi(u)$$

In a finite medium this may not follow, but in a large reactor it should be a good approximation. In many cases ξ is nearly constant and resonance capture is fairly small so that $\Sigma_t(u)\,\phi(u) = B_0^c \phi(u)$ should be slowly varying. It may be that $B_{L'}^c(u)\phi_L(u)$ for $L'>0$ is not slowly varying, but one hopes that it is slowly varying enough in one collision interval to permit the following Taylor Series expansion of $B_{L'}^c(u)\phi_L(u)$ about $u = u'$ (a Maclaurin series in U):

$$B_{L'}^c(u)\phi_L(u) = \sum_\nu \frac{(u'-u)^\nu}{\nu!} \frac{\partial^\nu}{\partial u^\nu}\left[B_{L'}^c(u)\phi_L(u)\right]$$

$$= \sum_\nu (-)^\nu \frac{U^\nu}{\nu!} \frac{\partial^\nu}{\partial u^\nu}\left[B_{L'}^c(u)\,\phi_L(u)\right] \qquad (3\text{-}13)$$

This series, of course, does not converge rapidly for hydrogen, for which U may be infinite. The series is best for heavy moderators

for which U takes on only small values. Deuterium moderation is a case for which the series converges slowly and a reasonable approximation may require more terms than could easily be handled. This problem will receive special attention later. Fortunately, scattering from hydrogen is nearly isotropic in C at reactor energies and the integrals run from 0 to ∞ on U so that this case is again easy to handle in a straightforward manner.

Upon inserting Equation (3-13) into Equation (3-8c), we have

$$J_L(k,u) = \sum_{L',\nu=0}^{\infty} \sum_i N_i \frac{\partial^\nu}{\partial u^\nu}\left[B_{L'}^{c,i}(u)\phi_L(k,u)\right]\int_0^{\ln\frac{1}{\alpha_i}} U^\nu T_{LL'}^i(U)\,dU$$

$$= \sum_i N_i \sum_{L',\nu=0}^{\infty} T_{LL'}^{\nu} \frac{\partial^\nu}{\partial u^\nu}\left[B_L^{c,i}(u)\phi_L(k,u)\right] \qquad (3\text{-}14a)$$

where the $T_{LL'}^{\nu}$ have been previously defined in Section I-25.

Using this expansion for all elements except hydrogen and deuterium, we have:

$$\Sigma_t(u)\phi_J(k,u) - \frac{ik}{2J+1}\left[J\phi_{J-1}(k,u) + (J+1)\phi_{J+1}(k,u)\right]$$

$$= N_H J_J^H(k,u) + N_D J_J^D(k,u) + \sum_{i\neq H,D} N_i \sum_{\nu,L'=0}^{\infty} T_{JL'}^{\nu i} \frac{\partial^\nu}{\partial u^\nu}\left[B_{L'}^{c,i}(u)\phi_J(k,u)\right] + S_J(u) \qquad (3\text{-}14b)$$

Quite often, for heavy elements, one is satisfied to retain all terms of

order γ, neglecting terms of higher order in γ. Selection may be made using Amster's Theorem, quoted in Section 25. For $j = 0$ and $j = 1$ only terms with $\nu = 0, 1$ need by kept, while for $j \geq 2$ all terms may be ignored in this approximation. Frequently, the $\nu = 1$ terms for $j = 1$ is also neglected, an approximation which is somewhat inconsistent* but which leads to some valuable results. In this approximation, $J_L(k, u)$ becomes

$$J_0(k,u) = \sum_i N_i \sum_{L'=0}^{\infty} \left[T_{0L'}^{0i} \, B_{L'}^{c\,i}(u) \phi_L(k,u) + T_{0L'}^{1i} \frac{\partial}{\partial u} \left[B_L^{c\,i}(u) \phi_L(k,u) \right] \right] \tag{3-15a}$$

$$J_1(k,u) = \sum_i N_i \sum_{L'=0}^{\infty} T_{1L'}^{0i} \, B_{L'}^{c\,i}(u) \phi_1(k,u) \tag{3-15b}$$

The sums $\sum_{L'} T_{LL'}^{\nu i} \, B_{L'}^{c}(u)$ may be evaluated using Equations (1-62a) and (1-62b)

$$J_0(k,u) = \Sigma_S(u) \phi_0(k,u) + \frac{\partial}{\partial u} \left[\xi \Sigma_S(u) \phi_0(k,u) \right] \tag{3-15c}$$

$$J_1(k,u) = \Sigma_S(u) \langle \mu \rangle \phi_1(u) \tag{3-15d}$$

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* It should be noted that T_{10}^{1}, the leading terms being dropped here to approximately $2\gamma/3$ for small γ.

C. The P_1 Approximation

9. The Neutron Age

It is clear that the most accurate P_1 approach should employ the full P_1 equations, but this set has been solved in closed form only a few problems. Many solutions to the P_1 equations have been obtained in various approximations given later, but the advent of large high-speed computers has made it possible to solve the complete P_1 equations numerically. Numerical methods cannot completely supplant analytical methods; the latter give insight into the problems so that the various methods supplement each other. Hence we shall endeavor to give analytical solutions whenever they are obtainable, and for problems which are as realistic as possible.

The P_1 equations follow from (3-10a) by setting $\varphi_2(k, u) = 0$.

$$\Sigma_t(u)\,\phi_0(k,u) - \iota k\,\phi_1(k,u) = \sum_i N_i J_0^i(k,u) + S(k,u) \qquad (3\text{-}16a)$$

$$\Sigma_t(u)\,\phi_1(k,u) - \frac{\iota k}{3}\,\phi_0(k,u) = \sum_i N_i J_1^i(k,u) \qquad (3\text{-}16b)$$

Where the $J_j(k, u)$ are written in the rigorous form, of Equation (3-8c). In most work heavy element scattering is approximated in some manner. If the Taylor series approximation is made for all elements (including hydrogen and deuterium), we have the so-called

age-diffusion approximation; if hydrogen is excluded from this approximation and is treated rigorously, the consistent P_1 Selengut-Goertzel (SG) approximation is obtained; if both hydrogen and deuterium are excluded a consistent P_1 approximation is obtained.

In many cases still another approximation is applied. This method, called the P_1 Greuling-Goertzel (GG) Method, reduces the problem of solving an equation with integrals over different energy ranges to a much simpler one in which all integrals extend to infinity by replacing the scattering frequencies of all elements except hydrogen by approximate kernels. The procedure is, of course, not necessary for hydrogen as the rigorous kernel is already of the type required. This method is particularly useful in problems involving deuterium moderation.

It is important to note that some sort of approximation is almost always made to heavy element scattering, but the difficulty in obtaining an accurate approximation for hydrogen slowing down and the simplicity of the kernel for hydrogen compels us to treat it rigorously. This last point is to be emphasized--that <u>hydrogen slowing down will always be treated rigorously</u>.

An important property of the P_1 approximation is that with it <u>one can calculate the age rigorously</u>; that is, angular Legendre moments of the flux higher than the first do not contribute to the second spatial moment of the flux. Accurate

calculation of the age is thus a criterion by means of which the validity of approximations to the P_1 equations may be examined. Later in the chapter, the results of some of the approximate calculations will be compared with each other and with experiment and it will be seen that the methods just mentioned do give the age accurately in the problems for which they are designed.

The fact that the age is given rigorously in the P_1 approximation will now be proven. First, each term in the P_1 equations is expanded in a power series in k, the Fourier Transform variable:

$$\phi_j(k,u) = \sum_{l=0}^{\infty} \varphi_{jl}(u) \frac{(\mu k)^l}{l!} \qquad (3\text{-}17a)$$

for the flux, and

$$J_j^i(k,u) = \sum_{l=0}^{\infty} J_{jl}^i(u) \frac{(\mu k)^l}{l!} \qquad (3\text{-}17b)$$

for the degradation integrals. Now, from Taylor's theorem the expansion coefficients of the flux are given by

$$\varphi_{jl}(u) = \frac{\partial^l}{\partial(\mu k)^l} \phi_j(k,u)\Big]_{k=0} = \int_{-\infty}^{\infty} (z)^l \phi_j(z,u)\, dz \qquad (3\text{-}17c)$$

where the $\phi_j(z, u)$ are the coefficients of the Legendre expansion of the flux in configuration (z) space.

Substitution of the flux expansion (3-17a) into the defi-

nition of $J_j(k, u)$, Equation (3-8a) shows that

$$J^i_{jl}(u) = \int_{u-\ell n \frac{1}{\alpha_i}}^{u} \varphi_{jl}(u') B^{o\,i}_{l}(u', \tau)\, du' \qquad (3\text{-}17d)$$

Also, from the definition of the age we have

$$\tau(u) = \frac{1}{2} \frac{\int_{-\infty}^{\infty} z^2 dz \int_{-1}^{1} d\mu\, \Phi(z, u, \mu)}{\int_{-\infty}^{\infty} dz \int_{-1}^{1} d\mu\, \Phi(z, u, \mu)} = \frac{1}{2} \frac{\varphi_{02}(u)}{\varphi_{00}(u)} \qquad (3\text{-}17e)$$

One further result is required before the statement made above can be proven, namely

$$\varphi_{jl}(u) = 0 \qquad \text{for } j > l \text{ or } j+l \text{ odd} \qquad (3\text{-}18a)$$

To show this is will be most convenient to use the spherical harmonics equations without resorting to the P_1 approximation although a group-theoretical proof is also possible. Substituting the expansions (3-17a,b) into the spherical harmonics Equations (3-10a) one obtains:

$$\Sigma_t(u) \sum_{l=0}^{\infty} \frac{(\lambda k)^l}{l!} \varphi_{0l}(u) - \lambda k \sum_{l=0}^{\infty} \frac{(\lambda k)^l}{l!} \varphi_{1l}(u) = \sum_{i=0}^{\infty} N_i \frac{(\lambda k)^l}{l!} J^i_{0l}(u) + S(u) \qquad (3\text{-}18b)$$

from the first equation, where it has been assumed that the source is a plane $\delta(z)$. In the expansion of the source in a power series in k only the first term is non-zero since S does not depend

upon k .

From the spherical harmonics equations with $j>0$,

one obtains:

$$\Sigma_t(u)\sum_{l=0}^{\infty}\frac{(ik)^l}{l!}\varphi_{jl}(u)-\frac{ik}{2j+1}\left[j\sum_{l=0}^{\infty}\frac{(ik)^l}{l!}\varphi_{j-1,l}(u)+(j+1)\sum_{l=0}^{\infty}\frac{(ik)^l}{l!}\varphi_{j+1,l}(u)\right]$$

$$=\sum_{l=0}^{\infty}\sum_{i}N_i\frac{(ik)^l}{l!}J^i_{jl}(u) \qquad (3\text{-}18c)$$

Now one can collect coefficients of the various powers of k in these equations and equate them. For example, from Equations (3-18c) if one collects powers of k^0 one obtains for any $j \neq 0$:

$$\Sigma_t(u)\,\varphi_{j0}(u)=\sum N_i\,J^i_{j0}(u)$$

which is a homogeneous Volterra Integral equation for $\varphi_{j0}(u)$ which has only the trivial solution:

$$\varphi_{j0}(u)=0$$

Using this result, one quickly finds by collecting the coefficients of k^1 in (3-18b) that

$$\varphi_{01}(u)=0$$

Continuing, collecting coefficients of k^2 in the $\ell = 1$ equation,

one has

$$\varphi_{21}(u) = 0$$

By iterating in this manner, always choosing to collect odd powers of k in the even j equations and even powers of k in the odd j equations, one arrives at the result (3-18a).

Now, collecting coefficients of k^0 and k^2 in the $j = 0$ equation and coefficients of k^1 in the $j = 1$ equation leads to a set of three coupled equations in the three lowest index non-zero $\varphi_{j\ell}(u)$:

$$\Sigma_t(u)\,\varphi_{00}(u) = S_0 + \sum_i N_i J_{00}^i(u) \qquad (3\text{-}19a)$$

$$\frac{1}{2}\Sigma_t(u)\,\varphi_{02}(u) - \varphi_{11}(u) = \frac{1}{2}\sum_i N_i J_{02}^i(u) \qquad (3\text{-}19b)$$

$$\Sigma_t(u)\,\varphi_{11}(u) - \frac{1}{3}\varphi_{00}(u) = \sum_i N_i J_{11}^i(u) \qquad (3\text{-}19c)$$

This set of equations, when taken together with the defining relations for the $J_{j\ell}^i(u)$, Equations (3-17d), three for each moderator present, is just sufficient to determine the quantities $\varphi_{00}(u)$ and $\varphi_{02}(u)$, and hence the age from Equation (3-17e). None of the $\varphi_{j\ell}(u)$ with $j>1$ enter Equations (3-19) since $\phi_2(k, u)$ contributes nothing to the coefficient of k^1 in the second of the equations, hence the neutron age can be calculated rigorously using the P_1 approximation.

10. Age Diffusion Theory

The simplest special case of the P_1 approximation is that for which the hydrogen and deuterium concentrations vanish, thus eliminating two terms on the right side of each of Equations (3-16). We are then dealing only with the case of "heavy" element (e.g., carbon, beryllium) moderation and the Taylor series expansion (3-13) can be expected to converge rapidly. It has been seen that the second and higher derivative terms in these equations have coefficients of order at least γ^2, i.e., neglect of them can be expected to introduce an error of approximately 1/81 in the beryllium, but would leave an error of magnitude 1/4 in deuterium. Hence, as a first approximation they may be neglected for heavy elements and we arrive at a consistent P_1 approximation for heavy elements:

$$\Sigma_t(u)\phi_0(k,u) - ik\phi_1(k,u) = \Sigma_s(u)\phi_0(k,u) - \frac{\partial}{\partial u}\sum \xi_i \Sigma_{s_i}^{(u)} \phi_0(k,u) + S_0(k,u) \tag{3-20a}$$

$$\Sigma_t(u)\phi_1(k,u) - \frac{ik}{3}\phi_0(k,u) = \sum_i \Sigma_{s_i}(u)\langle\mu\rangle\phi_1(k,u) + \frac{\partial}{\partial u}\sum_i \langle\mu v\rangle_i \phi_1(k,u) \tag{3-20b}$$

Although this set can be reduced to a single second order differential equation for $\varphi_0(u)$, in practice this is rarely done because of the great difficulty involved; the set is sometimes solved numerically however. Dropping the last term in the second equation (a procedure

which was seen to be inconsistent) leads to a simple linear relationship between $\phi_0(k, u)$ and $\phi_1(k, u)$, i.e., between the Fourier Transforms of the flux and the current

$$\phi_1(k,u) = \frac{ik\,\phi_0(k,u)}{3\left[\Sigma_t(u) - \sum_i \Sigma_{si}\langle\mu\rangle_i\right]} = ik\,D(u)\,\phi_0(k,u) \qquad (3\text{-}21a)$$

The significance of

$$D(u) = \left[3\left(\Sigma_t(u) - \sum_i \Sigma_{si}(u)\langle\mu\rangle_i\right)\right]$$

may be seen more easily if we take the inverse Fourier Transform:

$$\phi_1(z,u) = -D(u)\frac{\partial}{\partial z}\phi_0(z,u) \qquad (3\text{-}21b)$$

which is Fick's Law,* used in Chapter I without derivation. Using Equation (3-21b) to eliminate $\phi_1(k, u)$ from Equation (3-16a) one obtains the extension of the usual "Fermi Age Equation"[8] to anisotropic scattering:

$$\left(D(u)k^2 + \Sigma_a(u)\right)\phi_0(k,u) = -\frac{\partial}{\partial u}\left(\bar{\xi}(u)\Sigma_s(u)\phi_0(k,u)\right) + S_0(k,u) \qquad (3\text{-}22)$$

where use has been made of the result of Chapter II:

$$\bar{\xi}(u) = \frac{\sum_i \Sigma_{si}(u)\,\xi_i}{\Sigma_s(u)}$$

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* This simple and desirable result is, of course, the reason why the last term in Equation (3-20b) is dropped. In the last analyses the only rationale for this procedure is its success in predicting the age.

[9] Glasstone & Edlund, op. cit., p.172 et. seq.

Equation (3-22) is the basic equation of "Age-Diffusion" or "Fermi Age" theory. It may be put into a more conventional form by means of some variable transformations. First, we define a quantity q(k, u) (shown below to be the slowing down density):

$$q(k,u) = \bar{\xi}(u)\,\Sigma_s(u)\,\phi_0(k,u) \qquad (3\text{-}23a)$$

which, when substituted in (3-22) yields:

$$\left[\frac{D(u)k^2 + \Sigma_a(u)}{\bar{\xi}\,\Sigma_s(u)}\right] q(k,u) = -\frac{\partial q(k,u)}{\partial u} + S_0(k,u) \qquad (3\text{-}23b)$$

In Chapter II, it was seen that the slowing down density in an infinite medium could be given to a good approximation by an expression of the form (3-23a) either for the case of slowing down in a single moderator or for the case of mixtures in which resonances were absent. It should be pointed out that in the latter case, the Taylor Series expansion fails to converge rapidly since at least some of the $B_L^c(u)$ are rapidly varying functions of lethargy. We shall have to live with this fact as one of the limitations of Age-Diffusion Theory, i.e. that the effects of resonances in cross sections can be treated only approximately.

Since Equation (3-23b) is for slowing down with absorption one might expect that it can be reduced to a problem without absorption by introducing the resonance escape probability appropriate to the case under consideration. This is indeed the case, for if we

set:

$$q(k,u) = q'(k,u)\, e^{-\int_{u'}^{u} \frac{\Sigma_a(u'')}{\xi \Sigma_s(u'')}\, du''} = q'(k,u)\, p(u' \to u) \qquad (3\text{-}24a)$$

and

$$S(k,u) = S'(k,u)\, e^{-\int_{u'}^{u} \frac{\Sigma_a(u'')}{\xi \Sigma_s(u'')}\, du''} = S'(k,u)\, p(u' \to u) \qquad (3\text{-}24b)$$

where q'(k, u) is a fictitious slowing down density that would obtain if there were no absorption, the absorption term disappears and we have

$$\frac{D(u)\, k^2}{\xi \Sigma_s(u)}\, q'(k,u) = -\frac{\partial q'(k,u)}{\partial u} + S_0(k,u) \qquad (3\text{-}25)$$

From the work of Chapter II

$$\exp\left\{ -\int_{u'}^{u} \frac{\Sigma_a(u'')}{\xi \Sigma_s(u'')}\, du'' \right\}$$

may be recognized as the resonance escape probability for small capture. One further transformation, namely a change in independent variable from u to:

$$\tau_F(u) = \int_0^u \frac{D(u')}{\xi \Sigma_s(u')}\, du' \qquad (3\text{-}26a)$$

with

$$S(\tau_F)\, d\tau_F = S(u)\, du \qquad (3\text{-}26b)$$

reduces (3-25) to the usual Fermi Age Equation[10]

$$\frac{\partial q'(k,\tau_F)}{\partial \tau_F} + k^2 q'(k,\tau_F) = S_0'(k,\tau_F) \qquad (3\text{-}26c)$$

τ_F is as yet a purely mathematical quantity, but as the symbol suggests, it is indeed an approximation to the age. This equation is readily solved by the methods employed in Chapter II to yield:

$$q'(k,\tau_F) = \int_0^{\tau_F} s'(\tau_F)\, e^{-k^2\tau_F}\, d\tau_F \qquad (3\text{-}27a)$$

which for a monoenergetic source $s(\tau_F) = \delta(\tau_F)$ reduces to

$$q'(k,\tau_F) = e^{-k^2\tau_F(u)} \qquad (3\text{-}27b)$$

allowing resonance absorption, but still neglecting the fast effect, we have

$$q(k,u) = e^{-k^2\tau_F(u)}\, p(0\to u) \qquad (3\text{-}27c)$$

The discussion of Chapter I allows us to identify $q(|\bar{r} - \bar{r}|, E)$ with the slowing down density kernel $P(|\underline{r} - \underline{r}'|, E)$. Hence, in light of our discussion of Chapter I, we can write

$$\overline{P_T}(B_g^2) = e^{-B_g^2\tau_F(u_T)} \in p(0\to u) \qquad (3\text{-}28)$$

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[10] As a historical note it may be noted that the name age arose from the similarity of Equation (3-27c) to the ordinary time-dependent diffusion equation (for heat, material etc.), where τ would ordinarily be the time variable. The term seems to be due to E. Fermi Ricerca Sci. 7, 13(1936)

where fast fission is now included. Hence, the criticality condition for a purely thermal bare asymptotic reactor may be written as

$$\frac{\eta f \epsilon p(0 \to u_T)\, e^{-B_g^2 \tau_F(u_T)}}{1 + L^2 B_g^2} = 1 \qquad (3\text{-}29)$$

under the assumptions made above, provided τ_F does not vary greatly within the fission spectrum. The fast fission factor, ϵ, has been arbitrarily re-introduced because fast fission was not provided for in the slowing down equations; the resonance escape probability was, of course, included. Equation (3-29) is the usual Fermi Age criticality condition. In this model the fast effect, ϵ, the resonance escape probability, $p(o \to u_T)$, and the fast non-leakage probability, are all independent, i.e., the total escape probability is the product of the individual escape probabilities. In Chapter I it was mentioned that this is not true in the actual physical case, nor is it true in the more sophisticated models, unless the individual factors are all quite close to unity, but the result does obtain here due to the simplicity of the model.

The inverse Fourier Transforms of some of the above expressions are familiar. For example, the inverse of (3-26c) is the well known Age Diffusion Equation*:

$$\nabla^2 q'(\underline{r}, \tau_F) = \frac{\partial q'(\underline{r}, \tau_F)}{\partial \tau_F} + S_o(\underline{r}, \tau_F) \qquad (3\text{-}30a)$$

* Here we take the three dimensional inversion, which is permitted because of the identity of the one- and three-dimensional Fourier Transforms.

while the inverse of Equation (3-27a) is its solution for a point source

$$q'(\underline{r}, \tau_F) = \int_0^{\tau_F} \frac{S'(\tau_F') \, e^{-r^2/4(\tau_F - \tau_F')}}{[4\pi(\tau_F - \tau_F')]^{3/2}} \, d\tau_F' \qquad (3\text{-}30b)$$

which for a monoenergetic source $\delta(\tau_F' - \tau_0)$ reduces to the well known Gaussian age kernel:

$$q'(\underline{r}, \tau_F) = \frac{e^{-r^2/4(\tau_F - \tau_0)}}{[4\pi(\tau_F - \tau_0)]^{3/2}} \qquad (3\text{-}30c)$$

or in one dimension (taking a one dimensional inversion) we have:

$$q'(z, \tau_F) = \frac{e^{-z^2/4(\tau_F - \tau_0)}}{[4\pi(\tau_F - \tau_0)]^{1/2}} \qquad (3\text{-}30d)$$

The mean square slowing down length will now be calculated to show that τ_F is indeed an approximation to the age as stated. The most convenient means of calculating the age is provided by combining Equations (3-17c) and (3-17e):

$$\langle z^2 \rangle = \left. \frac{-\frac{\partial^2 q(k,u)}{\partial k^2}}{q(k,u)} \right|_{k=0} = -2 \left. \frac{\frac{\partial q(k^2,u)}{\partial (k^2)}}{q(k^2,u)} \right|_{k=0} \qquad (3\text{-}31a)$$

For a monoenergetic source we have using Equation (3-27b):

$$\langle z^2 \rangle = 2\tau_F(u) = \int_0^u \frac{D(u')}{\xi \Sigma_s(u')} \, du' \qquad (3\text{-}31b)$$

so that the quantity $\tau_F(u)$ defined by Equation (3-26a) is identical to the neutron age, defined previously, in the Age Diffusion Approximation. It will therefore be denoted simply by τ henceforth.

If the source it not monoenergetic the non-leakage probability must be written:

$$P_T(B_g^2) = \frac{q_f(B^2,\ \tau(u_T))}{q_f(0,\ \tau(u_T))} = \frac{\int_0^{\tau(u_T)} S(\tau')\, e^{-B^2(\tau-\tau')}\, p(\tau' \to \tau)\, d\tau'}{\int_0^{\tau(u_T)} S(\tau')\, p(\tau' \to \tau)\, d\tau'} \qquad (3\text{-}32a)$$

and the age becomes

$$\tau(u) = \frac{1}{2}\langle z^2(u)\rangle = \frac{\int_0^{\tau} (\tau-\tau')\, S(\tau')\, p(\tau' \to \tau)\, d\tau'}{\int_0^{\tau} S(\tau')\, p(\tau' \to \tau)\, d\tau'} \qquad (3\text{-}32b)$$

and is found by applying the formula (3-31a) to Equation (3-28a).

A connection between these formulae and a more commonly quoted result is obtained in the limit of small B^2 *. In this limit

$$\bar{P}_T(B^2) \approx \frac{\int_0^{\tau(u_T)} S(\tau')\left[1 - B^2(\tau(u_T)-\tau')\right] p(\tau' \to \tau(u_T))\, d\tau'}{\int_0^{\tau(u_T)} S(\tau')\, p(\tau' \to \tau(u_T))\, d\tau'}$$

$$= 1 - B^2 \frac{\int_0^{\tau(u_T)} (\tau(u_T)-\tau)\, S(\tau')\, p(\tau' \to \tau(u_T))\, d\tau'}{\int_0^{\tau(u_T)} S(\tau')\, p(\tau' \to \tau(u_T))\, d\tau'}$$

If resonance capture is very small of if it occurs far from the source this reduces to

$$\bar{P}_T(B^2) = 1 - B^2 \int_0^{\tau(u_T)} [\tau(u_T) - \tau]\, S(\tau')\, d\tau'$$

$$\approx e^{-B^2 \tau_{av}(u_T)} \qquad (3\text{-}33a)$$

where the source average value of $\tau(u_T)$, $\tau_{av}(u_T)$ is

$$\tau_{av}(u_T) = \int_0^{\tau(u_T)} S(\tau')\, [\tau(u_T) - \tau']\, d\tau' \qquad (3\text{-}33b)$$

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* This was pointed out by M. Levine, unpublished.

This manipulation has been carried out in order to show the connection between the correct formula for the fast escape probability (3-32a) and Equation (3-33a) which is frequently used in the literature, but is only approximate.

A few interesting properties of the Fermi Age may be discovered here: First it is additive; that is the Fermi Age for slowing down from lethargy 0 to lethargy u is just the sum of the age for slowing down from $u = 0$ to $u = u'$ plus the age for slowing down from $u = u'$ to $u = u$, where u' is any lethargy between 0 and u. This is also a general property of the neutron age.

Secondly, in age-diffusion theory absorption has an effect on the spatial shape of the slowing down density only through the slight dependence of D on Σ_a. This is essentially the statement that the processes of resonance escape and fast leakage are independent. The effect of absorption is to reduce the number of neutrons available at any particular lethargy but their spatial distribution is almost independent of the number which have been absorbed. Of course, this is not a true description of the physical processes occurring in a reactor, and it is a difficulty inherent in the method.

This difficulty is indicated by the fact that the resonance escape probability calculated by this method is that for the small absorption limit. An explanation of this phenomenon will be delayed until later.

11. The Selengut Goertzel Method[11]

The approach employed in the previous section is called Age Diffusion Theory because it assumes the linear relation between the neutron current, $\phi_1(r, u)$, and the gradient of the flux, $\phi_0(r, u)$, which is basic to diffusion theory. We were unable, however, to treat hydrogen or deuterium slowing down by that model as the truncation of the Taylor Series expansion required is a poor approximation for these moderators.

It will later be shown how Age-Diffusion Theory can be derived in a manner which yields more physical insight into the nature of the approximations. In essence, age-diffusion theory implies that neutrons make an infinite number of infinitesimal flights in travelling any finite distance; alternatively, it assumes that a neutron gains only an infinitesimal lethargy in a given collision. This last statement is the reason that the method employed in the previous section is sometimes referred to as the continuous slowing down model. More will be said about the implications of these considerations after the differences between the Selengut-Goertzel and Age-Diffusion results have been derived and discussed.

To begin with, instead of discarding the $J_0^H(k, u)$ term from the first of the P_1 equations, we will include it in its rigorous form; deuterium slowing down, which is best treated by the

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[11] D. Selengut and G. Goertzel, unpublished.

method of the succeeding section, is ignored for the present. In the second equation, in order to obtain Fick's Law, one is forced to make the Taylor Series expansion for all elements, thus yielding Equation (3-21a) modified to include hydrogen, i.e., the diffusion coefficient D contains terms arising from hydrogen scattering. Treating heavy elements as in the previous section, we arrive at the basic equation:

$$\left[D(u)k^2 + \Sigma_a^{(u)} + \Sigma_s^H(u)\right]\phi_0(k,u) = J_0^H(k,u) - \frac{\partial}{\partial u}\left(\xi\Sigma_s'(u)\phi_0(k,u)\right) + S_0(k,u) \quad (3\text{-}34)$$

Here

$$\Sigma_s'(u) = \Sigma_s(u) - \Sigma_s^H(u)$$

and $\bar{\xi}(u)$ retains its previous definition and still does not include the effects of hydrogen. Of course, a new unknown, $J_0^H(k, u)$, has been added to the equation, so that another equation relating it to the flux, $\phi_0(k, u)$, is required. This is conveniently supplied by Equation (3-11) with $j = 0$, but for numerical calculations it is sometimes easier to use the equation obtained by differentiating the $j = 0$ Equation (3-11):

$$J_0^H(k,u) + \frac{\partial J_0^H(k,u)}{\partial u} = \Sigma_s^H(u)\phi_0(k,u) \quad (3\text{-}35)$$

This method is sometimes called the Diffusion Selengut-Goertzel or Inconsistent P_1 Selengut-Goertzel Method for reasons that are probably already plain. A consistent P_1 method similar to the

Selengut-Goertzel scheme is sometimes used and employs the following set of equations

$$[\Sigma_a(u)+\Sigma_s^H(u)]\,\phi_0(k,u)-ik\phi(k,u)=J_0^H(k,u)-\frac{\partial}{\partial u}\left(\xi(u)\Sigma_s'(u)\,\phi_0(u)\right)+S_0(k,u) \tag{3-36a}$$

and

$$[\Sigma_t(u)-\Sigma_s(u)\langle\mu\rangle+\Sigma_s^H\langle\mu\rangle_H]\,\phi_1(k,u)-\frac{ik}{3}\phi_0(k,u)=J_1^H(k,u)-\frac{\partial}{\partial u}\left(\langle\mu v\rangle\Sigma_s'(u)\,\phi_1(k,u)\right) \tag{3-36b}$$

in which hydrogen slowing down is treated rigorously throughout, and the $T_{1L'}^{1}$ terms have been retained. Introduction of the fourth dependent variable $J_1^H(k, u)$ requires use of Equation (3-11) with $j = 1$.

The quantity $J_0^H(k, u)$ has the same physical interpretation as in Chapter II. Again consider the slowing down density $q(k, u)$ due to a particular nuclear type which, from Equation (1-32b), is equal to

$$q(k,u)=\int_{u-\ln\frac{1}{\alpha}}^{u}du'\int_{u}^{u'-\ln\frac{1}{\alpha}}\Sigma_s(u')\,\phi_0(k,u')\,F(u'\to u'')\,du''$$

for isotropic scattering in the center-of-mass system this becomes:

$$q(k,u)=\int_{u-\ln\frac{1}{\alpha}}^{u}\Sigma_s(u')\,\phi_0(k,u)\,\frac{e^{-(u-u')}}{1-\alpha}\,du' \tag{3-37a}$$

For the particular case of hydrogen this is also $J_0^H(k, u)$, Equation (3-11). Hence, $J_0^H(k, u)$ is the slowing down density of neutrons whose last collision was with a hydrogen nucleus. An Analytical solution

of the Diffusion Selengut-Goertzel equations is possible if $\xi = 0$, i.e., if hydrogen slowing down dominates. Diffusion due to collisions with other elements is permitted, but they are assumed so heavy that their contribution to the slowing down density may be neglected compared to that of hydrogen.

First, the age is calculated; the power series expansion method is again the simplest.[12] However, in the SG method, one must distinguish between two different "ages," the "flux age" and the "slowing down density age" defined by

$$\tau_N = \frac{1}{2} \lim_{k \to 0} \frac{\partial \phi(k,\mu)/\partial(k^2)}{\phi(k,\mu)} = \frac{1}{2} \frac{\phi_{02}(\mu)}{\phi_{00}(\mu)} = \frac{1}{2} \frac{\int_{-\infty}^{\infty} z^2 \phi(z,\mu)\,dz}{\int_{-\infty}^{\infty} \phi(z,\mu)\,dz} \qquad (3\text{-}37b)$$

and

$$\tau_q = \frac{1}{2} \lim_{k \to 0} \frac{\partial q(k,\mu)/\partial(k^2)}{q(k,\mu)} = \frac{1}{2} \frac{J_{02}^{\#}(\mu)}{J_{00}(\mu)} = \frac{1}{2} \frac{\int_{-\infty}^{\infty} z^2 q(z,\mu)\,dz}{\int_{-\infty}^{\infty} q(z,\mu)\,dz} \qquad (3\text{-}37c)$$

These two definitions are not equivalent in the SG Approximation, although they are in the Age Diffusion Approximation. The difference between them leads, however, to some interesting results. Under the approximations made, the equations required for the age calculation are:

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[12] This method was used by H. Hurwitz, Jr., and P.F. Zweifel, J. Appl. Phys., 26, 8, 923 (1955) and originally by R. Marshak, op. cit.

$$\left[\Sigma_s^H(u) + \Sigma_a(u)\right]\varphi_{00}(u) = J_{00}(u) + S(u) \qquad (3\text{-}38a)$$

$$J_{00}(u) + \frac{\partial J_{00}(u)}{\partial u} = \Sigma_s^H(u)\,\varphi_{00}(u) \qquad (3\text{-}38b)$$

$$-2D(u)\,\varphi_{00}(u) + \left[\Sigma_a(u) + \Sigma_s^H(u)\right]\varphi_{02}(u) = J_{02}(u) \qquad (3\text{-}38c)$$

$$J_{02}(u) + \frac{\partial J_{02}(u)}{\partial u} = \Sigma_s^H(u)\,\varphi_{02}(u) \qquad (3\text{-}38d)$$

These four differential equations for the four required quantities may readily be solved. Simultaneous solution of the first two yields $J_{00}(u)$ and $\varphi_{00}(u)$:

$$J_{00}(u) = \int_0^u \frac{\Sigma_s^H(u')}{\Sigma_s^H(u') + \Sigma_a(u')}\, S(u')\, e^{-\int_{u'}^{u} \frac{\Sigma_a(u'')}{\Sigma_a(u'') + \Sigma_s(u'')}\, du''} \qquad (3\text{-}39a)$$

and

$$\varphi_{00}(u) = \frac{1}{\Sigma_a(u) + \Sigma_s^H(u)}\left[J_{00}(u) + S(u)\right] \qquad (3\text{-}39b)$$

which may be used to solve the last two of Equations (3-38). Before proceeding to the actual calculations, it will be instructive to determine the difference between the two ages defined above. We have

$$\tau_N = \frac{1}{2}\frac{\varphi_{02}(u)}{\varphi_{00}(u)} = \frac{D(u)}{\Sigma_a(u) + \Sigma_s^H(u)} + \frac{1}{2}\frac{J_{02}(u)}{\left[\Sigma_a(u) + \Sigma_s^H(u)\right]\varphi_{00}(u)} \qquad (3\text{-}39c)$$

if there are no sources at lethargy u. But, from Equation (3-38c) we immediately find:

$$\tau_q = \frac{1}{2}\frac{J_{02}(u)}{J_{00}(u)} = \frac{1}{2}\frac{J_{02}(u)}{[\Sigma_a(u)+\Sigma_s^H(u)]\varphi_{00}(u)} \qquad (3\text{-}39d)$$

It is thus apparent that the difference between the flux age and the slowing down age is just $D/(\Sigma_a + \Sigma_s^H)$ evaluated at the lethargy of measurement; this term arises from the fact that a neutron travels a finite distance at lethargy u before experiencing the collision which will either absorb it or slow it down further, and is therefore called the "last flight correction."

The physical significance of this correction is that a neutron contributes to the slowing down density instantaneously upon reaching or crossing lethargy u, but continues to contribute to the flux until it is degraded to lethargies above u. From one-speed diffusion theory it is known that the mean square distance travelled by a diffusing neutron is $6D/\Sigma a = 6L^2$, but the effective "absorption" cross section here is $[\Sigma_a(u) + \Sigma_s^H(u)]$ since either a true absorption or a slowing down collision will remove the neutron from the lethargy of interest. The added contribution to the flux age is just one-sixth of this mean square distance.

Let us now calculate τ_q. Eliminating $\varphi_{02}(u)$ from the last two of Equations (3-38) and then using Equation (3-39b) to eliminate $\varphi_{00}(u)$, one finds by straightforward integration:

$$J_{02}(u) = 2\int_0^u \left[\frac{D\Sigma_s^H}{(\Sigma_a+\Sigma_s^H)^2}\right]_{u'} \left[J_{00}(u')+S(u')\right] e^{-\int_{u'}^{u}\left(\frac{\Sigma_a}{\Sigma_a+\Sigma_s^H}\right)_{u''}du''} \qquad (3\text{-}40a)$$

Then τ_q can be found by dividing $J_{02}(u)$, Equation (3-40a), by $J_{00}(u)$, Equation (3-39a). As the result is complicated only the monoenergetic source case will be investigated. The Selengut-Goertzel slowing down density age, becomes, under this assumption:

$$\tau_q = \int_0^u \left[\frac{D\Sigma_s^H}{(\Sigma_a+\Sigma_s^H)^2}\right]_{u'} du' + \left[\frac{D}{\Sigma_a+\Sigma_s^H}\right]_{u=0} \qquad (3\text{-}40b)$$

Two points of difference between this expression and the Fermi Age expression are noted. First, an additional term $D/(\Sigma_a + \Sigma_s^H)$ evaluated at the source lethargy is included. It is the contribution to the age due to the distance that neutrons travel at the source energy before starting to slow down and hence is designated the "first flight correction." That the first flight correction should be $D/(\Sigma_a + \Sigma_s^H)$ can be verified by the method used in considering the last flight correction.

Secondly, the integrand of the first term on the right-hand side of Equation (3-40b) contains a term $\Sigma_s^{H2}/(\Sigma_a + \Sigma_s^H)^2$ that was not found in the Fermi Age expression.

Flight corrections arise from a failing in the Age Diffusion approximation that was mentioned previously. Age Diffusion Theory assumes that neutrons travel an infinitesimal distance between con-

secutive collisions. This may be a reasonable approximation for neutrons which have started to slow down and thus are not all at one energy. However, at the source energy, neutrons scatter with the one flight collision distribution

$$\frac{e^{-\Sigma_t(0)\, r}}{4\pi r^2} \qquad (3\text{-}41)$$

before they actually start to slow down if all elements present are assumed to slow down. If the first flight kernel represents only a short flight of the neutrons from the source, little error is introduced by neglecting this effect. Hydrogen, however, is once again peculiar; its scattering cross section falls off rather rapidly above 1 mev (see Figure 3) so that the first flight correction is quite considerable at fission energies. This is further aggravated by the fact that slowing down in hydrogen requires relatively few collisions so that the age tends to be relatively low in hydrogenous systems. In other moderators this effect is not nearly so pronounced; in fact, the last flight correction is small even for hydrogen.

Even the Diffusion Selengut-Goertzel method does not treat the first and last flight corrections properly. It has been seen that the SG theory predicts these corrections as $[D/(\Sigma_a + \Sigma_s^H)]_{u=0}$ and $[D\,(\Sigma_a + \Sigma_s^H)]_u$ respectively, i.e., it gives the diffusion theory result; the rigorous correction will be demonstrated later. The nature of the flight correction suggests that the flux in the SG approximation, as given above, is the convolution of an age kernel and two one-speed

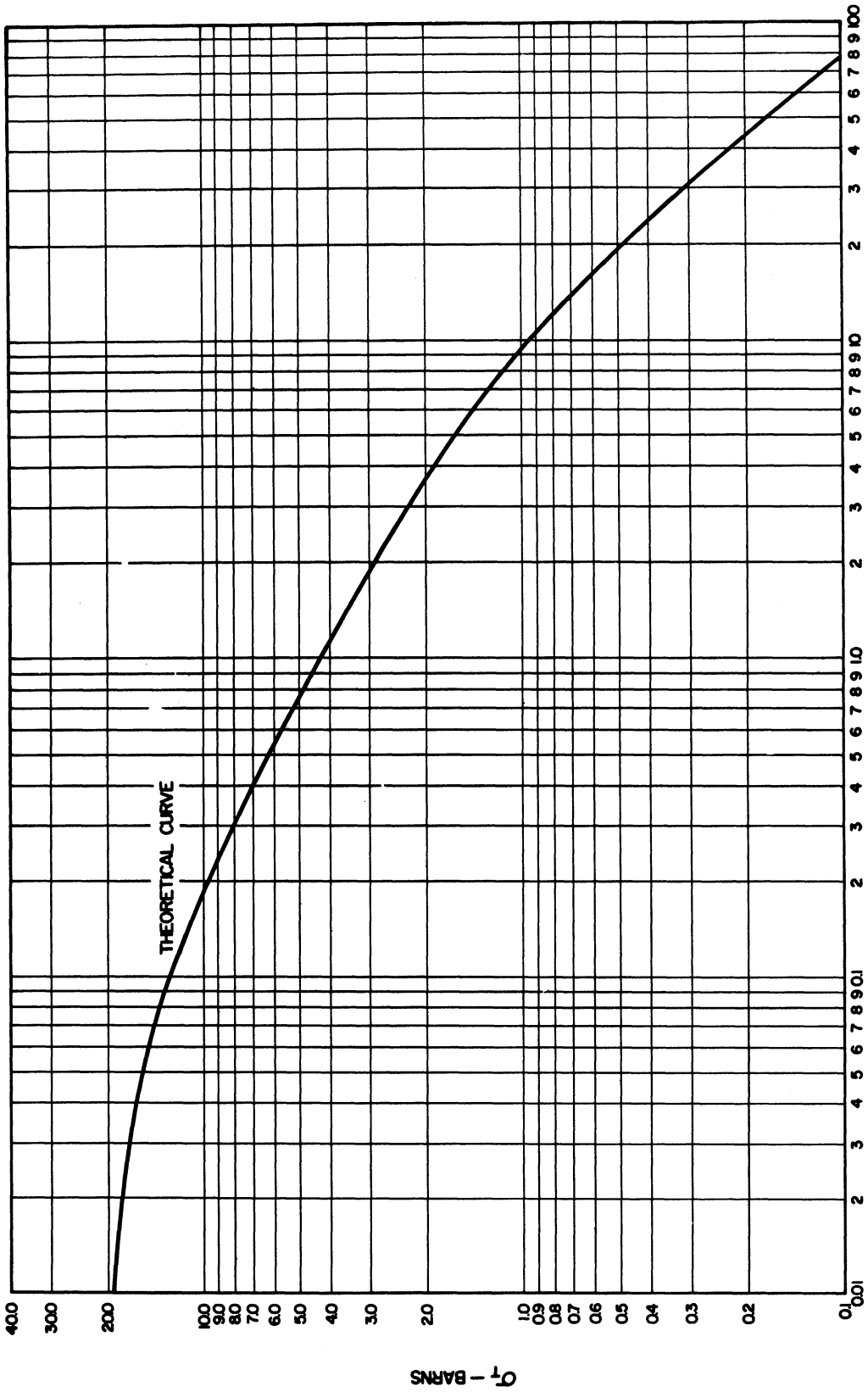

Figure III-3 The Total Cross Section of Hydrogen.

assumes that neutrons travel an infinitesimal distance between con-

diffusion kernels:

$$\phi_0(r \leftarrow r,u) = \int_{r'''} d^3r''' \int_{r''} d^3r'' \frac{e^{-|r''-r'|/L(0)}}{4\pi D(0)|r''-r'|} \frac{e^{-|r'''-r''|/4\tau}}{(4\pi\tau)^{3/2}} \frac{e^{-|r'''-r|/L(u)}}{4\pi D(u)|r'''-r|} \tag{3-42}$$

where

$$L^2(0) = \frac{D(0)}{\Sigma_a(0)+\Sigma_s^{tr}(0)}$$

$$L^2(u) = \frac{D(u)}{\Sigma_a(u)+\Sigma_s^{tr}(u)}$$

and one would expect that the more rigorous result for the slowing down density would be a similar convolution involving a single one flight kernels(at lethargy zero). If one calculates the second moment of this distribution, he does indeed obtain the age previously given. This distribution can also be derived by direct integration of the Selengut-Goertzel Equation.

The Fourier Transform of the slowing down kernel required for the Asymptotic Reactor Theory critical condition can be found by transforming the convolution for the slowing down density mentioned above or by solving Equations (3-34) and (3-35) directly. The result is, for a mono-energetic source:

$$\overline{P}(B^2) = \left(\frac{\Sigma_s^{tr}}{\Sigma_s^{tr}+DB^2+\Sigma_a}\right)_{u=0} \exp\left\{-\int_0^{u_{th}} \left(\frac{DB^2+\Sigma_a}{DB^2+\Sigma_a+\Sigma_s^{tr}}\right)_{u'} du'\right. \tag{3-43a}$$

Note that here the kernel does not separate into the product of a resonance escape probability and a non-leakage probability as in the

Age Diffusion case. Only in the limit $B^2 \to 0$ does this separation occur, for then one can neglect DB^2 in the denominators in Equation (3-43a) to obtain:

$$\bar{P}(B^2) = \left(\frac{\Sigma_s^H}{\Sigma_s^H + \Sigma_a}\right)_{u=0} e^{-\int_0^{u_{th}} \left(\frac{\Sigma_a}{\Sigma_a+\Sigma_s^H}\right)_{u'} du'} e^{-B^2 \int_0^{u_{th}} \left(\frac{D}{\Sigma_a+\Sigma_s^H}\right) du'}$$

$$= p\, e^{-B^2 \int_0^{u_{th}} \left(\frac{D}{\Sigma_s^H+\Sigma_a}\right) du'} \approx p e^{-B^2 \tau_{th}} \qquad (3-43b)$$

12. The Greuling-Goertzel Procedure[13, 14]

The simplicity of the equations that arise in hydrogen moderation problems and the subsequent ease of solution of the equations for such systems suggests seeking similar approximate equations for applications to systems containing other moderators. In particular, one would like to have an equation analogous to Equation (3-35) of the type*

$$\phi_f(k,u) + \lambda(u) \frac{\partial \phi_f(k,u)}{\partial u} = \xi(u) \Sigma_s(u) \phi_0(k,u) \qquad (3-44)$$

for all moderators. One hopes the parameters λ and ξ can be chosen such that the error inherent in the approximation will be minimized, e.g., proportional to γ^2 instead of γ as in the Age-

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[13] E. Greuling and G. Goertzel, Nuc. Sci. Eng., 7, 69 (1960).

[14] The development here closely parallels that of H. Amster, J. Appl. Phys., 29, 623 (1958).

* The symbol λ here is frequently denoted by γ in the literature.

Diffusion method. The symbol ξ will be shown to retain its previous meaning. This approximation may be applied to any element other than hydrogen but the success of the Age-Diffusion Model for heavy element moderation has limited its use almost exclusively to deuterium, which is in the anomolous position of being too light to permit application of age theory and yet does not enjoy the simple scattering kernel of hydrogen.

The derivation given here is rather formal but is in some respects simpler than that given by the originators of the method. In a rather arbitrary fashion, a new function $\eta_L(k,u)$ is defined by a Taylor series expansion for each element:

$$\eta_L(k,u) = -\sum_{n=0}^{\infty} \frac{\partial^n}{\partial u^n} \sum_{L'=0}^{\infty} T_{LL'}^{n+1} B_{L'}^{c}(u) \phi_L(k,u) \qquad (3\text{-}45a)$$

then, by differentiation:

$$\frac{\partial \eta_L(k,u)}{\partial u} = -\sum_{n=0}^{\infty} \frac{\partial^{n+1}}{\partial u^{n+1}} \sum_{L'=0}^{\infty} T_{LL'}^{n+1} B_{L'}^{c}(u) \phi_L(k,u) \qquad (3\text{-}45b)$$

For notation purposes, indices referring to particular nuclear types are suppressed. In general, however, a summation over all nuclear types is to be implied. Multiplying Equation (3-45b) by a parameter, λ_L (which may be a function of u), and adding it to Equation (3-45a)

we obtain, after some rearrangement,

$$\eta_L(k,u) + \lambda_L \frac{\partial \eta_L(k,u)}{\partial u} = -\sum_{L'=0}^{\infty} T^1_{LL'} B^c_{L'}(u) \phi_L(k,u) \left(1 - \frac{d\lambda_L}{du}\right)$$

$$- \frac{\partial}{\partial u} \sum_{L'=0}^{\infty} B^c_{L'}(u) \phi_L(k,u) \left[T^2_{LL'} + \lambda_L T^1_{LL'}\right]$$

$$- \sum_{n=2}^{\infty} \sum_{L'=0}^{\infty} \left[\frac{\partial^n}{\partial u^n}\left(B_{L'}(u) T^{n+1}_{LL'}\right) + \lambda_L \frac{\partial^n}{\partial u^n}\left(B^c_{L'}(u) \phi_L(k,u) T^n_{LL'}\right)\right] \quad (3\text{-}45c)$$

The parameters λ_L may now be chosen such that the second term on the right-hand side of Equation (3-45c) vanishes, i.e., all first derivatives of the flux drop out*:

$$\lambda_L(u) = -\frac{\sum_{L'=0}^{\infty} T^2_{LL'} B^c_{L'}(u)}{\sum_{L'=0}^{\infty} T^1_{LL'} B^c_{L'}(u)} = \frac{\langle U^2 P_L(\mu) \rangle}{\langle U P_L(\mu) \rangle} \quad (3\text{-}45d)$$

Now since all of the components of the third term on the right-hand side of Equation (3-45c) are of order γ^2 or smaller, this term may be neglected to the required degree of approximation. Thus we have:

$$\eta_L(k,u) + \lambda_L \frac{\partial \eta_L(k,u)}{\partial u} = -\left(1 - \frac{\partial \lambda_L}{\partial u}\right) \phi_L(k,u) \sum_{L'=0}^{\infty} T^1_{LL'} B^c_{L'}(u) \quad (3\text{-}45e)$$

λ_0 is denoted simply as λ ; for isotropic scattering in the center-of-mass system it is a constant, so that the $L = 0$ Equation (3-45e) will be the desired result (3-45a) if it can be demonstrated that $\eta_0(k, u) = q(k, u)$, the slowing down density.

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* In general, a sum over all elements present is required.

At this point, we shall digress momentarily to show the equivalence of η_o and q and also display the physical significance of the $\eta_L(k, u)$[15]. First the concept of an angular dependent slowing down density is required. This quantity, designated by $q(\underline{r}, u, \mu)$, is defined as the number of neutrons slowing down past lethargy u per unit volume at $\underline{r}$ per second which are travelling in direction μ (per unit μ) after the scattering collision. By the arguments given in the derivation of Equation (1-32b) for $q(\underline{r}, u)$ (which is now seen to be the zeroth angular moment of $q(\underline{r}, u, \mu)$) we can write

$$q(\underline{r}, u, \mu) = \int_{u-\ln\frac{1}{\alpha}}^{u} du' \int_{u}^{u'+\ln 1/\alpha} du'' \int d\mu' \, \Sigma_s(u' \to u'', \mu' \to \mu) \Phi(\underline{r}, u', \mu') \qquad (3-46a)$$

Now if the flux and scattering cross section are expanded in Legendre Polynomials according to Equations (3-7a and c) and the addition theorem (3-7e) is applied, it is possible to reduce the above expression for $q(\underline{r}, u, \mu)$ much as the expression for the degradation integral $J(\underline{r}, u, \mu)$ was reduced in the development of the spherical harmonics method. The calculations, which are very similar to those used in the spherical harmonics development, are not shown here but the result is quoted:

$$q(\underline{r}, u, \mu) = \sum_{L=0}^{\infty} \frac{2L+1}{2} P_L(\mu) \sum_{L'=0}^{\infty} \int_{u-\ln\frac{1}{\alpha}}^{u} du' \, \phi_{L'}(\underline{r}, u') B_{L'}^{c}(u') \int_{u}^{u'+\ln\frac{1}{\alpha}} T_{LL'}(U) dU' \qquad (3-46b)$$

where all of the quantities involved have been previously defined.

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[15] The following was suggested by H. Amster, private communication.

Now by changing the integration variables from u'' to U = u'' - u' in the second integral and from u' to U' = u - u' in the first integral we have

$$q(r,u,\mu)=\sum_{L=0}^{\infty}\frac{2L+1}{2}P_L(\mu)\sum_{L'=0}^{\infty}\int_0^{\ln\frac{1}{\alpha}}dU\,\phi_L(u-U')B_{L'}^c(u-U')\int_{U'}^{\ln\frac{1}{\alpha}}T_{LL'}(U)dU \qquad (3\text{-}46c)$$

Now expanding $\phi_L(u - U')B^c_{L'}(u - U')$ in a Taylor series as in Equation (3-13), this becomes

$$q(r,u,\mu)=\sum_{L=0}^{\infty}\frac{2L+1}{2}P_L(\mu)\sum_{n,L'=0}^{\infty}\frac{\partial^n}{\partial u^n}\left[B_{L'}^c(u')\phi_L(u')\right]\int_0^{\ln\frac{1}{\alpha}}\frac{(-U')^n}{n!}dU'\int_{U'}^{\ln\frac{1}{\alpha}}T_{LL'}(U)dU \qquad (3\text{-}46d)$$

Finally, one does the U' integral by parts, viz.

$$\int_0^{\ln\frac{1}{\alpha}}dU\frac{(-U')^n}{n!}\int_{U'}^{\ln\frac{1}{\alpha}}dU\,T_{LL'}(U)=\frac{(-)^n}{(n+1)!}\left[U'^{n+1}\int_{U'}^{\ln\frac{1}{\alpha}}T_{LL'}(U)\,dU\right]_0^{\ln\frac{1}{\alpha}}$$
$$-\int_0^{\ln\frac{1}{\alpha}}dU'\frac{(-U')^{n+1}}{(n+1)!}T_{LL'}(U') \qquad (3\text{-}46e)$$

The first term is clearly zero while the second is just the definition of $-T^{n+1}_{LL'}$, Equation (1-56), so that we now have

$$q(r,u,\mu)=-\sum_{L=0}^{\infty}\frac{2L+1}{2}P_L(\mu)\sum_{n=0}^{\infty}\sum_{L'=0}^{\infty}T^{n+1}_{LL'}\frac{\partial^n}{\partial u^n}\left[B^c_{L'}(u)\phi_L(r,u)\right] \qquad (3\text{-}46f)$$

a comparison of the Fourier Transform of Equation (3-46f) with the definition of $\eta_L(k, u)$, Equation (3-45a) reveals that

$$q(k,u,\mu)=\sum_{L=0}^{\infty}\frac{2L+1}{2}\eta_L(k,u)P_L(\mu) \qquad (3\text{-}46g)$$

Thus the $\eta_L(k, u)$ defined so off handedly earlier are seen to be the Legendre Coefficients of the angular slowing down density. In

particular

$$\eta_0(k,u) = g(k,u) \qquad (3\text{-}46k)$$

Another important relationship can be derived by comparing Equations (3-14a) and (3-45b):

$$J_L(k,u) = \frac{-\partial \eta_L(k,u)}{\partial u} + \phi_L(k,u) \sum_{L'=0}^{\infty} T^{\circ}_{LL'} B^{c}_{L'}(u) \qquad (3\text{-}47a)$$

We are now in a position to write the desired equations. The slowing down density has been written in the desired form (3-44) and its relation to the degradation integral has been found. All one now need do is to find $\eta_L(k, u)$ in terms of $\phi_L(k, u)$, construct $J_L(k, u)$ from Equation (3-47a) and substitute it into the P_L equations. The mechanics of this operation follow. Solving Equation (3-45e) for $\eta_L(k, u)$ we have

$$\eta_L(k,u) = -\sum_{L'=0}^{\infty} T'_{LL'} \int_0^u du' \phi_L(k,u') \left(1 - \frac{\partial \lambda_L}{\partial u}\right) \frac{B^{c}_{L'}(u')}{\lambda_L(u')} e^{-\int_{u'}^{u} \frac{du''}{\lambda_L(u'')}} \qquad (3\text{-}47b)$$

And, on differentiating one obtains:

$$\frac{\partial \eta_L(k,u)}{\partial u} = -\sum_{L'=0}^{\infty} T'_{LL'} \phi_L(k,u) \left(1 - \frac{\partial \lambda_L}{\partial u}\right) \frac{B^{c}_{L'}(u)}{\lambda_L(u)}$$
$$+ \sum_{L'=0}^{\infty} \frac{T'_{LL'}}{\lambda_L(u)} \int_0^u \phi_L(k,u') \left(1 - \frac{\partial \lambda_L}{\partial u}\right) \frac{B^{c}_{L'}(u')}{\lambda_L(u')} e^{-\int_{u'}^{u} \frac{du''}{\lambda_L(u'')}} du' \qquad (3\text{-}47c)$$

which may be substituted into Equation (3-47a) to yield $J_L(k, u)$

which, in turn, may be substituted into the P_L Equations (3-10) to yield the desired modified set:

$$\Sigma_{mj}(u)\phi_j(k,u) - \frac{ik}{2j+1}\left[j\phi_{j-1}(k,u) + (j+1)\phi_{j+1}(k,u)\right]$$

$$= S_0\delta_{j0} - \sum_{L'=0}^{\infty} \frac{T^1_{jL'}}{\lambda_j(u)} \int_0^u \phi_j(k,u') \frac{\left(1 - \frac{d\lambda_j}{du'}\right)}{\lambda_j(u')} B^c_{L'}(u') e^{-\int_{u'}^{u} \frac{du''}{\lambda_j(u'')}} \qquad (3\text{-}47d)$$

Summation over the various moderators present is again understood and a new cross section has been introduced:

$$\Sigma_{mj} = \Sigma_t - \sum_{L'=0}^{\infty} \left[T^0_{jL'} - \frac{T^1_{jL'}}{\lambda_j(u)}\left(1 - \frac{d\lambda_j}{du}\right)\right] B^c_{L'}(u) \qquad (3\text{-}47e)$$

These are the basic equations of the Greuling-Goertzel Method. The motivation behind this method and the explanation of some of the recent interest in it is now becomes clear. The Equations (3-47d) strongly resemble the equations for slowing down in hydrogen in that the lethargy interval (u - ln $1/\alpha$, u) has been mapped into the region (0, u) by altering the scattering frequency. The actual and modified scattering frequencies are compared in Figure 4. The advantage is that we are now dealing with integral equations of a type which are more readily solved. Analytical solutions are possible for some simplified problems and, more importantly perhaps, numerical solution is considerably simplified. In fact, computer codes developed for treating slowing down in hydrogen are readily modified for solutions of the

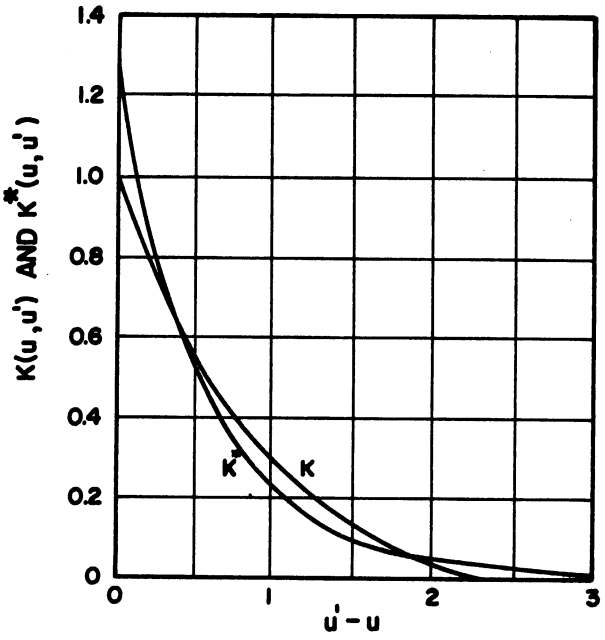

Figure III-4 Comparison of Exact and Greuling-Goertzel Kernels.

Greuling-Goertzel (GG) equations. Thus far, application has been made only to the P_1 case, for which a set of two coupled integral equations is obtained. An alternate procedure is to use the P_1 equations with $J_L(k, u)$ given by Equation (3-47a) in conjunction with the differential equations (3-45e) for the $\eta_L(k, u)$. Clearly, these schemes are completely equivalent, the choice generally being made on the basis of ease of programming for numerical solution. The set is written down in order to permit companson of this method and previous ones that have been investigated. Substituting Equation (3-47a) into the P_1 equations gives:

$$\Sigma_a(u)\phi_0(k,u) - ik\phi_1(k,u) = S_0(k,u) - \frac{\partial q_1(k,u)}{\partial u} \qquad (3\text{-}48a)$$

and

$$\Sigma_t(u)\phi_1(k,u) - \frac{ik}{3}\phi_0(k,u) - J_1(k,u) = \frac{\partial \eta_1(k,u)}{\partial u}$$

$$+ \sum_{L'=0}^{\infty} T^0_{1L'} B^0_{L'}(\omega)\phi_1(k,u) = \frac{\partial \eta_1}{\partial u} + \Sigma_s(\mu)\phi_1 \qquad (3\text{-}48b)$$

or combining terms:

$$\Sigma_{tr}(u)\phi_1(k,u) - \frac{ik}{3}\phi_0(k,u) = \frac{\partial \eta_1(k,u)}{\partial u} \qquad (3\text{-}48c)$$

Now remembering that

$$\sum_{L'=0}^{\infty} T^{1}_{0L'} B^{c}_{L'}(u) = \xi(u)\sigma_s(u) \qquad (3\text{-}48d)$$

and defining

$$\sum_{L'=0}^{\infty} T^{1}_{1L'} B^{c}_{L'}(u) = \sigma_s \langle \mu U \rangle = \sigma_s \zeta \qquad (3\text{-}48e)$$

Equations (3-45e) for $L = 0, 1$ can be written:

$$q(k,u) + \lambda_0(u) \frac{\partial q(k,u)}{\partial u} = \phi_0(k,u)\left(1 - \frac{\partial \lambda_0}{\partial u}\right)\xi(u)\Sigma_s(u) \qquad (3\text{-}48f)$$

$$\eta_1(k,u) + \lambda_1(u) \frac{\partial \eta_1(k,u)}{\partial u} = \phi_1(k,u)\left(1 - \frac{\partial \lambda_1}{\partial u}\right)\xi(u)\Sigma_s(u) \qquad (3\text{-}48g)$$

For isotropic scattering, the λ_L become constants

$$\lambda_L = -\frac{T^{2}_{L0}}{T^{1}_{L0}} \qquad (3\text{-}49a)$$

and in particular

$$\lambda_0 = -\frac{T^{2}_{00}}{T^{1}_{00}} = \frac{1 - \alpha\left[1 + \ln\frac{1}{\alpha} + \frac{1}{2}\ln^2\frac{1}{\alpha}\right]}{1 - \alpha\left(1 + \ln\frac{1}{\alpha}\right)} \rightarrow \frac{4\gamma}{3} \qquad (3\text{-}49b)$$

$$\lambda_1 = -\frac{T^{2}_{10}}{T^{1}_{10}} \longrightarrow \frac{4\gamma}{5} \qquad (3\text{-}49c)$$

the arrows indicating the limits for small γ. These values will allow us to compare the GG method with others.

Both consistent and inconsistent GG calculations may be ultilized. The former is the set of Equations (3-48) just written, while the latter may be derived from (3-48) by setting $\partial\eta_1/\partial u = 0$ in Equation (3-48b). Inspection reveals the following features of these equations:

a) If $\lambda_0 = 1$, $\lambda_1 = 3/2$, the consistent GG equations are identical to the consistent P_1 equations for hydrogen, i.e., hydrogen is treated rigorously by the GG method;

b) If $\lambda_0 = 1$, the inconsistent GG set is identical to the Selengut-Goertzel equations and

c) If $\lambda_0 = 0$, the inconsistent GG set reduces to the Age Diffusion equation.

An analytical solution is possible for the inconsistent P_1 GG set of equations when λ is constant, i.e., scattering is isotropic.* It is solved here to give an expression for the age, which will facilitate comparison, at least qualitatively, with other methods. In this approximation Equation (3-48g) has no significance, while (3-48b) simply becomes Fick's Law. When Fick's Law is applied to Equation (3-48a) and Equation (3-47c) is used to evalute $\partial q/\partial u$, a single diffusion equation results:

$$\left[\Sigma_a(u) + D(u)k^2 + \sum_{\lambda_0}\Sigma_s(u)\right]\phi_0(k,u) = S(k,u) + \frac{\Sigma}{\lambda_0^2}\int_0^u \Sigma_s(u')\,\phi(u')\,e^{-(u-u')/\lambda_0}\,du' \quad (3\text{-}50a)$$

* One need not restrict the solution to the case of a single element, provided λ is properly defined and constant.

which is identical to Equation (2- 29a) if Σ_a (u) is replaced by $[\Sigma_a$ (u) + D (u) $k^2]$. Hence, the solution can be written down practically by inspection. Once again, only monoenergetic sources are considered for simplicity. The solution for $\phi_o(k, u)$ is:

$$\phi_o(k,u) = \left[\frac{1}{\lambda_0(\Sigma_a + Dk^2) + \xi\Sigma_s}\right]_u \left[\frac{\xi\Sigma_s}{\lambda_0(\Sigma_a + Dk^2) + \xi\Sigma_s}\right]_{u=0} \exp\left\{-\int_0^u \frac{\Sigma_a(u') + D(u')k^2}{\lambda_0(\Sigma_a(u') + D(u')k^2) + \xi\Sigma_s(u')} du'\right\} \quad (3\text{-}50b)$$

The observation that Σ_a (u) is replaced by $[\Sigma_a$ (u) + D (u) $k^2]$ is a result frequently obtained and applies to the diffusion approximations discussed earlier. Since this term arises from neutron leakage and in a bare reactor $k^2 = B^2$, this often leads to the interpretation of D (u) B^2 as a "leakage cross section" for these systems. For reflected systems, one must, of course, be more careful about making this interpretation.

The age may be obtained by either of the methods previously employed. Having already obtained an explicit expression for ϕ_o (k, u), it is probably more convenient to differentiate (3-50b) directly rather than to employ the power series method. The result for τ_N is

$$\tau_N(u) = \left.\frac{D\lambda_0}{\lambda_0\Sigma_a + \xi\Sigma_s}\right|_u + \left.\frac{D\lambda_0}{\lambda_0\Sigma_a + \xi\Sigma_s}\right|_{u=0} + \int_0^u \frac{\xi\Sigma_s D}{(\lambda_0\Sigma_a + \xi\Sigma_s)^2} du' \quad (3\text{-}50c)$$

Again, the terms may be interpreted as a last flight correction, a first flight correction and a modified Fermi Age formula. τ_q, as might be inferred from the previous section, is given by $\tau_N(u)$ minus the first term on the right-hand side of (3-50c). The interesting point here is the introduction of a new fictitious absorption cross section given by λ_o times the true absorption cross section. This result is exactly the analytical result obtaines by the Selengut-Goertzel method if $\lambda_o = \xi = 1$, the values for hydrogen. Thus, in a way, the GG procedure is a generalization of the Selengut-Goertzel method to all moderators. Values of λ_o were given in Table I, Chapter II. As will be seen later in this chapter, this method in its more rigorous form yields better results than the previously described methods, particularly for deuterium (heavy water) moderated reactors.

13. The Age in Hydrogen

Explicit expressions for the age may be obtained analytically in several special cases. The first of these is the rather important case in which hydrogen is the only moderator. (This case was discussed in relation to the SG method earlier; again it is assumed that all slowing down is due to hydrogen but other elements may affect neutron transport.) For such a case one replaces $N^n J_o^n(k, u)$ by $\Sigma_s^n(u)\, \phi_o(k, u)$ and $N^n J_1^n(k, u)$ by $\langle\mu\rangle_n \Sigma_s^n \phi_1(k, u)$ for all elements except hydrogen. Making these substitutions, Equations (3-19)

lead to the following simplified equations:

$$[\Sigma_a(u)+\Sigma_s^H(u)]\varphi_{00}(u) = S_0 + N_H J_{00}^H(u) \qquad (3\text{-}51a)$$

$$\tfrac{1}{2}[\Sigma_a(u)+\Sigma_s^H(\omega)]\varphi_{02}(u) - \varphi_{11}(u) = \tfrac{1}{2} N_H J_{02}^H(u) \qquad (3\text{-}51b)$$

$$[\Sigma_{tr}(u)+\Sigma_s^H\langle\mu\rangle_H]\varphi_{11}(u) - \tfrac{1}{3}\varphi_{00}(u) = N_H J_{11}^H(u) \qquad (3\text{-}51c)$$

where $\langle\mu\rangle_H = 2/3$ to a very good approximation. The solution of the set of Equations (3-51) and the defining equations for the $J_{j\ell}^H(u)$ is straightforward, if rather tedious, and yields the well-known "Marshak Formula" for the age.[16, 17] Only the $\varphi_{j\ell}(u)$ are given here as the $J_{j\ell}^H(u)$, being simply linear combinations of the $\varphi_{j\ell}(u)$, are easily obtained from (3-51) using the results quoted below.

$$\tfrac{1}{2}\varphi_{02}(u) = \frac{1}{\Sigma_a(u)+\Sigma_s^H(u)}\left[\varphi_{11}(u)+\int_0^u (1-s(u'))\,\varphi_{11}(u')\,e^{-\int_{u'}^u s(u'')\,du''}\right] \qquad (3\text{-}52a)$$

$$\varphi_{11}(u) = \frac{1}{3\left(\Sigma_{tr}(u)+\frac{2}{3}\Sigma_s^H(u)\right)}\left[\varphi_{00}(u)+\tfrac{3}{2}\int_0^u (1-\lambda(u'))\,\varphi_{00}(u')\,e^{-\frac{3}{2}\int_{u'}^u \lambda(u'')\,du''}\right] \qquad (3\text{-}52b)$$

$$\varphi_{00}(u) = \frac{1}{\Sigma_a(u)+\Sigma_s^H(u)}\left[S(u)+\int_0^u (1-s(u'))\,S(u')\,e^{-\int_{u'}^u s(u'')\,du''}\right. \qquad (3\text{-}52c)$$

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[16] R. E. Marshak, op. cit.

where the following symbols have been employed:

$$S(u) = \frac{\Sigma_a(u)}{\Sigma_a(u) + \Sigma_s^H(u)} \qquad (3\text{-}52d)$$

$$\lambda(u) = \frac{\Sigma_{tr}(u)}{\Sigma_{tr}(u) + \frac{2}{3}\Sigma_s^H(u)} \qquad (3\text{-}52e)$$

The values of τ_N (or τ_q, if desired) obtained from these formulae are rigorous for the case treated here, which, while it may not seem to have much application to an experimental situation, actually approximates slowing down in water rather well.* Here, the formula obtained for the age is not easily interpretable unless one invokes assumptions so drastic as to render the expression obtained almost meaningless. Some discussion of this result is to be found in the literature.[18]

The previously derived inconsistent P_1 SG results are obtained by using Fick's Law

$$\varphi_{11}(u) = \frac{\varphi_{00}(u)}{\Sigma_{tr}(u)}$$

instead of Equation (3-52b). Stated another way, the exponential in the

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* This is, in part, due to some of the effects of oxygen cancelling each other out.

[18] Ibid.

integral (3-52b) is replaced by a delta function

$$e^{-\frac{3}{2}\int_{u'}^{u}\lambda(u'')du''} \longrightarrow \frac{2}{3}\,\frac{\delta(u-u')}{\lambda(u')}$$

It may also be shown that for the special case of no absorption, $\Sigma_a = 0$, the first flight correction is given by

$$\left.\frac{\lambda(u)}{3\Sigma_s(u)\Sigma_{tr}(u)}\right]_{u=0} = \left.\frac{1}{3\left[\Sigma_{tr}+\frac{2}{3}\Sigma_s^H\right]\Sigma_s}\right]_{u=0} \qquad (3\text{-}53)$$

which is smaller than the SG result because $2/3\,\Sigma_s^H(u)\left(=\Sigma_s^H\langle\mu\rangle_H\right)$ is added to the transport cross section. This phenomenon is explained by the fact that hydrogen scattering changes the lethargy of source neutrons and therefore effectively "absorbs" them. Equation (3-53) is the rigorous first flight correction under the assumption that heavy elements do not slow down.

14. The Age in Pure Heavy Elements[19]

It is also possible to rigorously calculate the age in a single heavy non-absorbing element. Here, it is more convenient to adopt another approach as the limits on defining integrals the $J_j^n(k, u)$ do not permit the easy conversion of the integral equation into a diffenrential equation that made the hydrogen case simple. First, the P_1 equations are written in terms of the collision density $\chi(k, u) = \Sigma_t(u)\phi(k, u)$. One has, for a monoenergetic sinusoidal source,

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[19] R.E. Marshak, op. cit.

and no absorption:

$$\chi_0(k,u) - ik\phi_1(k,u) = \int_{u-\ell n\frac{1}{\alpha}}^{u} \chi_0(k,u')F_0(u-u')du' + \delta(u) \qquad (3\text{-}54a)$$

$$\chi_1(k,u) - \frac{ik}{3}\phi_0(k,u) = \int_{u-\ell n\frac{1}{\alpha}}^{u} \chi_1(k,u')F_1(u-u')du' \qquad (3\text{-}54b)$$

where F_0 and F_1 are the first two Legendre moments for the scattering frequency. In order to facilitate use of Laplace Transforms, the scattering frequencies F_0 and F_1 are defined as zero for $u > u' + \ell n\, 1/\alpha$ and the integrals in (3-54) are extended to zero. Then the integrals in Equations (3-54) are convolutions and the Laplace Transforms of the equations may be taken:

$$\bar{\chi}_0(k,s) - ik\bar{\phi}_1(k,s) = \bar{\chi}_0(k,s)\bar{F}_0(s) + 1 \qquad (3\text{-}55a)$$

$$\bar{\chi}_1(k,s) - \frac{ik}{3}\bar{\phi}_0(k,s) = \bar{\chi}_1(k,s)\bar{F}_1(s) \qquad (3\text{-}55b)$$

where s is again the transform variable and the barred quantities are the Laplace transforms of the unbarred quantities in appearing in Equations (3-54). Now the expansions of the $\phi_j(k, u)$ in power series in k as given by Equation (3-17a) may be transformed to yield an analogous series expansion for $\bar{\phi}_j(k, s)$

$$\bar{\phi}_j(k,s) = \sum_{\ell=j,j+2\ldots} \bar{\varphi}_{j\ell}(s)\,\frac{(ik)^\ell}{\ell!} \qquad (3\text{-}56a)$$

A similar series may be obtained for $\chi_j(k, s)$ by multiplying Equation (3-17a) by $\Sigma_t(u)$ before transforming:

$$\bar{\chi}_j(k,s) = \sum_{\ell=j,j+2\ldots} \bar{\chi}_{j\ell}(s)\,\frac{(ik)^\ell}{\ell!} \qquad (356b)$$

Again, use is made of Equation (3-17e) to determine the age, noting that either the $\varphi_{j\ell}(u)$ or $\chi_{j\ell}(u)$ may be used; the $\chi_{j\ell}(u)$ are of course simply the inverse transforms of the $\bar{\chi}_{j\ell}(s)$. These latter quantities are determined by equating coefficients of the various powers of k after the power series expansions have been inserted into Equations (3-55). They are:

$$\bar{\chi}_{00}(s) = \frac{1}{1-\bar{F}_0(s)} \qquad (3\text{-}57a)$$

$$\bar{\chi}_{11}(s) = \frac{\bar{\phi}_{00}(s)}{3\left(1-\bar{F}_1(s)\right)} \qquad (3\text{-}57b)$$

$$\bar{\chi}_{02}(s) = \frac{2\bar{\phi}_{11}(s)}{1-\bar{F}_0(s)} \qquad (3\text{-}57c)$$

A formal solution is possible if $\chi_{00}(u)$ is written as the inverse Laplace Transform of $(1 - \bar{F}_0[s])^{-1}$ and is denoted by $\kappa_0(u)$.

Then the last two quantities may be written as convolutions involving $K_0(u)$, which is a known function:

$$\chi_{11}(u) = \frac{1}{3}\int_0^u K_{11}(u-u')\,\frac{K_0(u')}{\Sigma_s(u')}\,du' \qquad (3\text{-}58a)$$

with

$$K_1(u) = \mathcal{L}^{-1}\left\{\frac{1}{1-F_1(s)}\right\} \qquad (3\text{-}58b)$$

and

$$\chi_{02}(u) = 2\int_0^u K_0(u-u')\,\frac{\chi_{11}(u')}{\Sigma_s(u')}\,du' \qquad (3\text{-}58c)$$

These may be combined to yield the rigorous age for slowing down in a single heavy element:

$$\tau(u) = \frac{1}{3K_0(u)}\int_0^u \frac{K_0(u-u')}{\Sigma_s(u')}\,du' \int_0^{u'} \frac{K_0(u'')K_1(u'-u'')}{\Sigma_s(u'')}\,du'' \qquad (3\text{-}59)$$

This formula, while rigorous, is quite formal and rather difficult to apply to a given situation, but does reduce to the formula of the previous section for hydrogen. Even in the case of isotropic elastic scattering, the forms of $K_0(u)$ and $K_1(u)$ are too complicated to allow (3-59) simple application in practical situations. As a matter of fact it may be noted that $K(u_0)$ is just the solution for the flux as a function of lethargy that was obtained in Chapter II; except for hydrogen it was in the form of an infinite series and is clearly difficult to apply here.

D. Methods Related to the P_L Approximations

15. The Gaussian Quadrature Procedure[2,21]

Probably the most used methods in reactor calculations are the P_L approximations, particularly the P_1 approximation and its modifications. Several other methods, which at first sight appear to be entirely new approaches, are in reality closely related to the P_L approximation and are also frequently employed. In few cases are they of greater value than the P_L approximation, but they do point out some of the difficulties inherent in the P_L methods; at times there is advantage in using these approximations for themselves.

An alternative to expansion of the angular neutron flux $\Phi(r, E, \underline{\Omega})$ in spherical harmonics is the approximation of the angular portion of the degradation integral by a quadrature formula. Many such schemes exist and have been applied to this problem. Of these, only two will be discussed here: the simplest scheme, which is based on the trapezoid rule, and is discussed later as the S_N method, and the scheme which gives the best approximation to the integral in a least mean squares sense, the Gauss Quadrature method. The latter method will now be discussed and its relation to the P_L method will be demonstrated.

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[20] G.C. Wick, Z. Physik, 121, 702 (1943).

[21] The Gauss Quadrature Method is discussed in many places, but the best discussion is probably S. Chandrasekhar, Radiative Transfer, New York; Dover (1960); see pp. 54-69.

In this method the angular integration in the degradation term in the Boltzmann Equation is approximated by the Gauss Quadrature Formula. In applying this procedure, however, one must be careful, since the Gauss Quadrature Formula using an odd number of points ("discrete ordinates") employs $\mu = 0$ as one of the points at which the integrand is evaluated. However, the angular flux $\Phi(z,E,\mu)$ need not be continuous in the $\mu = o$ direction.[22] For example, consider a plane moderator-vacuum interface. At the surface there will be no neutrons in the vacuum travelling parallel to the interface, but there may be some in the moderator. Then $\Phi(z, E, \mu)$ is not a continuous function of μ at $\mu = 0$ at the boundary. Therefore, this procedure may be successfully employed only in an approximation using an even number of points. Applying the $L + 1$ point (L odd) Gauss formula to the Fourier Transformed one-dimensional Boltzmann Equation, we obtain the equation

$$\Sigma_t(u)\oint(k,u,\mu) - ik\mu\oint(k,u,\mu) = S_0(u) + \int_{u-e^{-\alpha}}^{u}\sum_{j=0}^{L} F(u'\to u, \mu_j\to\mu)\Sigma_s(u')\oint(k,u',\mu_j) \qquad (3-60)$$

Here the μ_j are the discrete ordinates of the $L + 1$ point Gauss

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22 This argument is for the one dimensional case and is related to the fact that the one dimensional Boltzmann Equation has a singular point at $\mu = 0$. For three dimensions the arguments are similar but more difficult to make. Also the authors must give credit to B.I. Spinrad, private communication.

Quadrature Formula which are the zeros of the Legendre Polynomial of degree $L + 1$, $P_{L+1}(\mu)$; the ω_j are the relative weights, or Christoffel numbers

$$\omega_j = \frac{1}{P'_{L+1}(\mu_j)} \int_{-1}^{1} \frac{P_{L+1}(\mu)}{\mu - \mu_j} d\mu$$

where the prime denotes differentiation. $F(u' \to u, \mu_j \to \mu)$, as before, is the probability for transition from μ_j to μ while scattering from u' to u, per unit μ per unit lethargy.

If, in particular, μ is chosen to be each of the μ_j consecutively, this procedure results in a set of $L + 1$ simultaneous equations in the $(L + 1)$ functions $\Phi(k, u, \mu_j)$. The angular flux $\Phi(k, u, \mu)$ for all μ is obtained by substituting into Equation (3-60). This method is strictly applicable only to the one-dimensional problem.

16. Relation to the P_L Method

The Gauss Quadrature Method is equivalent to the P_L method in some approximation.[23] Noting that $F(u' \to u, \mu_j \to \mu_i)$ is a function only of the angle between the vectors $\underline{\Omega}$ and $\underline{\Omega}'$ we can write, using the addition theorem (3-7e) (the terms depending on the azimuthal angle are deleted as they drop out when the expansion is inserted into the degradation integral and the azimuthal integration is carried

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[23] R. Gast, "On the Equivalence of the Gauss Quadrature and P_L Methods" (WAPD-TM-118).

out):

$$F(u' \to u, \mu_j \to \mu_i) = \sum_{n=0}^{\infty} \frac{2n+1}{2} F_n(u' \to u) P_n(\mu_j) P_n(\mu_i) \qquad (3\text{-}61a)$$

Furthermore, it is always possible to write

$$\Phi(k, u, \mu_i) = \sum_{l=0}^{L} \frac{2l+1}{2} \phi_l(k, u) P_l(\mu_i) \qquad (3\text{-}61b)$$

since the right-hand side is a polynomial of degree L in μ_i and can always be made to pass through the L + 1 points, $[\mu_i, \Phi(k, \mu_i, u)]$ by suitable choice of the L + 1 $\phi_l(k, u)$. Using these expansions, which show some similarity to the expansion used in the P_L method, we can now rewrite Equation (3-60) as

$$\Sigma_t(u) \Phi(k, u, \mu_i) - ik\mu_i \Phi(k, u, \mu_i) = S_0(u)$$

$$+ \int_{u-\ln\frac{1}{\alpha}}^{u} du' \Sigma_s(u') \sum_{n=0}^{\infty} \frac{2n+1}{2} F_n(u' \to u) P_n(\mu_i) \left[\sum_{l=0}^{L} \frac{2l+1}{2} \phi_l(k, u') \sum_{j=0}^{L} \omega_j P_n(\mu_j) P_l(\mu_j) \right] \qquad (3\text{-}62a)$$

The last summation (over the index j) is recognized as the L + 1 point Gauss Quadrature of the integral

$$\int_{-1}^{1} P_n(\mu) P_l(\mu) d\mu$$

Now it may be noted[24] that the L + 1 point Gauss Formula rigorously evaluates integrals of polynomials of degree 2L + 1 or less. Then

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[24] Chandrasekhar, op. cit., p. 61.

if n is no greater than $L + 1$, the integrand of (3-62b) will be a polynomial of degree no greater than $2L + 1$ (since $n \leq L$) and the sum over j in Equation (3-62a) will be rigorously equal to (3-62b). But this integral is just the orthogonality integral for Legendre Polynomials so that the entire quantity in the bracket in Equation (3-62a) is just $\phi_n(k, u')$. Using this along with the recursion relation (3-10b) for Legendre polynomials and the definition of $\phi_n(k, u')$, we obtain from Equation (3-60)

$$-\sum_{l=0}^{L}\left\{\mu_k\left[(l+1)\phi_{l+1}(k,u)P_l(\mu_i)(1-\delta_{lL}) + l\,\phi_{l-1}(k,u)P_l(\mu_i)\right]\right.$$

$$+\Sigma_t(u)(2l+1)\phi_l(k,u)P_l(\mu_i) - (2l+1)\int_0^u B_l^o(u',v)\phi_l(k,u')P_l(\mu_i)du'$$

$$\left. - S_l(u)\delta_{l0}P_l(\mu_i)\right\} = 0 \qquad (3\text{-}63)$$

Finally, each term on the left hand sides of these equations is a polynomial of degree $L + 1$; hence Equations (3-63) can be satisfied only if the coefficients of each Legendre Polynomial are equated to zero. The P_L equations then result.

Thus we have shown that the P_L approximation and the $(L + 1)$ point quadrature method are equivalent provided the scattering kernel (and the source, if it is anisotropic, although this was not shown), can be expressed in terms of the first $L + 1$ Legendre polynomials.

In light of the above, it is apparent that the even P_L

approximations, which are equivalent to odd-point quadrature schemes, are not as useful as the even P_L methods. They suffer from the fact that discontinuity of the flux at $\mu = o$ cannot be tolerated.[25]

17. The Double P_L and Double Gauss Quadrature Methods[26]

As pointed out, the methods of the previous section lead to difficulties near $\mu = 0$. One reason was given earlier: a possible flux discontinuity at $\mu = 0$ is difficult to describe by a series of continuous functions. Furthermore, in the Gauss Quadrature Method, the discrete ordinates selected, the zeros of $P_L(\mu)$, tend to cluster more closely to $\mu = \pm 1$ than to $\mu = 0$. Thus, while the method gives the best overall convergence in a least mean squares sense, it may not give the best convergence at any particular given point. This has, in fact, been demonstrated mathematically. Probably the most obvious means of overcoming this difficulty is to use different expansions for the flux on either side of $\mu = 0$ or, what is the same thing, to apply the quadrature formula separately to each region. A discontinuity of the flux at $\mu = 0$ is then of no consequence; even the lowest order approximation will be capable of dealing with a step discontinuity. In this way, one arrives at the Double P_L (DP_L) and

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[25] Other reasons for not using even L approximations, based on arguments concerning boundary conditions are given by Davison, op. cit.

[26] J. Yvon, J. Nuc. Ener., 4, 305 (1957)

Double Gauss Quadrature (DGQ) approximations. As it is readily shown[27] that these schemes are equivalent in the sense of the last section, only the DP_L procedure is discussed. As yet, the methods have not seen much application in slowing down theory per se, but as multigroup methods are essentially schemes for adapting one-velocity transport theory to multi-energy problems, the methods see some application to slowing down in this sense.

First, the μ space $[-1, 1]$ is divided into two subspaces $[-1, 0]$ and $[0, 1]$. For each subspace, the angular flux and scattering functions are expanded in Legendre Polynomials, but, in order to retain the orthogonality properties, the expansion is made in terms of polynomials of $2\mu-1$ for $\mu>0$ and of $2\mu+1$ for $\mu<0$. This insures that the $P_L(\mu)$ will be orthogonal on the regions of interest. These expansions will be then substituted into the Boltzmann equation written in the following form:

$$\left(\Sigma_t(u) - ik\mu\right)\Phi(k,u,\mu) = \int_{u-\ln\frac{1}{\alpha}}^{u} du' \left[\int_{-1}^{0} d\mu' \Phi(k,u,\mu')\Sigma_s(u'\to u, \mu'\to\mu) + \int_{0}^{1} d\mu' \Phi(k,u,\mu')\Sigma_s(u'\to u, \mu'\to\mu)\right] + S_0(u) \tag{3-64}$$

As before, the expansion of the scattering frequency may be

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[27] Gast, op. cit.

simplified by means of the addition theorm (3-8), yielding:

$$\Sigma_s(u' \rightarrow u, \mu_0) = \sum_{j=0}^{\infty} \frac{2j+1}{2} \Sigma_{sj}(u' \rightarrow u) P_j(\mu') P_j(\mu) \qquad (3\text{-}65a)$$

where the terms involving the azimuthal angle ϕ have been suppressed as they will again integrate to zero when inserted into the degradation integral. To obtain the desired form, however, it is necessary to express the $P_j(\mu)$ as functions of the Legendre Polynomials of $2\mu + 1$. Two expansions are required:

$$P_j(\mu) = \sum_{l=0}^{j} a_j^l P_l(2\mu+1) \qquad \mu < 0$$

$$= \sum_{l=0}^{j} b_j^l P_l(2\mu-1) \qquad \mu > 0 \qquad (3\text{-}65b)$$

Only j terms are needed in this expansion since $P_j(\mu)$ is a polynomial of degree j. The constants a_j^l and b_j^l appearing in these equations could be determined by using the orthogonality properties but more straightforward means are available. In this manner, one obtains four different expansions for the scattering frequency:

$$\Sigma_s(u'\to u, \mu'\to\mu) = \sum_{j=0}^{\infty} \frac{2j+1}{2} \Sigma_{sj}(u'\to u) \sum_{l=0}^{j} b_j^l P_l(2\mu'+1) \sum_{g=0}^{j} b_j^g P_g(2\mu+1) \qquad \begin{matrix}\mu'<0\\ \mu<0\end{matrix}$$

$$= \sum_{j=0}^{\infty} \frac{2j+1}{2} \Sigma_{sj}(u'\to u) \sum_{l=0}^{j} b_j^l P_l(2\mu'+1) \sum_{g=0}^{j} a_j^g P_g(2\mu-1) \qquad \begin{matrix}\mu'<0\\ \mu>0\end{matrix}$$

$$= \sum_{j=0}^{\infty} \frac{2j+1}{2} \Sigma_{sj}(u'\to u) \sum_{l=0}^{j} a_j^l P_l(2\mu'-1) \sum_{g=0}^{j} b_j^g P_g(2\mu+1) \qquad \begin{matrix}\mu'>0\\ \mu<0\end{matrix}$$

$$= \sum_{j=0}^{\infty} \frac{2j+1}{2} \Sigma_{sj}(u'\to u) \sum_{l=0}^{j} a_j^l P_l(2\mu'-1) \sum_{g=0}^{j} a_j^g P_g(2\mu-1) \qquad \begin{matrix}\mu'>0\\ \mu>0\end{matrix}$$

(3-66)

In a similar manner, the flux expansion may be written

$$\Phi(k,u,\mu) = \sum_{l=0}^{\infty} (2l+1)\, \Psi_l(k,u)\, P_l(2\mu-1) \qquad \mu>0$$

$$= \sum_{l=0}^{\infty} (2l+1)\, \chi_l(k,u)\, P_l(2\mu+1) \qquad \mu<0$$

where the expansion coefficients are now expressible as integrals on the intervals $[-1, 0]$ and $[0, 1]$; it is convenient to define them as zero elsewhere:

$$\Psi_l(k,u) = \int_0^1 \Phi(k,u,\mu) P_l(2\mu-1)\, d\mu \qquad \mu>0$$

$$= 0 \qquad \mu<0$$

and

$$\chi_l(k,u) = \int_{-1}^{0} \Phi(k,u,\mu)\, P_l(2\mu+1)\, d\mu \qquad \mu<0$$

$$= 0 \qquad \mu>0$$

There expansions may be inserted into the Boltzmann Equation, which then separates into two sets of coupled equations in the $\chi_l(k, u)$

and $\psi_\ell(k, u)$; sources are again assumed to be isotropic:

$$-\mu k\left[\frac{j}{2j+1}\psi_{j-1}(k,u)-\psi_j(k,u)+\frac{j+1}{2j+1}\psi_{j+1}(k,u)\right]+2\Sigma_t(u)\psi_j(k,u)$$

$$=\int_{u-\ln\frac{1}{\alpha}}^{u}du'\sum_{\ell=0}^{\infty}\left[\chi_\ell(k,u')\sum_{k=0}^{\infty}\frac{2k+1}{2j+1}\Sigma_{sk}(u'\to u)a_k^j b_k^\ell\right.$$

$$\left.+\psi_\ell(k,u')\sum_{k=0}^{\infty}\frac{2k+1}{2j+1}\Sigma_{sk}(u'\to u)\,a_k^j b_k^\ell\right]+S_0(k,u) \qquad (3\text{-}67a)$$

and

$$-\mu k\left[\frac{j}{2j+1}\chi_{j-1}(k,u)-\chi_j(k,u)+\frac{j+1}{2j+1}\chi_{j-1}(k,u)\right]+2\Sigma_t(u)\chi_j(k,u)$$

$$=\int_{u-\ln\frac{1}{\alpha}}^{u}du'\sum_{\ell=0}^{\infty}\left[\chi_\ell(k,u')\sum_{k=0}^{\infty}\frac{2k+1}{2j+1}\Sigma_{sk}(u'\to u)\,b_k^j b_k^\ell\right.$$

$$\left.+\psi_\ell(k,u')\sum_{k=0}^{\infty}\frac{2k+1}{2j+1}\Sigma_{sk}(u'\to u)\,a_k^\ell b_k^j\right] \qquad (3\text{-}67b)$$

Again, an infinite set of integro-differential equations has been obtained. In this case, the coupling assumes a slightly more complicated form; all of the $\psi_j(k, u)$ and $\chi_j(k, u)$ are coupled to all of the others. This set cannot be truncated in the same manner as were the spherical harmonics equations. Here, one

must set $\psi_j(k, u) = \chi_j(k, u) = 0$ for all $j>L$ to obtain the Double PL (DPL) equations. Alternatively, one could set $\Sigma_{sk}(u' \rightarrow u) = 0$ for $k>L$ and $\psi_{L+1}(k, u) = \chi_{L+1}(k, u) = 0$ since, by definition, the a_k^ℓ and b_k^ℓ are zero if $\ell>k$. It is evident that a combination of these is also possible.

In contrast to the properties of the P_L approximation, the DP_o equations may be applied to finite medium problems. The DP_o equations merely assume a step function for the angular variation of the flux, and, in fact, for some problems involving plane interfaces the DP_o approximations has been found to give results which are as accurate as the P1 results.[28] Similarly, the DP_1 equations give results of accuracy comparable to that of the P_3 equationsin such problems. Another important point is that the even L-DPL equation do not possess the inherent difficulties of the even L-P_L equations and may be successfully employed.

The equivalence of the DP_L and DGQ methods may be demonstrated without resort to the kernel and source truncations that were necessary for the analogous proof with the ordinary GQ method.[29] Thus, it will be advantageous to retain extra terms in the expansion of the scattering kernel. A reasonable estimate is that $2L + 1$ terms should be retained: The DP_L scheme employs (in DGQ notation)

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[28] Ibid.

[29] Ibid.

$2L + 2$ discrete ordinates; comparable accuracy is obtained only if $2L + 1$ terms of the expansion of the scattering frequency are retained.

The DP_L equations may be set up in geometries other than plane following the method used here; in multigroup calculations of reflected reactors such developments are highly necessary, particularly if non-planar boundaries are present. For these developments, the reader is referred to the work of Schiff and Ziering.[30]

It has been suggested by Schiff and Ziering[31] that higher order multiple P_L equations, in which the angular region is broken into more than two parts, could be developed, but there is some doubt that the advantages gained are worth the increase in complexity that accompanies it. For example, in a quadruple P_L approximation, sixteen separate expansions of the scattering frequency are required.

18. The B_L Approximation

Another useful and a more rapidly converging approximation may be obtained from the spherical harmonics expansions of the Boltzmann Equation [Equation (3-9)]. To obtain it, before multiplying Equation (3-9) by $P_j(\mu)$ and integrating over μ, the entire equation is divided by $\left(1 - \frac{ik\mu}{\Sigma_t} \right)$. This results in a set of coupled integral

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[30] S. Schiff and S. Ziering, Nuc. Sci. Eng., 3, 635 (1958)

[31] S. Schiff and S. Ziering, Nuc. Sci. Eng., 1, 172 (1960)

equations different from the P_L equations:

$$\Sigma_t(u)\,\phi_j(k,u) = \sum_{l=0}^{\infty}(2l+1)A_{jl}(\eta)\Big[N_H J_l^H(k,u) + N_D J_l^D(k,u) + \sum_{i\neq H,D} N_i J_l^i(k,u) + S_0(k,u)\delta_{l0}\Big] \qquad (3\text{-}68a)$$

where the $A_{jl}(\eta)$ are defined by

$$A_{jl}(\eta) = A_{lj}(\eta) = \frac{1}{2}\int_{-1}^{1}\frac{P_j(\mu)P_l(\mu)}{1-\eta\mu}\,d\mu \qquad (3\text{-}68b)$$

and the parameter η is defined by

$$\eta = \sim y = \frac{2k}{\Sigma_t(u)} \qquad (3\text{-}68c)$$

By applying the same operation to Equation (3-10b), the recursion relation for Legendre polynomials, recursion relations for the A_{jl} may be obtained. For the relation relative to the second index we have:

$$\frac{2l+1}{\eta}A_{jl}(\eta) - (l+1)A_{j,l+1}(\eta) - lA_{j,l-1}(\eta) = \frac{\delta_{jl}}{\eta} \qquad (3\text{-}69a)$$

Since the $A_{jl}(\eta)$ are symmetric in j and l, the relation on the first index is quite similar

$$\frac{2j+1}{\eta}A_{jl}(\eta) - (j+1)A_{j+1,l}(\eta) - jA_{j-1,l} = \frac{\delta_{jl}}{\eta} \qquad (3\text{-}69b)$$

By successive use of these two recursion relations, any of the $A_{j\ell}(\eta)$ may be expressed in terms of $A_{00}(\eta)$ which can be found by direct integration:

$$A_{00}(\eta) = \eta^{-1}\tanh^{-1}\eta = \frac{Q_0(\frac{1}{\eta})}{\eta} \qquad (3\text{-}69c)$$

where $Q_\ell(x)$ is a Legendre function of the second kind.[32] In general, it may be shown that[33]

$$A_{j\ell}(\eta) = \frac{Q_j(\frac{1}{\eta})P_\ell(\frac{1}{\eta})}{\eta} \qquad (3\text{-}69d)$$

Numerical values of the first few $A_{j\ell}(\eta)$, up to $A_{22}(\eta)$ have been tabulated by Bethe, Tonks, and Hurwitz,[34] who also wrote them out explicitly:

$$A_{01} = \frac{A_{00}-1}{\eta}$$

$$A_{11} = \frac{A_{00}-1}{\eta^2}$$

$$A_{02} = \frac{3}{2\eta^2}\left[A_{00}\left(1-\frac{\eta^2}{3}\right)-1\right]$$

$$A_{12} = \frac{A_{02}}{\eta} \qquad A_{22} = A_{02}\left[\frac{3}{2\eta^2}-\frac{1}{2}\right]$$

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[32] E.T. Whittaker and G.N. Watson, "A Course in Modern Analyses", Oxford (1950).

[33] I. Waller, Arkiv. Math. Astron. Fysik, 34, 3, 1 (1947).

[34] H.A. Bethe, L. Tonks, and H. Hurwitz, Jr., Phys. Rev., 80, 11 (1950).

Before proceeding, let us look into the nature of this scheme. The operation of dividing by $(1 - ik\mu/\Sigma_t)$ in Fourier Transform space corresponds, in ordinary configuration space, to the operation of multiplying by the operator $(1 + \frac{\mu\partial/\partial z}{\Sigma_t})^{-1}$, the inverse of the "streaming" operator in the Boltzmann Equation. Stated less abstractly, this operation amounts to the conversion of the integro-differential Boltzmann Equation to a pure integral equation as was done in Section 2 Chapter II. Hence the above analysis is really equivalent to making a Legendre analysis of the integral form of the Boltzmann Equation. In configuration space this analysis is rather difficult to make; the results would clearly be the same as that obtained by taking the inverse Fourier Transforms of Equations (3-68) and would lead to rather involved convolutions of the Legendre Components of the flux, $\phi_j(\underline{r}, u)$ with the inverse transforms of the $A_{j\ell}(\eta)$, which are exponential integral functions of some complexity. It is for this reason that the approximations obtained by truncating the set of Equations (3-68), called the B_L Approximations,[35] are applied mainly to special problems, as for example the calculation of moments of the flux (e.g., the age) or the computation of group constants for multigroup calculations (see Chapter IV). Criticality calculations can be made by this method if one is willing to characterize the system

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[35] The name "B_L Approximation" appears to be due to H. Hurwitz, Jr., and P.F. Zweifel, J. Appl. Phys., 26, 923 (1956)

by a geometric buckling by setting $k^2 = B_j^2$, but it is difficult to use the method for determining flux distributions.

A low order approximation to the infinite set of coupled equations may be obtained by setting

$$J_\ell(k, u) = 0 \quad \text{for all} \quad j>L$$

This is the B_L approximation mentioned above. Again, a set of $L + 1$ coupled integral equations is obtained. In contrast to the method of uncoupling the equations in the P_L case, it is here essential to set all the $J_\ell(k, u)$ above the L-th equal to zero. In practice, this makes little difference since the physically interesting quantities are just the flux $\phi_0(k, u)$ and the current $\phi_1(k, u)$.

19. Relation to the P_L Approximation[36]

A relation between the P_L and B_L approximation is readily obtained. From Equations (3-68a) and (3-69d) it can be seen that if $J_j(k, u) = 0$ for all $j>L$, then

$$\frac{\phi_\ell(k,u)}{\phi_{\ell+1}(k,u)} = \frac{Q_\ell(\frac{1}{\eta})}{Q_{\ell+1}(\frac{1}{\eta})} \qquad \ell \geq L \qquad (3\text{-}70a)$$

The B_L equations may, in fact, be obtained by setting

$$\phi_{L+1}(k,u) = \frac{Q_{L+1}(\frac{1}{\eta})}{Q_L(\frac{1}{\eta})}\phi_L(k,u) \qquad (3\text{-}70b)$$

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[36] The bulk of the results quoted in this section were originally given by Hurwitz and Zweifel, Ibid.

in the spherical harmonics expansion of the Boltzmann Equation, instead of setting $\phi_{L+1} = 0$ as in the P_L approach.

It is also possible to cast the P_L equations in a form similar to that of the B_L equations by replacing the $A_{j\ell}(\eta)$ by $A'_{j\ell}(\eta)$, defined by *

$$A'_{j\ell} = \frac{1}{2}\int_{G_{L+1}} \frac{P_j(\mu)P_\ell(\mu)}{1-\eta\mu}\,d\mu \qquad (3\text{-}71a)$$

The subscript G_{L+1} on the integral indicates that the Gaussian Quadrature formula with $L + 1$ discrete ordinates is to be used in evaluation of the integral. In other words, the P_L equations can be rearranged in the form:

$$\Sigma_t(u)\,\phi_j(k,u) = \sum_{\ell=0}^{L} A'_{j\ell}(\eta)(2\ell+1)\left[J_\ell(k,u) + S_0\delta_{0\ell}\right] \qquad (3\text{-}71b)$$

This procedure gives another, and perhaps clearer, means of viewing the inconsistencies in even L-P_L approximation. First, it is to be noted that the $A'_{j\ell}(\eta)$ satisfy the same recursion relations as the $A_{j\ell}$ so, in effect, the P_L equations may be obtained by replacing A_{00} by A'_{00}. Now, a property of Fourier Transforms is that the transform of a bounded function must go to zero for large k. But, in the $L + 1$ point Gaussian integration scheme where $L + 1$ is odd, $\mu = 0$ is always one of the discrete ordinates chosen; the denominator of the integrand of (3-71a) is always unity at $\mu = 0$ so A'_{00} does not go to zero for large k. This, in turn prevents

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* For a proof see Appendix F.

$\phi_0(k, u)$ from going to zero in this limit, but instead makes it to go to a constant, and introduces delta functions in the spatial variation of the flux. This behavior does not obtain when $L + 1$ is even.

It is interesting to note, however, that in the B_L method there is special merit in dealing with even L approximations. The argument is made with a particular case, but is not limited to it. Rewrite the power series expansion (3-13) for the hydrogen degradation integral, $J_j^H(k, u)$ as

$$J_j^H(k,u) = \sum_{n=0}^{\infty} T_{j0H}^n \frac{\partial^n}{\partial u^n}\left(\Sigma_s^H(u)\phi_j(k,u)\right) \qquad (3\text{-}72)$$

Noting that the most important terms are those with $n = 0$, we have, from Equation (1-54a):

$$T_{00}^0 = 1 \qquad T_{30}^0 = T_{50}^0 = 0$$
$$T_{10}^0 = \frac{2}{3}$$
$$T_{20}^0 = \frac{1}{4} \qquad T_{40}^0 = -\frac{1}{24}$$

and, in general,

$$T_{2l+1,0}^0 = 0 \qquad l \geq 1$$

and

$$T_{2l,0}^0 = \frac{(-)^{l+1}(2l-3)!}{2^{2l-2}(l-2)!\,(l+1)!} \longrightarrow \left(\frac{e}{l}\right)^{3/2} \frac{(-)^{l+1}}{2\sqrt{\pi}}$$

in the limit of large ℓ . For hydrogen $T^{o}_{j\ell}$ with ℓ different from zero need not be considered since scattering is isotropic in C. In general, higher ℓ must be considered but they are usually small compared with the $\ell = 0$ terms. Thus, in going from the B_{L-1} approximation to the B_L approximation for L odd, the extra contributions come only from the derivative terms (n>1) in Equation (3-72) and the improvement is relatively small since the $T^{1}_{j\ell}$ are generally smaller than the $T^{o}_{j\ell}$. In the P_n case, on the other hand, there is an additional improvement in going from the P_{n-1} approximation to the P_n approximation due to the fact that the $A_{j\ell}$ are evaluated by the $n + 1$ point rather than the n-point Gaussian formula.

The smallness of the T^{o}_{LO} contributes to the superiority of the B_L method over the P_L method since in the P_L case one ignores ϕ_{L+1} whereas in the B_L scheme the most important neglected term is $T^{o}_{L+1,0}\,\phi_{L+1}(k, u)$.

Intuitively, one expects the B_L approximation to be superior to the P_L approximation as the latter ignores $\phi_{L+1}(k, u)$ while the former ignores the integrals of $\phi_{L+1}(k, u)$ multiplied by an oscillating function $B^{o}_{L}(u', U)$ [see Equation (1- 49c)].

Considering specifically the P_1 and B_1 approximations,

one notes that the two point Gauss Scheme gives

$$A'_{oo} = \left(1 + \frac{y^2}{3}\right)^{-1} = 1 - \frac{y^2}{3} + \frac{y^4}{9} + \cdots \qquad (3\text{-}73a)$$

where A_{oo} is, as before, given by

$$A_{oo} = y^{-1} \tanh^{-1} y = 1 - \frac{y^2}{3} + \frac{y^4}{5} + \cdots \qquad (3\text{-}73b)$$

so that for small y (small k, and hence large reactors) the two methods become equivalent. In general, the expansions of A_{oo} and A'_{oo} agree to terms of order y^{2L}, which is a consequence of the theorem that integration using the $L + 1$ point Gaussian quadrature is rigorous for any polynomial of degree up to and including $2L + 1$. In particular, both the B_1 and P_1 methods give the age rigorously.

The Age Diffusion, Selengut-Goertzel, and Greuling-Goertzel Inconsistent P1 approximations have analogs in the B_1 approximation. In the absence of sources, Fick's Law may again be obtained by replacing $J_1(k, u)$ by $\Sigma_s(u)\bar{\mu}\,\phi_1(k, u)$, i.e., by retaining only one term of the Taylor Series Expansion of $J_o(k, u)$. However, in this case the diffusion coefficient is found to be:

$$D \rightarrow {}'D' = \frac{1}{3'\Sigma_{tr}'} = \frac{1 - A_{oo}(y)}{y^2\left[A_{oo}(y)\Sigma_t(u) - 3A_{11}(y)\langle\mu\rangle\Sigma_s(u)\right]} \qquad (3\text{-}74a)$$

Note that as $y \to 0$, $'\Sigma_{tr}' \to \Sigma_{tr}$. Expanding $'\Sigma_{tr}'$ in powers of y, one finds

$$'\Sigma_{tr}' = \Sigma_{tr} + \Sigma_s \left(\frac{4}{15} y^2 + \frac{9}{25} y^4 + \cdots \right) \qquad (3-74b)$$

In a similar manner a B_1 Selengut-Goertzel calculation may be set up.

The B_1 adaptations of the inconsistent approximations may be used provided the lethargy expansions that lead to them are valid. On the other hand, the validity of the P_1 versions of these approximations depends not only on the validity of this expansion, but also on errors arising from the approximate evaluation of the $A_{j\ell}(\eta)$. This last mentioned error is large when $(4/15)\Sigma_s(u)y^2$ is large compared to $\Sigma_{tr}(u)$. Thus, for small reactors, the B_1 approximations are considerably superior to their P_1 analogs.

20. The Moments Method[37]

The moments method, originally devised by Fermi for his early work on slowing down in parafin,[38] is equivalent to the P_L method already discussed, although its outward appearance is quite different. The starting point here is the Legendre-analyzed, one-dimensional Boltzmann Equation, which may be obtained by inverting the Fourier

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[37] J.E. Wilkins, Jr., R. Hellens and P.F. Zweifel, PICG P/ (1955).

[38] E. Fermi, Ricerca Scientifica, 7 (2), 13 (1936).

Transformed Equations (3-10a):

$$\Sigma_t(u)\phi_j(z,u) - \frac{j}{2j+1}\frac{\partial \phi_{j-1}(z,u)}{\partial z} - \frac{j+1}{2j+1}\frac{\partial \phi_{j+1}(z,u)}{\partial z} = \sum_i N_i J_j^i(z,u) + S_0 \delta_{0j} \tag{3-75}$$

Instead of taking Fourier Transforms, Equation (3-75) is multiplied by z^n and integrated over all z. The moments of the flux $\phi_{jn}(u)$ are now defined as

$$\varphi_{jn}(u) = \frac{1}{n!}\int_{-\infty}^{\infty} z^n \phi_j(z,u)\,dz = \frac{1}{n!}\int_{-\infty}^{\infty} z^n dz \int_{-1}^{1} d\mu\, \Phi(z,u,\mu) P_j(\mu) \tag{3-76a}$$

and are the j-th Legendre and n-th spatial moments of the angular neutron flux. For the case of a plane unit isotropic source, we obtain, upon taking the spatial moments of Equations (3-75),

$$\Sigma_t^{(u)} \varphi_{jn}(u) = \frac{(j+1)\phi_{j+1,n-1}^{(u)} + j\phi_{j-1,n-1}^{(u)}}{2j+1} + S(u)\delta_{n0}\delta_{j0} + \sum_i N_i J_{jl}^i(u) \tag{3-76b}$$

where the moments of the degradation integral $J_{jn}(u)$ are defined by:

$$J_{jn}^i(u) = \int_{u-\ln\frac{1}{\alpha_i}}^{u} du\; \varphi_{jn}(u')\, B_j(u;U) \tag{3-76c}$$

The set of coupled integral equations arising out of this method is identical to the set previously obtained from the Fourier-Transformed Boltzmann Equation by expansion of the $\phi_j(k, u)$ in power series in k. When coefficients of the various powers of k are equated in those equations, the set of Equations (3-76b) results;

the first few of these are equations (3-19). It was, in fact, shown that [see Equation (3-17c)] the Taylor Series expansion coefficients are identically the moments defined by (3-76a). Hence, the two methods are really only different derivations of the same set of equations.

Clearly, many of the results previously obtained apply to this method. For example, Equation (3-18a) reads:

$$\varphi_{jn} = 0 \qquad \begin{array}{l} \text{if } j+n \text{ is odd} \\ \text{or if } n > j \end{array}$$

The moments method is particularly useful for obtaining the flux at large distances from the source (as is important, for example, in shielding applications). The reason is that for large z, small values of k are most important (Tauberian theorem),[39] and the moments expansion of the flux (3-17a) will converge rapidly for small k. For values of k of importance in most reactor applications, the moments expansion does not converge sufficiently rapidly to $\bar{\phi}_o(k^2)$ for practical application. Of course, for comparison with measurement of the age or of higher flux moments, the moments method is ideal. For comparison with the flux distribution at short and intermediate distances, the moments method is probably about equivalent in difficulty to inversion of the Fourier Transform solutions.

Naturally, the Age Diffusion, Selengut-Goertzel, and Greuling-Goertzel approximations may be adapted for use in the moments method. They are obtained by making approximations to the $J_{jn}(u)$ which parallel those made in the P_1 approach. In view of the exact analogy of the two methods, these approximations will not be developed here.

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[39] N. Weiner, The Fourier Integral and Certain of its Applications. New York: Dover, 1958.

21. Polynomial Approximations

The P_L approximation to the Boltzmann Equation is the one most frequently used and is, historically, the most important, having been developed long before its application to nuclear reactors. Other approximations are, of course, possible and many have been developed. Expansions in Legendre polynomials are chosen most often because of their simple orthogonality relation on the interval of interest and the addition theorem (3-7e) which makes handling of the scattering integral particularly simple. This is not to say that Legendre Polynomials necessarily give the best approximation for a given number of terms in the series. It can, in fact, be shown that Legendre Polynomials give the best approximation in the sense of a least squares fit, that is, the mean square error in the angular distribution of the flux is minimal for a given number of terms when Legendre Polynomials are used. However, the error at an individual point may be very great. We have seen that transport theory does not require continuity of the neutron flux at $\mu = 0$ and that in some cases discontinuities are observed. Yvon's method, covered in Sec. 16 was specially devised to counteract such difficulties.

It can be shown that if the aim of a polynomial approximation is to minimize the maximum error at any μ, the expansion should be carried out in terms of Tchebycheff Polynomials.[40]

[40] W. Conkie, Nuc. Sci. Eng., 6, 260 (1959).

However, in practice, this method suffers so much from the lack of a simple addition theorem that its use must be restricted to problems involving isotropic scattering in the lab system. For this reason, it is unlikely that Tchebycheff Polynomial Approximations will see any great use in the future.

E. Other Approximations to the Boltzmann Equation

22. The S_N Method[41]

We now come to a method which was designed specifically for use on high-speed computers, the so-called S_N procedure. In this method, no attempt is made at obtaining analytical results. Rather, the techniques used are selected so as to minimize the difficulty in solving the Boltzmann Equation numerically, that is, for ease in programming for computer solution. Since analytical results are not sought by this method, calculations utilizing it always employ "group" methods. Thus, it will be sufficient to consider the one-velocity Boltzmann Equation as the starting point; it is to be understood that group methods will generally be used to supply the physical constants required as well as the source term.

The one velocity - one dimension Boltzmann can be written:

$$\Sigma_t(u)\,\phi(z,\mu) + \mu\frac{\partial\phi(z,\mu)}{\partial z} = \int_{-1}^{1}\phi(z,\mu')\Sigma(\mu'\to\mu)\,d\mu' + S(z,\mu) \qquad (3\text{-}77)$$

[41] B. G. Carlson and G. I. Bell, PICG P/2386 (1958).

This equation can be set up for numerical solution once a procedure for evaluating the integral term has been specified. The Gaussian scheme already used is one such method and has advantages that were pointed out earlier. However, as nearly all reactor calculations are currently done by computers, there is some advantage in using a method which sacrifices accuracy for simplicity. That is to say, it may be more economical to use a scheme which requires a greater number of terms for convergence in which the terms are simpler and easier to program.

As a start, the interval $[-1, 1]$ in μ space is divided into N intervals, $[\mu_{i-1}, \mu_i]$, which are generally equal in size but need not be (unequal intervals are rarely employed). Most often, the number of intervals is even; S_2, S_4, S_8, and S_{16} are the most frequently used approximations. Within each sub-interval the variations of the flux is assumed to be linear:

$$\phi(z,\mu) = \left[\frac{\mu - \mu_{i-1}}{\mu_i - \mu_{i-1}} \phi(z,\mu_{i-1}) + \frac{\mu_i - \mu}{\mu_i - \mu_{i-1}} \phi(z,\mu_i) \right] \quad (3\text{-}78a)$$

$$\mu_{i-1} \le \mu \le \mu_i \quad i = 1, 2 \cdots N$$

where μ_i is the end of the i^{th} interval and $\mu_o = -1$. A similar expression may be written for the source if it is anisotropic:

$$S(z,\mu) = \left[\frac{\mu - \mu_{i-1}}{\mu_i - \mu_{i-1}} S(z,\mu_{i-1}) + \frac{\mu_i - \mu}{\mu_i - \mu_{i-1}} S(z,\mu_i) \right] \quad (3\text{-}78b)$$

When these expressions are substituted into (3-77) and the equation integrated from μ_{i-1} to μ_i a set of N coupled equations results:

$$\left[\frac{\mu_i-\mu_{i-1}}{2}\right]\Sigma_t\left[\phi(z,\mu_i)+\phi(z,\mu_{i-1})\right]+\left[\frac{\mu_i-\mu_{i-1}}{6}\right]\left[(2\mu_i+\mu_{i-1})\frac{\partial}{\partial z}\phi(z,\mu_i)\right.$$
$$\left.+(\mu_i+2\mu_{i-1})\frac{\partial}{\partial z}\phi(z,\mu_{i-1})\right]=\sum_{j=1}^{N}\int_{\mu_{j-1}}^{\mu_j}d\mu'\,\phi(z,\mu')\int_{\mu_{i-1}}^{\mu_i}d\mu\,\Sigma(\mu'\to\mu)+\frac{(\mu_i-\mu_{i-1})}{2}\left[S(z,\mu_i)\right.$$
$$\left.+S(z,\mu_{i-1})\right] \qquad (3\text{-}79a)$$

Explicit expressions for the scattering-in term are obtained if one applies the trapezoid rule to the μ' integral; $F(\mu' \to \mu)$ is then approximated by expansions of the form (3-78) on both the μ and μ' variables and ϕ is approximated as above. As this leads to rather complicated algebraic expressions without adding a great deal to the development, we shall consider, for convenience, the case of isotropic scattering in the laboratory system.* Then

$$F(\mu' \to \mu) = 1/2$$

and Equation (3-79a) becomes

$$\Sigma_t\left[\phi(z,\mu_i)+\phi(z,\mu_{i-1})\right]+\frac{(2\mu_i-\mu_{i-1})}{3}\frac{\partial\phi(z,\mu_i)}{\partial z}+\frac{(\mu_i+2\mu_{i-1})}{3}\frac{\partial\phi(z,\mu_{i-1})}{\partial z}$$
$$=\frac{1}{2}\sum_{j=1}^{N}(\mu_j-\mu_{j-1})\left[\phi(z,\mu_j)+\phi(z,\mu_{j-1})\right]+\left[S(z,\mu_i)+S(z,\mu_{i-1})\right] \qquad (3\text{-}79b)$$

Equations (3-79b) for a set of N coupled ordinary differential equations; there are, however, (N + 1) μ_i ; hence, one more equation involving the $\phi(z, \mu_i)$ is required. Such an equation is obtained by setting $\mu = -1$ in Equation (3-77)

$$\Sigma_t\,\phi(z,-1)-\frac{\partial}{\partial z}\phi(z,-1)=\frac{1}{4}\sum_{j=1}^{N}(\mu_j-\mu_{j-1})\left[\phi(z,\mu_{j-1})+\phi(z,\mu_j)\right]+S(z,-1) \qquad (3\text{-}79c)$$

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* Most currently used SN Codes to not allow for an isotropic scattering. A few, however, replace Σ_t by Σ_{tr} , a trick which accounts for anisotropic scatter in the same way as diffusion theory.

This then completes the set of S_N equations. Evidently, the solution is not complete until boundary conditions are specified. From the correct boundary condition

$$\phi(R_S , \mu) = 0 \qquad (3\text{-}80a)$$

for R_S on the boundary and direction μ pointing in from the boundary, it is clear that a satisfactory proper boundary condition is

$$\phi(R_S , \mu_i) = 0 \qquad (3\text{-}80b)$$

for all μ_i pointing in from the boundary. Also, of course, one must insist on $\phi(z, \mu_i)$ being continuous (except possibly for $\mu_i = 0$) everywhere inside the reactor. Schemes for adapting the S_N method to other geometries have been given and are frequently useful but space does not permit their inclusion here.[42]

A number of one-speed neutron transport test problems were solved by Carlson.[43] Clearly the accuracy of a given S_N calculation will depend on flux anisotropy and hence on reactor dimensions, but it was found that for systems approximately the size of existing reactors, the S_4 method gives the criticality to within about one per cent of that obtained by nearly exact variational calculations. Since one generally does not care to calculate k_{eff} to an accuracy better than this (due to uncertainties in cross sections and in reactor composition) Carlson recommends the S_4 method for general calculational purposes. Higher order S_N procedures are generally reserved for specialized problems.

[42] B. Duane, The DSN Programs

[43] B. Carlson, op. cit.

Carlson further states that the accuracy of the S_2 method is comparable to that of the P_3 method and that of the S_4 method to that of the P_5 method in one speed transport problems. These statements were based on test problems in which it was found that the P_L approximations usually yielded values lower than the exact results.

F. Statistical Methods

23. Monte Carlo[44]

All of the methods discussed up to now are schemes for solving slowing down problems by means of some approximation to the Boltzmann Equation. Here, we give a brief outline of methods which are frequently used but which are based on the fact that, after all, the physical processes occurring in a reactor are probabilistic in nature.

In all of the previous work in this book several implicit statistical assumptions were made. In treating the neutron density,

$$n(\underline{r}, E, \underline{\Omega}) = \frac{\Phi(\underline{r}, E, \underline{\Omega})}{v}$$

it was assumed that at criticality a steady state existed such that a time independent neutron density could be assigned to every $\underline{r}$, E, and $\underline{\Omega}$. Actually, even in a critical reactor the neutron density fluctuates somewhat about the average value; in reality we have described only the behavior of the average neutron density. Use is made of this fact in the first method given, the Monte Carlo method, so-called because of its dependence on chance events.

[44] An excellent description of the principles of this method as well as some of the techniques employed in shortening the computation and improving convergence are to be found in an article by G. Goertzel and M. Kalos in Progress in Nuclear Energy, Vol. I, New York: Pergamon Press, 1956. A further list of references is also found there.

Instead of attempting to study the statistical behavior of large numbers of neutrons directly, as use of the Boltzmann Equation implies, we shall study the behavior of individual neutrons and obtain the individual characteristics; their energies, positions, and directions of travel. These properties may then be averaged over many "histories" (neutrons). For statistical reliability, one must study and average the required properties over many neutrons histories; naturally, this is possible only on a large computer. Perhaps the method can best be illustrated by a simple example (not connected with slowing down), the determination of the diffusion length. For further simplification, plane geometry will be chosen.

Suppose a neutron emanates from a plane isotropic source at $z = 0$. The probability of its being emitted in a direction $\theta = \cos^{-1}\mu$ relative to the z axis is

$$P(\mu)\,d\mu = \frac{d\mu}{2} = \frac{\sin\theta}{2}\,d\theta \qquad (3\text{-}81a)$$

To insure that after large numbers of neutrons have been considered, they will have this distribution, use may be made of random numbers. A new variable y is introduced whose distribution $Q(y)$ is related to $P(\mu)$ by

$$Q(y)\,dy = P(\mu)\,d\mu \qquad (3\text{-}81b)$$

In order to facilitate recourse to random numbers, it is necessary to have y randomly distributed, or mathematically:

$$Q(y) = 1 \qquad 0 \leq y \leq 1 \tag{3-81c}$$

for y may then be selected from a set of random numbers between zero and unity. Clearly, this can be only if

$$dy = P(\mu)\, d\mu \tag{3-81d}$$

or, on integrating, one may write

$$y = \int_{-1}^{\mu} P(\mu')\, d\mu' = \frac{\mu+1}{2} \tag{3-81e}$$

Then, having chosen a random number for y, one obtains the required value of μ by inverting Equation (3-81e)

$$\mu = 2y + 1 \tag{3-81f}$$

Having this, one then wants to know how far the neutron travels before experiencing a collision; this is easily done by applying the above technique to the distribution for path lengths:

$$P(r)\, dr = e^{-\Sigma r} \Sigma dr \tag{3-81g}$$

The question of whether the collision is a scattering or an absorption is answered by choosing a third random number. If this number is less than Σ_a/Σ_t the collision is assumed an absorption; if not, the collision is taken to be a scattering. Proceeding in this manner, one may use random numbers to decide: (1) with what type of nucleus

the collision takes place, and (2) if the collision is a scattering, the new direction of motion. By repeating this process for each flight, always recording its position, the neutron may be followed until it is absorbed. At this point the distance z from the source may be computed and squared. By averaging this value over many such histories, one can obtain a value for L^2.

This scheme is called "straight" or "analog" Monte Carlo. While it is a valid procedure, a considerable amount of computation is required in order to obtain sufficient histories for statistically reliable results. Statistical theory predicts that the relative error should be inversely proportional to the square root of the number of histories so that approximately 10,000 histories are required for one per cent accuracy. Many improvements to this basic scheme have been suggested. Generally, they achieve better accuracy for a given amount of computation by changing the relative probabilities of certain events and then compensating for this by wieghting the neutron histories accordingly when averages are taken. As a discussion of these techniques would require a chapter by itself, it is not given here. Instead, the reader is referred to the review article by Goertzel and Kalos quoted in footnote 44 where a complete set of references may be found.

This method is generally used to best advantage in solving problems that are difficult to solve analytically, such as those involving heterogeneous media or rapidly varying cross sections. Due to their

nature, Monte Carlo problems of any difficulty require large digital computers and even then they frequently require large amounts of machine time. This is one of the major drawbacks in the method, others being the lack of generalized results that enable one to apply the results of one calculation to other problems and the inability to obtain results as functions of parameters without extremely large expenditures of computer time.

24. Stochastic Process Methods

In the previous section a description of the processes undergone by individual neutrons was given in which the process of neutron diffusion was represented as being quite similar to diffusion of other types of particles and to Brownian Motion. A general theory has been developed to treat such problems which involve stochastic processes, i.e., those governed by probabilistic considerations.[45] As this method is almost entirely unrelated to those preceding it here, only a brief introduction to the method may be attempted here. Readers interested in this approach will find considerable material in the references already given[45] and in the work of Doob.[46]

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45 An excellent review article by S. Chandrasekhar, Revs. Mod. Phys., 15, 1, (1943), reprinted in Noise and Stochastic Processes, N. Wax, ed., New York: Dover, 1954, is available. Also of particular value is the work of M. C. Wang and G. E. Uhlenbeck, Revs. Mod. Phys., 17, 323 (1945) also reprinted in the above. The first application of this method to neutron problems was made by C. N. Klahr, Nuc. Sci. Eng., 3, 269 (1958).

46 J. Doob, Stochastic Processes, New York: Wiley, 1953.

First of all, one notes that neutron slowing down and diffusion is a Markoff Process, that is, a neutron's future may be predicted from a knowledge of its present state without referring to its past history. This allows the application of Markoff's Method to the problems.

Secondly, all calculations of this nature necessarily involve time dependence; the method strictly applies only to the calculation of the space energy coordinates of a neutron with increasing time. Thus, the attack will have to be that of solving the problem for a pulsed (delta function in time) source and then to treat this solution as a Green's Function for any time dependent, e.g., a constant, source.

For a Markoff Process, one can write the Smoluchowski Equation:

$$P(\underline{R},t) = \int P(\underline{R}-\Delta\underline{R},t-\Delta t)\,\rho(\underline{R}-\Delta\underline{R},\Delta\underline{R},t) + S(R,t) \qquad (3\text{-}82)$$

Here $P(\underline{R}, t)\, d\underline{R}$ is the probability that a neutron will be in the phase space volume element $d\underline{R}$ ($= d^3r\, d\,\underline{\Omega}\, du$) at $\underline{R}$ ($= \underline{r}, \underline{\Omega}, u$) at time t after having been emitted from an isotropic source at the origin at $t = 0$ and $\rho(\underline{R}, \Delta\underline{R}, \Delta t)$ is the probability that a neutron at $\underline{R}$ will suffer displacement $\Delta\underline{R}$ in time Δt. The major part of the task is that of finding the displacement function $\rho(\underline{R}, \Delta\underline{R}, \Delta t)$.

To this attempt, Markoff's method may be applied. The essence of this method if the following (not derived here for reasons of space), quoted from the work of Chandrasekhar.* If $\tau(\Delta\underline{R}_i)\, d\Delta\underline{R}_i$ is the

*See footnote 42.

probability that the i^{th} flight will lie in the volume element $d\Delta\underline{R}_i$ about $\underline{R}_i$, and if all flights have this same distribution, the N flight distribution function $W_N(\underline{R})\, d\underline{R}$, i.e., the probability that a neutron will lie in volume element $d\underline{R}$ at $\underline{R}$ after N flights, may be calculated as follows:

First, take the multi-dimensional Fourier Transform of $\tau(\underline{R})$:

$$A(\underline{\rho}) = \int_{\text{all } \underline{R}} e^{i\underline{\rho}\cdot\Delta\underline{R}}\, \tau(\Delta\underline{R})\, d\Delta\underline{R} \qquad (3\text{-}83a)$$

Then take the n^{th} power of $A(\underline{\rho})$ and invert the Fourier Transform

$$W_N(\Delta\underline{R}) = \frac{1}{(2\pi)^n}\int_{\text{all } \underline{\rho}} e^{-i\underline{\rho}\cdot\Delta\underline{R}}\, [A(\underline{\rho})]^N d\underline{\rho} \qquad (3\text{-}83b)$$

For the limit of very large N, one may find $[A(\underline{\rho})]^N$ approximately by expanding $e^{i\underline{\rho}\cdot\Delta\underline{R}}$ in the integral defining $A(\underline{\rho})$ and keep only the first three terms. One then has:

$$[A(\underline{\rho})]^N \approx \left[1 + i\sum_{j=1}^{n}\langle\Delta x_j\rangle\rho_j - \frac{1}{2}\sum_{j,k=1}^{n}\langle\Delta x_j\Delta x_k\rangle\rho_j\rho_k\right]^N$$

$$\approx \exp\left\{iN\sum_{j=1}^{n}\langle\Delta x_j\rangle\rho_j - \frac{N}{2}\sum_{j,k=1}^{n}\langle\Delta x_j\Delta x_k\rangle\rho_j\rho_k\right. \qquad (3\text{-}83c)$$

where the averages $\langle\Delta x_j\Delta x_k\rangle$ are defined by

$$A_i = \langle\Delta x_i\rangle = \int\Delta x_i\,\tau(\Delta\underline{R})\, d\Delta\underline{R}$$

$$B_{jk} = \langle\Delta x_j\,\Delta x_k\rangle = \int\Delta x_j\,\Delta x_k\,\tau(\Delta\underline{R})\, d\Delta\underline{R} \qquad (3\text{-}83d)$$

Now, taking the inverse transform of Equation (3-83c) one obtains a Gaussian Distribution for $W_N(\underline{R})$

$$W_N(\underline{R}) = \prod_{i=1}^{n} \frac{1}{2\pi N \langle \Delta X_i^2 \rangle} e^{-\langle \Delta X_i \rangle^2 / 2N \langle \Delta X_i^2 \rangle} \qquad (3\text{-}83e)$$

provided one neglects the average of products $\langle \Delta x_j \, \Delta x_k \rangle$.* If one now assumes that neutrons make many collisions while suffering small changes in position, lethargy, or direction, $W_N(\underline{R})$ as given by Equation (3-83e) may be taken as the required function $\rho(\underline{R}, \Delta\underline{R}, \Delta t)$.

The assumption that only small changes in a neutron's coordinates occur in a small time interval is rather severe and implies that slowing down in light elements cannot be properly treated by this method, since light moderators lead to large lethargy changes; also, the angular variation of the neutron density should not be given correctly by the method as a neutron always suffers large angular changes in any collision. Equation (3-83e) may be cast into a more convenient form if one defines m as the mean number of collisions a neutron suffers per unit time (approximtely $v\Sigma_t$) so that

$$N = m\Delta t$$

and Equation (3-83c) becomes

$$\rho(\underline{R}, \Delta\underline{R}, \Delta t) = \prod_{i=1}^{N} \frac{1}{2\pi m \Delta t \langle \Delta X_i^2 \rangle} e^{-\langle \Delta X_i \rangle^2 / 2m\Delta t \langle \Delta X_i^2 \rangle} \qquad (3\text{-}83f)$$

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* These terms may readily be included but are omitted to make the development somewhat neater.

Now, upon substituting Equation (3-83f) into the Smoluchowski Equation (3-82) and expanding $p(\underline{R} - \Delta\underline{r}, \underline{R}, t - \Delta t)$ in a Taylor Series about $\underline{R}$ and $\underline{t}$, keeping only second derivative terms, one obtains the Fokker-Planck equation.

$$\frac{\partial p}{\partial t} = \sum_i \left[-\frac{\partial}{\partial x_i}\left[m\langle \Delta x_i \rangle p\right] + \frac{1}{2}\frac{\partial^2}{\partial x_i^2}\left[m\langle \Delta x_i^2 \rangle p\right]\right] + S \qquad (3\text{-}84\,a)$$

It may be noted here that if the cross product averages $\langle \Delta x_i \, \Delta x_j \rangle$ had not been neglected, we would have arrived at the more general equation:

$$\frac{\partial p}{\partial t} = \sum_i \frac{\partial}{\partial x_i}\left[m\langle \Delta x_i \rangle p\right] + \sum_{i,j} \frac{\partial^2}{\partial x_i \partial x_j}\left[m\langle \Delta x_i \, \Delta x_j \rangle p\right] + S \qquad (3\text{-}84\,b)$$

Equation (3-84b) is the basic equation of the stochastic process method.

As an example, we shall neglect the angular variables. Now we define

$$\frac{1}{6} m\langle r^2 \rangle = \frac{1}{2} m\langle \Delta x^2 \rangle = \frac{1}{2} m\langle \Delta y^2 \rangle = \frac{1}{2} m\langle \Delta z^2 \rangle = D \qquad (3\text{-}85\,a)$$

and

$$\langle u^2 \rangle = \gamma \qquad (3\text{-}85\,b)$$

We have previously defined

$$\langle u \rangle = \xi \qquad (3\text{-}85\,c)$$

As defined above, D will be found to be the previously defined diffusion coefficient divided by v. Treating only the case of one space dimension and ignoring, somewhat inconsistently $\langle \Delta u \, \Delta x \rangle$, we arrive

at the equation

$$\frac{\partial p}{\partial t} = -m\xi \frac{\partial p}{\partial u_1} + \frac{m\gamma}{2} \frac{\partial^2 p}{\partial u^2} + D\frac{\partial^2 p}{\partial x^2} + \delta(u)\delta(x)\delta(t) \qquad (3\text{-}86)$$

for a pulsed monoenergetic plane source of neutrons. It is interesting to note that Equation (3-86) is just the time-dependent age-diffusion equation without absorption if $\gamma = 0$, since $m = \Sigma_s v$. In this manner the Age-Diffusion equation has been derived from a completely different approach which makes some of the assumptions implicit in it more comprehensible. In particular, the statements that Age Diffusion theory implies small lethargy changes in collisions and small flights between collisions have been validated in a manner which shows the nature of the approximation more explicitly.

Differences between the Age-Diffusion equation and Equation (3-86) are readily pointed out. The results given here are not derived but are quoted from Klahr.[47] Solving Equation (3-86) one has

$$p(x, u, t) = \frac{1}{2\pi t}\sqrt{\frac{1}{\gamma D m}}\, e^{-\left[\frac{x^2}{4Dt} + \frac{\xi^2}{\gamma m t}\left(\frac{u}{\xi} - mt\right)\right]} \qquad (3\text{-}87a)$$

Integration of this result in time yields the solution for a steady state source

$$p(x, u) = \int_0^\infty p(x, u, t)\, dt = \frac{1}{2\pi}\sqrt{\frac{1}{\gamma D m}}\, e^{\xi u/\gamma}\, K_0\left[\frac{\xi}{\gamma}\left(\frac{\gamma m x^2}{2D} + u^2\right)^{1/2}\right] \qquad (3\text{-}87b)$$

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[47] Klahr, op. cit.

where $K_o(x)$ is the modified Bessel Function of the second kind. This result is rather difficult to work with as it stands. It is interesting to note that the Fermi Age kernel is yielded in the limit

$$\frac{m\gamma x^2}{2Du^2} = \frac{x^2/\langle\Delta x^2\rangle}{u^2/\langle\Delta u^2\rangle} << 1 \qquad (3\text{-}87c)$$

for Equation (3-87b) then yields, as expected,

$$m\xi\, p(x,u) = q(x,u) = \frac{1}{\sqrt{4\pi\tau}}\, e^{-x^2/4\tau} \qquad (3\text{-}87d)$$

for the slowing down density. This is precisely what is expected since this limit is that for which Equation (3-86) reduced to the Age-Diffusion equation. Also, we note that for heavy moderators:

$$\langle\Delta u^2\rangle \approx \frac{2\xi}{3} = \frac{4}{3A}$$

$$\langle\Delta x^2\rangle = \frac{2}{\Sigma^2}$$

so that

$$\frac{\langle\Delta u^2\rangle}{\langle\Delta x^2\rangle} = \frac{2}{3}\frac{\Sigma^2}{A}$$

that is, this limit is valid for heavy elements and for large cross sections, i.e., it is valid when age-diffusion theory is valid.

Extensions of this method for use in reactor calculations are being made.[48] This method does not, however, appear to have any significant advantages at the present time over the methods already given.

[48] C. N. Klahr and K. Held, "Stochastic Process Method Calculation of Neutron Flux Spectra," Reports TRG 13-28 TRG 112:QPR7-8 (1959).

G. SMALL SOURCE THEORY

Heterogeneous Method

The final method presented here is one designed specifically for application to heterogeneous systems. As it treats fuel assemblies as line (or point) sources and sinks, it has been named "Small Source Theory" by W. A. Horning[49] who developed it in the United States independently of S. M. Feinberg[50] who devised it in the U.S. S.R. This method, too, has undergone considerable development as a tool for reactor calculations in recent years; hence, only a bare outline of the method can be given here.

As stated above, in a cylindrical system fuel assemblies are assumed line sources and sinkis infinite in the axial direction.* Ignoring epithermal fission, the source strength S_k, i.e., the number of neutrons emitted per second by the k^{th} rod, is related to a_k, the number of absorptions per second in the k^{th} rod by

$$S_k = \eta_k a_k \qquad (3\text{-}88a)$$

where η_k is the number of fast neutrons emitted by the k^{th} rod per thermal neutrons absorbed. Note that this is not necessarily equal to

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[49] W. A. Horning, HW 34021 (Hanford).

[50] S. M. Feinberg, PICG P/669 (1955).

* Neutron leakage in the axial direction is generally treated by diffusion theory.

η, the fuel efficiency previously defined, unless the actual rod size is negligible, i.e., if there is no fast fission.

If $P_T(|\underline{r} - \underline{r}'|)$ is the thermal slowing down density kernel (assumed a displacement kernel) as defined in Chapter I, the slowing down density into the thermal group at point $\underline{r}$ will be

$$S_k \, P_T(|\underline{r}-\underline{r}'|) \approx S_k \frac{e^{-|\underline{r}-\underline{r}'|^2/4\tau}}{4\pi\tau} \qquad (3\text{-}88b)$$

if Age Diffusion theory may be used to describe slowing down. The kernel $P_T(|\underline{r}-\underline{r}'|)$ should be defined with respect to the neutron spectrum emerging from the rods, but the fission spectrum kernel is usually quite accurate enough.

The thermal diffusion kernel $f(\underline{r}, \underline{r}')$ is now introduced and defined as the probability per unit volume at $\underline{r}$ that a neutron thermalized at $\underline{r}'$ will diffuse to $\underline{r}$. For line sources:

$$f(\underline{r},\underline{r}') = \frac{K_0\left(\frac{|\underline{r}-\underline{r}'|}{L}\right)}{2\pi \Sigma_a D} \qquad (3\text{-}88c)$$

is the required kernel in the diffusion approximation. Defining the convolution of the slowing down density and diffusion kernel as

$$F(\underline{r},\underline{r}') = \int_{\underline{r}'} P_T(|\underline{r}''-\underline{r}'|) f(|\underline{r}''-\underline{r}|) \, d^2\underline{r}' \qquad (3\text{-}88d)$$

and noting that each rod absorbes a_k thermal neutrons per second, we can write the thermal flux

$$\phi_T(\underline{r}) = \sum_k \left[s_k F(\underline{r}, \underline{r}_k) - a_k f(\underline{r}, \underline{r}_k) \right]$$

$$= \sum_k a_k \left[\eta_k F(\underline{r}, \underline{r}_k) - f(\underline{r}, \underline{r}_k) \right] \quad (3\text{-}89a)$$

using relation (3-88a). It has been assumed that the effect of the rods on slowing down can be ignored. This method has difficulty in dealing with resonance absorption accurately in a simple way. However, as resonance absorption is usually important, one treats epithermal absorption artificially by assuming that it all takes place at one energy; a relatively simple means of handling resonance capture can then be obtained.

For a point $\underline{r}_n$ on the surface of a rod, say the n^{th}, the distance to the k^{th} rod may be approximated by the distance between centers, except when n = k. For n = k, one has the "distance" to the rod, the radius of the rod ρ_n. Thus

$$\phi_T(\underline{r}_n) \simeq \sum_{n \neq k} a_k \left[\eta_k F(|\underline{r}_n - \underline{r}_k|) - f(|\underline{r}_n - \underline{r}_k|) \right]$$

$$+ a_n \left[\eta_n F(\rho_n) - f(\rho_n) \right] \quad (3\text{-}89b)$$

The essence of the method lies in the assumption that a linear relationship exists between a_n and $\phi(\underline{r}_n)$, i.e., between the absorption in the rod and the flux on the surface.

$$a_n = \frac{1}{\gamma_n} \phi_T(\underline{r}_n) \quad (3\text{-}89c)$$

Then, equating $\phi_T(\underline{R}_n)$ in Equations (3-89b) and (3-89c) one has

$$\gamma_n a_n = \sum_{n \neq k} a_k \left[\eta_k F(|\underline{r}_n - \underline{r}_k|) - f(|\underline{r}_n - \underline{r}_k|) \right] + a_n \left[\eta_n F(\rho_n) - f(\rho_n) \right] \qquad (3\text{-}90a)$$

or, for simplicity we set

$$\alpha_{kn} = \eta_k F(|\underline{r}_n - \underline{r}_k|) - f(|\underline{r}_n - \underline{r}_k|) \qquad k \neq n$$

$$= \eta_n F(\rho_n) - f(\rho_n) \qquad k = n \qquad (3\text{-}90b)$$

to obtain

$$\gamma_n a_n = \sum_k \alpha_{kn} a_k$$

This is a set of homogeneous linear equations in the a_n, there being as many a_n and equations as there are rods in the system. A solution will exist only if the determinant

$$A = \begin{vmatrix} \alpha_{11} - \gamma_1 & \alpha_{12} & \cdots & \\ \alpha_{21} & \alpha_{22} - \gamma_2 & & \\ \vdots & \vdots & \ddots & \\ & & & \alpha_{NN} - \gamma_N \end{vmatrix}$$

is set equal to zero. This is then the critical equation for the system.

It is presumed that L and τ are well known. In a typical calculation one wants to find a combination $\underline{r}_n - \underline{r}_k$, ρ_n, and the number of rods N which makes the system critical. This is clearly possible only if the two parameters η_k and γ_k are known. For the case of

identical rods they need be known for only one rod.

Herein lies the advantage of this method. One need only measure the parameters η and γ for one rod, say in a thermal column, to be able to calculate the critical size of a reactor. It is possible to include resonance absorption, epithermal fission, and any other effect of interest by adding more parameters of this type, although it should again be mentioned that the treatment is generally quite artificial.

Most reactors currently being built do not meet the conditions required for application of the method. Of the many types currently under consideration,, heavy water- or graphite-moderated reactors can be said to definitely fall into this category.

The method is still relatively new and has not been tested too rigorously as yet. Hence, its use is still largely restricted compared with methods previously given.

CHAPTER IV

NUMERICAL SOLUTIONS OF THE BOLTZMANN EQUATION

A. The Multigroup Approach

1. Failure of Analytical Methods

Most of the calculational methods of the first three chapters rested on assumptions which are not generally valid in existing reactors. First, it was assumed that the reactor consists of a single region in which the composition is uniform, or at least periodic with a period small compared to the overall dimensions of the system. In such systems all neutrons leaving the outer surface of the reactor never return, since the systems were assumed to be surrounded by an infinite vacuum. These assumptions led to a rather simple exposition of reactor theory in general and of slowing down in particular, which was useful for pointing out many basic principles. However, from the reactor designer's point of view, the disappearance of the neutrons which leave the reactor leaves fewer behind for maintaining the critical chain reaction. To compensate for the lost neutrons, more neutrons must be produced in the reactor and hence more fuel must be used. As fuel is generally more expensive than moderator, this is a rather uneconomical mode of operation.

If, instead of allowing the neutrons to escape, we provide some means of returning the escaped neutrons to the reactor, i.e., of reflecting them, the fuel requirements of the "core" should be smaller. It can readily be seen that a reflector should be constructed of materials with absorption cross sections as low as possible. Furthermore, since much of the neutron leakage from a reactor will be leakage of fast neutrons and since thermal neutrons are generally more valuable for causing fission, an

additional advantage is gained if the reflector is also a good moderator. Thus, the reflector materials most frequently employed are the common moderators, i.e., hydrogen, deuterium, beryllium, carbon, and/or their compounds.

In fast reactors, the situation is somewhat different. Here, a moderating reflector is frequently a disadvantage; one of the greatest advantages of fast reactors is their ability to breed, which is a direct consequence of the facts that η is higher and absorption cross sections of structural materials are lower for fast neutrons. The fuel loading of fast reactors is generally much larger than that of thermal reactors so that reflection would not be as important as in thermal systems. A better scheme is to surround the system with fertile materials (e.g., U-238 and Th-232) in which neutron capture leads to production of more fuel (here Pu-239 and U-233); thus the breeding ratio may be increased at no penalty to the core. Here, the material surrounding the reactor is generally called a "blanket" rather than a reflector.

It was pointed out in Chapter I that the methods of the first three chapters do not apply to fast reactors. This is a consequence of the fact that whatever moderation is present in fast systems is due to largely to inelastic scattering in structural materials, fuel and coolants (usually liquid metals). Inelastic scattering reduces the energy of the scattered neutrons rather drastically on a single collision and is difficult to describe analytically. Another approach is required if one is to be able to handle such systems.

Finally, the spatial distribution of the flux (and hence the power) in the type of reactor discussed in the first three chapters is

highly peaked near the center of the reactor. This means that more heat is produced there (which is in itself poor from an engineering standpoint) and that the fuel near the center will be depleted more rapidly. Consequently, the limitations of the system, either decrease in reactivity or metallurgical limits, will be reached rather quickly. To overcome this, it is advantageous to "flatten" the flux shape. Reflection tends to aid in this attempt as it replenishes the neutrons near the boundaries, where the flux in a bare reactor is smallest. Further flattening must, however, be accomplished by making the core itself non-uniform.

For reactors in which any of the above difficulties arise (and this includes almost all reactors), one must resort to numerical solutions of the Boltzmann Equation; the Boltzmann Equation will have to be approximated in some way that is convenient for machine computation. This is not to say that the development of the first three chapters is invalid or useless. It, in fact, contains many of the approximations frequently used in numerical reactor calculations. For example, numerical methods usually employ diffusion theory of the P_L approximations, although some of the other methods of Chapter III also find frequent application.

The general approach will be essentially that of using finite difference approximations in treating the space and energy (or lethargy) variations of the flux. For the lethargy, the treatment is very similar to the "one group" approximation applied to thermal neutrons in Chapter I, but is applied to the fast neutron group as well. The major difference is that fast neutrons are not usually treated by one group theory, but

are generally treated as though they possess only a finite number of discrete energies. This is the multigroup approach.

After making the multigroup approximation, finite differences techniques will be applied to the spatial variation of the neutrons in each group. The Boltzmann Equation will then have been reduced to a form suitable for numerical computation.

2. The Adjoint Flux

The concept of an adjoint flux can be quite a useful in reactor physics. Basically, the concept is a mathematical one but the adjoint flux does have a direct physical interpretation. The procedure here will be to define the adjoint flux and derive the equation governing it in a somewhat mathematically abstract manner and then to state its physical significance. As a start, we define the scalar product (Ψ, X) of two functions Ψ and X by

$$(\Psi, X) = \int \Psi X \, d\tau \qquad (4\text{-}1a)$$

where the integration is understood to be taken over the complete range of variables for which the functions are defined; $d\tau$ represents the product of differentials of all variables involved. For example, if Ψ is the neutron flux $\Phi(\underline{r}, u, \underline{\Omega})$, and if X is another function defined over the same range of variables, $\underline{r}$, u and $\underline{\Omega}$, the integration would extend over the reactor (R) in configuration space, over all lethargies from zero to infinity and over all solid angles $\underline{\Omega}$.

Now, if L is a linear operator[1] which, when operating on a function defined over these variables, say X , produces another function defined over the same variables, one can then define the scalar product $(\Psi, L X)$. The operator adjoint to L , denoted by L^+ , may then be defined by the relation

$$(\Psi, L X) = (L^+ \Psi, X) \qquad (4\text{-}1b)$$

i.e., L^+ is the operator which makes (4-1b) hold. Here the boundary condition on the function Ψ will, in general, be different from those on X . These "adjoint" boundary conditions will, for any given case, be chosen along with the operator L^+ , to make Equation (4-1b) hold. In this sense, the boundary condition may be considered to be part of the definition of the operators L and L^+ . As an illustration of an adjoint operator and of how it may be found, we shall take the Boltzmann Equation for a critical reactor, which may be written as:

$$B\,\Phi(\underline{r}, u, \underline{\Omega}) \equiv \underline{\Omega}\cdot\underline{\nabla}\,\Phi(\underline{r}, u, \underline{\Omega}) + \Sigma_t(\underline{r}, u)\,\Phi(\underline{r}, u, \underline{\Omega})$$
$$- \int du' \int d\underline{\Omega}'\; \Phi(\underline{r}, u', \underline{\Omega}')\; \Sigma_s(u' \to u, \underline{\Omega}' \to \underline{\Omega})$$
$$- f(u) \int d\underline{\Omega}' \int du'\; \nu(u')\,\Sigma_f(u')\; \Phi(\underline{r}, u', \underline{\Omega}) = 0 \qquad (4\text{-}2a)$$

where f(u) is the fission spectrum previously defined (see Section 9, Chapter I) and B is, by definition, the Boltzmann operator. The scalar

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[1] That is, it has the property $L(A\Psi + Bx) = AL\Psi + BLX$ for any pair of functions Ψ and X and constants A and B . For the properties of such operators see, for example, R. Courant and D. Hilbert, Methods of Mathematical Physics, Vol.I, Interscience, New York (1953).

product of Equation (4-2a) with $\Psi(\underline{r}, u, \underline{\Omega})$, is now taken (i.e., Equation (4-2a) is multiplied by $\Psi(\underline{r}, u, \underline{\Omega})$ and integrated over the reactor volume, all u and Ω). The operator B^+, which obeys the following equation

$$(B^+ \Psi, \Phi) = (\Psi, B\Phi) = 0 \qquad (4\text{-}2b)$$

is then the adjoint of the Boltzmann operator B.

In particular, Equation (4-2b) will be satisfied if Ψ is a function such that

$$B^+ \Psi = 0 \qquad (4\text{-}2c)$$

and obeys the appropriate boundary conditions which will be discovered later. The solution of this equation will be denoted by $\Phi^+(\underline{r}, u, \underline{\Omega})$ and is called the adjoint flux. We now derive the adjoint operator B^+; in the course of the derivation the correct boundary conditions will be discovered.

Since each operator comprising the Boltzmann operator is itself linear and since linear operators obey the relation

$$(L_1 + L_2)^+ = L_1^+ + L_2^+$$

we may consider each term separately. From Gauss' Theorem we have:

$$\int d\underline{\Omega} \int du \int_R \nabla \cdot \underline{\Omega} (\Phi \Phi^+) d^3r = \int du \int d\Omega \int_S \Phi \Phi^+ \underline{\Omega} \cdot \hat{n} dS \qquad (4\text{-}3a)$$

where S is the surface of the reactor and n is a unit outward normal. If one then applies the boundary condition (which will be seen to be the

correct adjoint boundary condition)

$$\Phi^{+}(\underline{r}, u, \underline{\Omega}) = 0 \quad \text{for} \quad \underline{\Omega}\cdot n > 0 \qquad \underline{r} \text{ on } S \qquad (4\text{-}3b)$$

and remembers the boundary condition:

$$\Phi(\underline{r}, u, \underline{\Omega}) = 0 \quad \text{for} \quad \underline{\Omega}\cdot n < 0 \qquad \underline{r} \text{ on } S \qquad (4\text{-}3c)$$

the right hand side of Equation (4-3a) is seen to be identically zero. Hence, on expanding the left hand side of Equation (4-3a), we have:

$$\int du \int d\underline{\Omega} \int_R d^3r \; \Phi^{+}(\underline{r}, u, \underline{\Omega})\, \underline{\Omega}\cdot\underline{\nabla}\, \Phi(\underline{r}, u, \underline{\Omega}) = -\int du \int d\underline{\Omega} \int d^3r \; \Phi(\underline{r}, u, \underline{\Omega})\, \underline{\Omega}\cdot\underline{\nabla}\, \Phi^{+}(\underline{r}, u, \underline{\Omega}) \qquad (4\text{-}3d)$$

Now, on taking the scalar product of the Boltzmann Equation (4-2a) with $\Phi^{+}(\underline{r}, u, \underline{\Omega})$, the first term is just the left hand side of Equation (4-3d). Hence the adjoint of $\underline{\Omega}\cdot\underline{\nabla}$ is $-\underline{\Omega}\cdot\underline{\nabla}$ (with the adjoint boundary conditions).

The second term obtained by taking the scalar product of Equation (4-2a) with Φ^{+} is

$$\iiint \Phi^{+}(\underline{r}, u, \underline{\Omega})\, \Sigma_t(\underline{r}, u)\, \Phi(\underline{r}, u, \underline{\Omega})\, d^3r\, du\, d\underline{\Omega} \equiv \iiint \Phi(\underline{r}, u, \underline{\Omega})\, \Sigma_t(\underline{r}, u)\, \Phi^{+}(\underline{r}, u, \underline{\Omega})\, d^3r\, du\, d\underline{\Omega} \qquad (4\text{-}4)$$

so that $\Sigma_t(r, u)$ is its own adjoint (i.e., it is <u>self adjoint</u>).

In the third term one has, by changing the names of the variables,

$$\int d^3r \int du \int d\underline{\Omega}\, \Phi^+(\underline{r},u,\underline{\Omega}) \int \Sigma_s(u'\to u,\underline{\Omega}'\to\underline{\Omega})\,\Phi(\underline{r},u',\underline{\Omega}')\,du'\,d\underline{\Omega}' =$$

$$-\int d^3r \int du \int d\underline{\Omega}\, \Phi(\underline{r},u,\underline{\Omega}) \int du' \int d\underline{\Omega}'\, \Sigma_s(u\to u',\underline{\Omega}\to\underline{\Omega}')\,\Phi^+(\underline{r},u',\underline{\Omega}') \qquad (4\text{-}5)$$

so that the adjoint of

$$\int \Sigma_s(u'\to u,\underline{\Omega}'\to\underline{\Omega})^{\circ}\,du'\,d\underline{\Omega}'$$

is*

$$\int \Sigma_s(u\to u',\underline{\Omega}\to\underline{\Omega}')^{\circ}\,du'\,d\underline{\Omega}' \,.$$

The fourth term is also converted in the same manner:

$$-\int d^3r \int d\underline{\Omega} \int du\, f(u)\,\Phi^+(\underline{r},u,\underline{\Omega}) \int du' \int d\underline{\Omega}'\, \nu\Sigma_f(\underline{r},u')\,\Phi(\underline{r},u',\underline{\Omega}') =$$

$$-\int d^3r \int d \int du\, \nu\Sigma_f(\underline{r},u)\,\Phi(\underline{r},u,\underline{\Omega}) \int d\underline{\Omega}' \int du'\, f(u')\,\Phi^+(\underline{r},u',\underline{\Omega}') \qquad (4\text{-}6)$$

so that the adjoint of

$$f(u)\int \nu\Sigma_f(\underline{r},u')^{\circ}\,du'\,d\underline{\Omega}'$$

is

$$\nu\Sigma_f(\underline{r},u)\int f(u')^{\circ}\,du'\,d\underline{\Omega}' \,.$$

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* Here the dot (°) inside the integral denotes that the effect of the operator on a function is obtained by inserting the function in place of the dot.

Combining these results, we have the adjoint Boltzmann Equation:

$$B^{+}\Phi^{+}(\underline{r},u,\underline{\Omega}) = -\underline{\Omega}\cdot\underline{\nabla}\,\Phi^{+}(\underline{r},u,\underline{\Omega}) + \Sigma_t(\underline{r},u)\,\Phi^{+}(\underline{r},u,\underline{\Omega})$$

$$-\int du'\int d\underline{\Omega}'\,\Phi^{+}(\underline{r},u',\underline{\Omega}')\,\Sigma_s(u\to u',\underline{\Omega}'\to\underline{\Omega}) \qquad (4\text{-}7)$$

$$+\nu\Sigma_f(\underline{r},u)\int d\underline{\Omega}'\int du' f(u')\,\Phi^{+}(\underline{r},u',\underline{\Omega}') = 0$$

The condition (4-3b) which is required in order to obtain this equation becomes the boundary condition which must be applied to Equation (4-7).

One may note the "upside down" nature of the adjoint equation. The first term has its sign reversed; the "adjoint neutrons" flow with the gradient of the flux, not against it. From the third term it is seen that "adjoint neutrons" gain energy in collisions whenever they lost energy in the original Boltzmann Equation (and vice versa at thermal energies). Finally, in the last term, the roles of the fission cross section and fission spectrum are reversed, that is, "adjoint neutrons" are absorbed at high energies and produced at thermal energies if the reverse is true in the original Boltzmann Equation. This is a general property of adjoint operators.

A direct physical meaning may be attached to the adjoint angular flux $\Phi^{+}(\underline{r}, u, \underline{\Omega})$; it is given here without proof as the proof is quite long[2]. It may be shown that $\Phi^{+}(\underline{r}, u, \underline{\Omega})$ is proportional to the number of fissions per second in a critical reactor at a much later time, caused by one neutron now at position $\underline{r}$ with lethargy u travelling in direction $\underline{\Omega}$. Hence, when properly normal-

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[2] H. Hurwitz, Jr., KAPL - 98 (1948).

ized*, it is equal to that quantity, and is called the Iterated Fission Probability and denoted by $F(\underline{r}, u, \underline{\Omega})$. Also, because it is a measure of how important a particular neutron is in maintaining the critical chain reaction, it is sometimes normalized differently and called the Importance Function[3].

This interpretation of the adjoint flux leads directly to its use in perturbation theory; from the above definition, one can quickly derive the effect of a small disturbance on a reactor. Thus, if, for example, one were to add an absorbing foil with macroscopic absorption cross section Σ_a to a critical reactor, the foil (considered to be small) would absorb $\Sigma_a(\underline{r}, u)\,\Phi(\underline{r}, u, \underline{\Omega})d^3r'd\underline{\Omega}$ neutrons in d^3r, $d\Omega$ and du per second. Then, if each of neutrons absorbed would eventually have caused F fissions per second to take place, the number of such fissions will be diminished by

$$\int F(\underline{r}, u, \underline{\Omega})\,\Sigma_a(\underline{r}, u)\,\Phi(\underline{r}, u, \underline{\Omega})\,d^3r\,du\,d\underline{\Omega}$$

Due to the normalization of F (see footnote on this page) this represents the fractional decrease in fissions at a later time due to the disturbance, i.e., it is the decrease in the multiplication factor.

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* The normalization is

$$f(\underline{r}, u, \underline{\Omega}) = \frac{\Phi^+(\underline{r}, u, \underline{\Omega}) \int \Sigma_f(\underline{r}', u')\,\Phi(\underline{r}', u', \underline{\Omega}')\,d\underline{r}'\,du'\,d\underline{\Omega}'}{\nu \int d^3r' \int \Sigma_f(\underline{r}', u')\,\Phi(\underline{r}', u', \underline{\Omega}')\,du'\,d\underline{\Omega}' \int \Phi^+(\underline{r}', u'', \underline{\Omega}'')\,f(u')\,du''\,d\underline{\Omega}''}$$

[3] The use of the adjoint flux in reactor theory is originally due to E.P. Wigner.

Similar arguments with respect to other types of perturbations lead to the usual perturbation theory formulae. Other derivations[4] rely on the mathematical properties of adjoint functions, and lead, as expected, to the same results.

3. Properties of the Adjoint Flux

Thus far, we have derived the equation adjoint to the Boltzmann Equation. However, as the earlier chapters have shown, reactor calculations always employ some approximation to the Boltzmann Equation. It is to be expected then that actual calculations of the adjoint flux will similarly employ approximations to the Adjoint Boltzmann Equation. A cursory look at Equation (4-7) will reveal that its structure is much the same as that of the Boltzmann Equation, so that procedures identical to those used for obtaining approximations to the Boltzmann Equation may be employed in obtaining workable approximations. An alternate approach is, of course, to derive the adjoint equations for a given approximation directly in a manner similar to that used above. In particular, the adjoints of matrix operators will be required in the multigroup approach. In fact, we have already employed a matrix operator in a somewhat concealed form when the P_L equations were written. That as, the P_L equations might have been written

$$\| P \| \, |\Phi| = 0$$

where $|\Phi|$ is a flux vector*:

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[4] See, for example, Weinberg and Wigner, op. cit., Chapter XVI.

* Vector in the sense of an L x 1 matrix.

$$|\phi| = \begin{pmatrix} \phi_0 \\ \vdots \\ \phi_L \end{pmatrix}$$

and $\|P\|$ is the matrix operator

$$\|P\| = \begin{pmatrix} \Sigma_t - \int \Sigma_{s_0}(u' \to u)\, du - \nu f \int \Sigma_f(u')\, du & \frac{\partial}{\partial z} & 0 & 0 & \cdots \\ \frac{1}{3}\frac{\partial}{\partial z} & \Sigma_t - \int \Sigma_{s_1}(u' \to u)\, du' & \frac{2}{3}\frac{\partial}{\partial z} & 0 & \cdots \\ 0 & \vdots & \vdots & & \end{pmatrix}$$

As finite difference techniques will be applied to the lethargy and spatial variables in the present chapter, the continuous operators with respect to these variables will be replaced by approximating matrix equivalents. Hence we shall require the extension of the concepts of scalar product and "adjointness" to matrices.

The scalar product of two vectors is, in N dimensions

$$(\chi, \psi) = |\chi|^+ |\psi| = \sum_{L=1}^{N} \chi_L^+ \psi_L$$

where the adjoint matrix X^+ is, in this case, simply the transposed matrix. Should the elements of these vectors be continuous functions of another variable (e.g., the ϕ_j are functions of $\underline{r}$ and u in the above example) integration over the appropriate range of those variables is also to be implied. The adjoint of a matrix operator is obtained by transposing the matrix and taking the adjoint of any operator appearing as an element of the matrix, e.g.,

$$\|P\|^{+} = \begin{pmatrix} \Sigma_t - \int \Sigma_{s_0}(u \to u')^{\circ} du' - \nu\Sigma_f \int f(u')^{\circ} du' & \frac{1}{3}\frac{\partial}{\partial z} & 0 & 0 \\ -\frac{\partial}{\partial z} & \Sigma_t - \int \Sigma_{s_1}(u \to u')^{\circ} du' & -\frac{2}{3}\frac{\partial}{\partial z} & \\ 0 & & & \end{pmatrix}$$

The use of adjoint operators and functions can aid materially in solving certain classes of problems. By way of illustration, suppose one wishes to find the multiplication constant k of a reactor but is not particularly desirous of obtaining accurate flux shapes.

To begin with, the multiplication constant, which does not appear in the Boltzmann Equation per se, must be introduced artificially in some manner. The usual scheme for doing this is to note that k must be proportional to ν, the mean number of neutrons per fission. Although ν is a natural constant, we may treat it as an eigenvalue, i.e., a constant to be determined by the calculation. Then we may set

$$\nu' = \frac{\nu}{k} \qquad (4\text{-}8a)$$

where ν' is the eigenvalue determined by the Boltzmann Equation. (It is the value which ν would have to take to make a non-critical reactor critical.) Then the Boltzmann Equation may be written

$$\underline{\Omega} \cdot \underline{\nabla} \Phi + \Sigma_t \Phi = \int \Sigma_s (u' \to u, \underline{\Omega}' \to \underline{\Omega}) \Phi(\underline{r}, u', \underline{\Omega}') du' d\Omega' = \nu' f(u') \int \Sigma_f \Phi du' d\Omega' \qquad (4\text{-}8b)$$

Now if the flux Φ were known, one could determine ν' by dividing Equation (4-8b) by $f\int \Sigma_f \Phi du' d\underline{\Omega}'$ and inserting the flux. This, however, is certainly equivalent to solving the complete Boltzmann Equation and

is generally quite impractical. For the sake of brevity, we shall rewrite Equation (4-8b) in abstract operator form as

$$\mathcal{L}\,\Phi = \nu' \mathcal{R}\,\Phi \qquad (4\text{-}8c)$$

where $\mathcal{L}$ and $\mathcal{R}$ represent the operators on the left and right hand sides of Equation (4-8b) respectively. The adjoint equation could similarly be written

$$\mathcal{L}^+ \Phi^+ = \nu' \mathcal{R}^+ \Phi^+ \qquad (4\text{-}8d)$$

where we have explicitly used the fact that operators with real eigenvalues have the same eigenvalues as their adjoints. Now the scalar product of Equation (4-8c) with Φ^+ yields

$$\nu' = \frac{(\Phi^+,\ \mathcal{L}\Phi)}{(\Phi^+,\ \mathcal{R}\Phi)} \qquad (4\text{-}8e)$$

The advantage in using Equation (4-8e) to calculate ν' is that it is a variational expression. That is, the error in ν' is proportional to the product of the errors in Φ and Φ^+, a result which is readily proved as follows.

Let us use "trial functions" Φ_t and Φ_t^+ which are guesses at the true values of the flux and its adjoint:

$$\Phi_t = \Phi + \delta\Phi$$
$$\Phi_t^+ = \Phi^+ + \delta\Phi^+ \qquad (4\text{-}9a)$$

and insert them into Equation (4-8b) in an attempt to calculate ν'. The resulting value of ν' is denoted by

$$\nu_t = \nu' + \delta\nu' \qquad (4\text{-}9a)$$

where the δ quantities represent the deviations from the correct values of the quantities. Substituting these into Equation (4-8e),

$$(\nu' + \delta\nu')(\Phi^+ + \delta\Phi^+, \mathcal{R}[\Phi + \delta\Phi]) = (\Phi^+ + \delta\Phi^+, \mathcal{L}[\Phi + \delta\Phi]) \qquad (4\text{-}9b)$$

or, expanding:

$$(\nu' + \delta\nu')[(\Phi^+, \mathcal{R}\Phi) + (\delta\Phi^+, \mathcal{R}\Phi) + (\Phi^+, \mathcal{R}\delta\Phi) + (\delta\Phi^+, \mathcal{R}\delta\Phi)] =$$

$$(\Phi^+, \mathcal{L}\Phi) + (\delta\Phi^+, \mathcal{L}\Phi) + (\Phi^+, \mathcal{L}\delta\Phi) + (\delta\Phi^+, \mathcal{L}\delta\Phi) \qquad (4\text{-}9c)$$

But, from Equation (4-8c) we have

$$\mathcal{L}\Phi = \nu'\mathcal{R}\Phi$$

while, from the properties of adjoint operators and Equation (4-8d) one has

$$(\Phi^+, \mathcal{L}\delta\Phi) = (\mathcal{L}^+\Phi^+, \delta\Phi) = \nu'(\mathcal{R}^+\Phi^+, \delta\Phi) = \nu'(\Phi^+, \mathcal{R}\delta\Phi).$$

So that Equation (4-9c) becomes, after elimination of equal terms on the left and right hand sides:

$$\delta\upsilon'\left[(\Phi^+, \mathcal{R}\Phi)+(\delta\Phi^+, \mathcal{R}\Phi)+(\Phi^+, \mathcal{R}\delta\Phi)+(\delta\Phi^+, \mathcal{R}\delta\Phi)\right]=$$

$$(\delta\Phi^+, \mathcal{L}\delta\Phi) - \upsilon'(\delta\Phi^+, \mathcal{R}\delta\Phi) \qquad (4\text{-}9d)$$

from which it is clear that the error in the eigenvalue, $\delta\nu'$, is proportional to the products of the errors in Φ and Φ^+ , i.e., Equation (4-8e) is a variational expression for ν' .

It is just this property which makes perturbation theory so powerful. One can be certain of an accurate value of the multiplication constant so long as any sort of reasonable guess at the flux is obtainable. In perturbation theory, for example, one assumes that the flux in a reactor differing only slightly from an existing one is that of the existing one, and is able to calculate reactivity differences with a rather high degree of accuracy.

The advantages of using Equation (4-8e) in reactor calculations should now be apparent, but will be discussed in detail later. Again the reader is reminded that expressions of the type (4-8e) are available in any calculational model.

4. The Multigroup Equations

Clearly, numerical procedures can be applied to any neutron transport problem and, indeed, computer solutions for almost every quantity of interest in reactor calculations have been obtained. Here, however, we will restrict our interest to criticality problems, that is, to time independent problems. This is not to say that these calculations can be applied only to the problem of calculating which configura-

tions will make a reactor critical. Frequently, the reactor designer wants to know how much excess reactivity defined as $[(k_{eff}-1)/k_{eff} = \rho]$ is built into a reactor in order that he may be able to insure that the effects of temperature feedback, fission product poisoning, and fuel burnup can be overcome and that the control rods can safely shut the reactor down. Such problems may be solved without resort to the time-dependent Boltzmann Equation in the following manner.

Consider a supercritical reactor $(k_{eff} > 1)$. On the average, each neutron in a given generation gives rise to k_{eff} neutrons in the next generation, according to the definition of the criticality factor. A steady state neutron flux cannot exist within the reactor unless $k_{eff} = 1$. If, however, one is not interested in the actual time behavior of the system but wants only to know k_{eff}, possibly for the reasons mentioned above, it is not necessary to solve the time dependent problem. Instead, one frequently allows ν to be an eigenvalue in the manner previously described and

$$k_{eff} = \frac{\nu}{\nu'} \qquad (4\text{-}10)$$

A note of caution should be injected here. As defined in this manner, the effective multiplication factor leads to the so-called static reactivity. It is not, however, the reactivity which is to be used in solving problems in reactor kinetics, which is the dynamic reactivity. The difference arises out of the facts that the effective delayed neutron fraction depends on the time behavior of the system and the delayed neutrons have a different energy spectrum from that of

the prompt neutrons.[5] The difference is, however, generally quite small.

Because multigroup calculations are expensive, they are rarely carried out for any but the simplest approximations for the Boltzmann Equation. Generally, diffusion theory is used for criticality calculations, but other P_L and L approximations and the S_N approximation are frequently used for specialized calculations. The current knowledge of many cross sections does not generally warrant use of high order approximations, so that the development will be carried out only for the P_1 approximation.

To start with, the thermal neutron group will be treated exactly as in Chapter I, i.e., all neutrons with energies below E_T are taken as a single group. It is possible to apply multigroup procedures within the thermal group itself[6], but this is outside the range of a work on slowing down. The problem of upscattering, that is, of a neutron's gaining energy in a collision, which arises in the treatment of thermal neutr complicates the problem somewhat and will not be treated here. Furthermore, the thermal group is almost always treated by diffusion theory. In a non-uniform reactor one can write

$$\underline{J}_T(\underline{r}) = -D_T(\underline{r})\nabla\phi_T(\underline{r})$$

where the diffusion coefficient is now position dependent. Thus, the

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5 E.E. Gross and J.H. Marable, Nuc. Sci. Eng., 7, 281 (1960).

6 The techniques employed in setting up the multigroup thermal equations are quite similar to the methods used here. The techniques, for solution are, however, slightly modified. See E. M. Gelbard.

thermal group equation becomes:

$$-\nabla \cdot D_T(\underline{r}) \underline{\nabla} \phi_T(\underline{r}) + \Sigma_{aT}(\underline{r}) \phi_T(\underline{r}) = g_T(\underline{r}) \qquad (4\text{-}11)$$

the symbols have been previously defined in Chapter I. Some discussion of the methods of obtaining the thermal group constants D_T and Σ_{aT} has been given in Chapter I; a more intensive discussion will be given later in this chapter (see Section 9).

For fast neutrons, we begin by writing the P_1 equations, which have been obtained in both Chapters I and III. In general they may be written:

$$\Sigma_t(\underline{r},u)\,\underline{\phi}_0(\underline{r},u) + \underline{\nabla} \cdot \underline{\phi}_1(\underline{r},u) = \int \Sigma_{s_0}(u' \to u)\,\phi_0(\underline{r},u')\,du' + S(\underline{r},u) \qquad (4\text{-}12a)$$

and

$$\Sigma_t(\underline{r},u)\,\underline{\phi}_1(\underline{r},u) + \tfrac{1}{3}\,\underline{\nabla}\,\phi_0(\underline{r},u) = \int \Sigma_{s_1}(u' \to u)\,\underline{\phi}_1(\underline{r},u')\,du' \qquad (4\text{-}12b)$$

As written in this form, inelastic scattering is included in the degradation terms; Σ_{s_0} and Σ_{s_1} contain the effects of slowing down by inelastic collisions. However, as has been seen, diffusion theory is a poor approximation when the energy loss in a single collision is large, which is the case for inelastic scattering events.

Since one usually wants to apply diffusion theory, this difficulty must be circumvented in some manner. A simple means of doing this is to treat inelastic scattering as if it were "fission." The inelastic scattering cross section is added to the absorption cross section; the neutrons thus "absorbed" are then added to the source. If, as has been written, a source term is included only in the first P_1 equation, the assumption that inelastic scattering is symmetric about 90° in the laboratory system is automatically made. In the Hauser-Feshbach theory[7], in which a continuum of energy states of the compound nucleus is assumed, the scattering does have this property in the center of mass system and since inelastic scattering is largely due to heavy elements, the center of mass and laboratory systems are almost equivalent. (For cases in which the Hauser-Feshbach theory does not obtain, a non-isotropic source term could be included in the P_1 equation.) Thus we let

$$\Sigma_a(\underline{r},u) + \Sigma_{in}(\underline{r},u) \rightarrow \Sigma_a(\underline{r},u) \qquad (4\text{-}13a)$$

and

$$\upsilon f(u)\int_0^\infty \Sigma_f(\underline{r},u)\phi_0(\underline{r},u)\,du + \int_0^u \Sigma_{in}(u'\rightarrow u)\,\phi_0(\underline{r},u')\,du' \rightarrow S(\underline{r},u) \qquad (4\text{-}13b)$$

where $\Sigma_{in}(u' \rightarrow u)$ is the inelastic scattering frequency and

$$\Sigma_{in}(u) = \int_u^\infty \Sigma_{in}(u\rightarrow u')\,du' \qquad (4\text{-}13c)$$

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[7] W. Hauser and H. Feshbach, Phys. Rev., 87, 366 (1952).

The multigroup equations are now readily obtained by dividing the lethargy interval from zero to u_T, the thermal cutoff, into several small intervals (u_{j-1}, u_j) where $j = 1, 2, \text{---} N-1$, N-1 being the number of fast groups desired. Naturally, $u_o = 0$ and $u_{N-1} = u_T$. The choice of the number of groups for a particular calculation will be discussed later, but, in general, the larger the number of groups, the more accurate the calculation. On the other hand, the expense of a calculation is approximately proportional to the number of groups so that an optimization must be made.

Equations (4-12) are now integrated in lethargy over group to obtain:

$$\int_{u_{j-1}}^{u_j} \Sigma_t(\underline{r},u)\,\phi_0(\underline{r},u) + \underline{\nabla}\cdot\int_{u_{j-1}}^{u_j} \underline{\phi}_1(\underline{r},u)\,du = \int_{u_{j-1}}^{u_j} du \int_0^u du'\,\Sigma_{s_0}(u'\to u)\,\phi_0(\underline{r},u') + \int_{u_{j-1}}^{u_j} S(\underline{r},u)\,du \qquad (4\text{-}14a)$$

and

$$\int_{u_{j-1}}^{u_j} \Sigma_t(\underline{r},u)\,\underline{\phi}_1(\underline{r},u)\,du + \tfrac{1}{3}\underline{\nabla}\int_{u_{j-1}}^{u_j} \phi_0(\underline{r},u)\,du = \int_{u_{j-1}}^{u_j} du \int_0^u du'\,\Sigma_{s_1}(u'\to u)\,\underline{\phi}_1(\underline{r},u') \qquad (4\text{-}14b)$$

Now in analogy to the treatment of the thermal group, group fluxes are defined

$$\phi_{0j}(\underline{r}) = \int_{u_{j-1}}^{u_j} \phi_0(\underline{r},\omega)\,du \qquad (4\text{-}14c)$$

$$\underline{\phi}_{1j}(\underline{r}) = \int_{u_{j-1}}^{u_j} \underline{\phi}_1(\underline{r},u)\,du \qquad (4\text{-}14d)$$

Also, by breaking up the integrals in the scattering-in terms:

$$\int du' \Sigma_{s_{0,1}}(\underline{r},u'\to u)\phi_{0,1}(\underline{r},u') = \sum_{i=1}^{j} \int_{u_{i-1}}^{u_i} \Sigma_{s_{0,1}}(\underline{r},u'\to u)\phi_{0,1}(\underline{r},u') \qquad (4\text{-}14e)$$

and defining

$$\Sigma_{t_{j0,1}}(\underline{r}) = \frac{\int_{u_{j-1}}^{u_j} du\,\Sigma_t(\underline{r},u)\,\phi_{0,1}(r,u)}{\phi_{j0,1}(\underline{r})} \qquad (4\text{-}14f)$$

$$\Sigma_{ijo,1}(\underline{r}) = \frac{\int_{u_{j-1}}^{u_j} du \int_{u_{i-1}}^{u_i} du'\,\Sigma_{s_{0,1}}(u'\to u)\,\phi_{0,1}(\underline{r},u)}{\phi_{i0,1}(\underline{r})} \qquad (4\text{-}14g)$$

as the group cross sections, and

$$S_j(\underline{r}) = \int_{u_{j-1}}^{u_j} S(\underline{r},u)\,du \qquad (4\text{-}14h)$$

as the group source, one finally arrives at the multigroup P_1 equations:

$$\Sigma_{tj0}(\underline{r})\,\phi_{0j}(\underline{r}) + \underline{\nabla}\cdot\underline{\phi}_{1j}(\underline{r}) = \sum_{i=1}^{j} \Sigma_{ijo}(\underline{r})\,\phi_{0i}(\underline{r}) + S_j(\underline{r}) \qquad (4\text{-}14j)$$

$$\Sigma_{t_{j,1}}(\underline{r})\,\underline{\phi}_{1,j}(\underline{r}) + \frac{1}{3}\underline{\nabla}\,\phi_{0,j}(\underline{r}) = \sum_{i=1}^{j} \Sigma_{ij,1}\,\underline{\phi}_{1,j}(\underline{r}) \qquad (4\text{-}14k)$$

which is the set we have been seeking. Frequently, the terms $\Sigma_{jj}\phi_j(\underline{r})$ appearing on the right-hand sides of Equations (4-14j) and (4-14k) are subtracted from the $\Sigma_{tj}\phi_j$ terms to yield a somewhat simpler set of equations. The resulting cross section may be interpreted as a cross section for removal from the group:

$$\Sigma_{Rj} = \Sigma_{tj} - \Sigma_{jj} = \Sigma_{aj} + \sum_{k>j} \Sigma_{jk}$$

Thus far, Equations (4-14j) and (4-14h) are rigorously equivalent to the original P_1 equations. The difficulty is that the group sections $\Sigma_{tj0,1}$ and the "transfer cross sections" $\Sigma_{ij0,1}$, are defined in terms of the spectra within the group and cannot rigorously be determined until the fluxes are known, i.e., until the P_1 equations have been solved. Also, note that even in a region of uniform composition, in which the cross sections are not functions of position, the group-averaged cross sections may be functions of position if the flux, ϕ_0, and the current, ϕ_1, are not seperable in space and energy. Separability was shown in Chapter I to obtain for an asymptotic reactor, i.e., a reactor containing only one region of uniform composition but, of course, for such a reactor there is no need to apply the multigroup scheme at all.

There are several possible solutions to these problems. One which immediately comes to mind is iteration, i.e., assuming flux and current spectra, averaging the cross sections, computing a new spectrum from the multigroup equations, recomputing the averages and using these to compute a new spectrum and continuing until the process converges. The difficulty here is that one obtains only a histogram of a spectrum from the multigroup equations; these must be converted into a continuous spectrum before the averages can be computed; hence this procedure is valid only if a large number of groups are used.

Another possible procedure is to use the methods of the previous chapter to compute the spectrum which would obtain in each region if it were isolated from the other regions. This, the so-called spectral procedure, may also be used iteratively, and is described in greater detail later. The spectrum so calculated can be used to generate group cross sections for the multigroup calculation.

A third procedure, often used in fast reactor design, is to assume a single spectrum for all reactors, average the cross sections once and for all, and use the cross sections so obtained in multigroup calculations. This procedure may be valid as cross sections generally do not vary rapidly at high energy. Ultimately, the test of any of these methods lies in comparison with critical or exponential experiments or with operating reactors. The results lead one to suspect correctly that reactor design is more of an art than a science at the present time.

Equation (4-14k) is frequently simplified by ignoring off-diagonal elements of Σ_l, i.e., $\Sigma_{ijl} = 0$ for $i \neq j$. This corresponds to the neglect of anisotropic slowing down and is thus an inconsistent P_1 approximation. One can then rewrite Equation (4-13k) as

$$\Sigma_{tr_j}(\underline{r})\,\underline{\phi}_{1,j}(\underline{r}) + \frac{1}{3}\nabla\phi_{0,j}(\underline{r}) = 0 \qquad (4\text{-}14m)$$

where

$$\Sigma_{tr_j} = \Sigma_{t,j} - \Sigma_{1,jj}$$

can be seen to be the equivalent of Σ_{tr} averaged over $\underline{\phi}_1(r, u)$. If we assume Fick's Law to be valid at all energies, Σ_{trj} becomes simply

$$\Sigma_{tr_j} = \frac{\int_{u_{j-1}}^{u_j} \nabla\phi_0(\underline{r}, u)\,du}{\int_{u_{j-1}}^{u_j} \frac{\nabla\phi_0(\underline{r}, u)\,du}{\Sigma_{tr}(u)}} \qquad (4\text{-}14n)$$

and if $\underline{\phi}_1(\underline{r}, u)$ is separable in space and energy this reduces further to

$$\Sigma_{tr_j} = \lambda_{tr_j}^{-1} \qquad (4\text{-}14p)$$

where λ_{trj} is the flux average of the reciprocal of the transport cross section. This definition, while awkward, is frequently used and in another application has been shown to give accurate results in the

calculation of the thermal diffusion length for water.[7] For a more complete discussion of some of these points see Reference 8.

Very often, the multigroup procedure is applied directly to the consistent P_1 Selengut-Goertzel or Greuling-Goertzel Approximations. The major difference between these schemes and the one given above is the presence of derivatives with respect to lethargy in the basic equations from which they are derived.

To illustrate the treatment of the derivative terms, let us start with the Age Diffusion Equation, rewritten here[9]:

$$\frac{\partial}{\partial u} q(\underline{r},u) + \Sigma_a(\underline{r},u)\,\phi(\underline{r},u) - \nabla\cdot D(\underline{r},u)\,\underline{\nabla}\phi(\underline{r},u) = S(\underline{r},u) \qquad (4\text{-}15a)$$

with

$$q(\underline{r},u) = \xi(\underline{r},u)\,\Sigma_s(\underline{r},u)\,\phi(\underline{r},u) \qquad (4\text{-}15b)$$

The same procedure is again followed. Equation (4-15a) is integrated in lethargy from u_{j-1} to u_j and group cross sections are defined as before

$$q(\underline{r},u_j) - q(\underline{r},u_{j-1}) + \Sigma_{a_j}(\underline{r})\phi_j(\underline{r}) - \underline{\nabla}\cdot D_j(\underline{r})\,\nabla\phi_j(\underline{r}) = S_j(\underline{r},u) \qquad (4\text{-}15c)$$

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7 C.D. Petrie, M.L. Storm and P.F. Zweifel, Nuc.Sci.Eng., 2, 728 (1957).

8 G. Ball, P.F. Zweifel, International Converence on Fast and Intermediate Reactors, Vienna, 1961.

9 This derivation is also found in R. Ehrlich and H. Hurwitz, Jr., Nucleonics, 12, 23, (1952).

where $\phi_j(r, u)$ and $S_j(\underline{r})$ are defined by Equations (4-14c) and (4-14h) respectively. Here the definition of D_j takes the form (4-14p) automatically if separability is assumed. Some authors prefer to use

$$\bar{\phi}_j(\underline{r}) = \frac{\phi_j(\underline{r})}{u_j - u_{j-1}} = \frac{\phi_j(\underline{r})}{\bar{u}_j} \qquad (4\text{-}15d)$$

as a variable; the choice is a matter of personal preference. To complete the multigroup set of equations, a relation involving $\phi_j(\underline{r})$, $q(\underline{r}, u_j)$ and $q(\underline{r}, u_{j-1})$ is required. To accomplish this, one may notice that $q(\underline{r}, u_j)$ is related to $\phi(u_j)$ by Equation (4-15b), that is,

$$q(\underline{r}, u_j) = \xi(\underline{r}, u_j)\Sigma_s(\underline{r}, u_j)\phi(\underline{r}, u_j) \qquad (4\text{-}15e)$$

It is then usually assumed that $\phi_j(\underline{r})$ can be expressed as a linear combination of the end point values

$$\phi_j(\underline{r}) = \omega_1 \phi(\underline{r}, u_{j-1}) + \omega_2 \phi(\underline{r}, u_j) \qquad (4\text{-}15f)$$

thus yielding a set of equations in the $\phi(\underline{r}, u_j)$.

Alternatively, one could use the relation

$$q_j(\underline{r}) = \left(\xi(\underline{r})\Sigma_s(\underline{r})\right)_j \phi_j(\underline{r}) \qquad (4\text{-}15g)$$

to write the set of equations (4-15c) in terms of the slowing down density. Then, $q_j(\underline{r})$ is expressed as a linear combination of the end point values $q(\underline{r}, u_j)$ and $q(\underline{r}, u_{j-1})$ a procedure which is usually

preferable as q shows less variation with lethargy than does ϕ. A discussion of various schemes for obtaining these auxilliary equations is deferred until later.

An alternate procedure for the derivation of the multigroup equation has been given by Calame and Brooks.[10] They derived variational principles for the Age Diffusion and Consistent P_1 Equations. That is, they found a bilinear functional of $\phi(\underline{r}, u)$ and $\phi^+(\underline{r}, u)$, which is variationally stationary with respect to small deviations of $\phi(\underline{r}, u)$ and $\phi^+(\underline{r}, u)$ from their correct values. By assuming that $\phi^+(\underline{r}, u)$ is constant in each lethargy interval (u_{j-1}, u_j), and by assuming a particular functional form for $\phi(\underline{r}, u)$ within that interval, they were able to derive a set of multigroup equations. Usually, this functional form is a linear combination of the fluxes or slowing down densities at u_{j-1} and u_j. When such a form is employed, the multigroup equations obtained are identical to those obtained by the method used earlier. This method has not as yet been exploited fully.

B. Simple Applications of the Method

5. The Two-Group Two-Region Problem

To make clearer the basic principles of the multigroup method, a simple example may be useful. The simplest non-trivial example is the so-called two-group two-region problem, in which only two groups (one fast and one thermal) are used and it is assumed that the reactor consists of a fuel-loaded core and a reflector which contains no fuel. Both regions

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[10] G.P. Calame and H. Brooks, Trans. Amer. Nuc. Soc., 2, 1, Paper 7-4 (June 1959).

are assumed homogeneous. To further simplify the problem, inelastic scattering is ignored.

For the thermal group (T) one has immediately in the core (C):

$$-D_{TC} \nabla^2 \phi_{TC}(\underline{r}) + \Sigma_{a_{TC}} \phi_{TC}(\underline{r}) = q_{TC}(\underline{r}) \quad (4\text{-}16a)$$

and in the reflector (R):

$$-D_{TR} \nabla^2 \phi_{TR}(\underline{r}) + \Sigma_{a_{TR}} \phi_{TR}(\underline{r}) = q_{TR}(\underline{r}) \quad (4\text{-}16b)$$

For the fast neutrons, noting that

$$q(u_0) = q(0) = 0$$

$$q(u_1) = q(u_T) = q_T$$

and that all fission neutrons are born into the fast group, one obtains the fast group (F) equations, in the Age Diffusion Approximation:

$$-D_{FC} \nabla^2 \phi_{FC}(\underline{r}) + \Sigma_{a_{FC}} \phi_{FC}(\underline{r}) + q_{TC}(\underline{r}) = \nu \Sigma_{f_{TC}} \phi_{TC}(\underline{r}) \quad (4\text{-}16c)$$

for the core and

$$-D_{FR} \nabla^2 \phi_{FR}(\underline{r}) + \Sigma_{a_{FR}} \phi_{FR}(\underline{r}) - q_{TR}(\underline{r}) = 0 \quad (4\text{-}16d)$$

for the reflector, since there is no fuel and hence no fast neutron source in the reflector. We can eliminate the quantities q_{TC} and q_{TR}

by noting:

$$q_T(\underline{r}) = q(\underline{r}, u_T) = \xi \Sigma_s(u_T)\, \phi(\underline{r}, u_T) \qquad (4\text{-}16e)$$

in either the core or the reflector and postulating relation between $\phi_F(\underline{r})$ and $\phi(\underline{r}, u_T)$. The simplest relation that one could employ is simple proportionality. Intuitively, this appears to be a resonable assumption, and leads to:

$$\phi(\underline{r}, u_T) = C\, \phi_F(\underline{r})$$

or:

$$q_T(\underline{r}) = C\xi \Sigma_s(u_T)\, \phi_F(\underline{r}) = \Sigma_R\, \phi_F(\underline{r}) \qquad (4\text{-}16f)$$

which is to be applied separately to each region. The new proportionality constant, Σ_R, is often called the slowing down or removal cross section. Using Equation (4-16f) and ignoring resonance (fast) absorption in the reflector, we arrive at the well known two-group two-region equations

$$-D_{FC}\nabla^2\phi_{FC}(\underline{r}) + \left(\Sigma a_{FC} + \Sigma_{RC}\right)\phi_{FC}(\underline{r}) = \nu\Sigma_{fTC}\,\phi_{TC}(\underline{r}) \qquad (4\text{-}17a)$$

$$-D_{TC}\nabla^2\phi_{TC}(\underline{r}) + \Sigma_{aTC}\,\phi_{TC}(\underline{r}) = \Sigma_{RC}\,\phi_{FC}(\underline{r}) \qquad (4\text{-}17b)$$

$$-D_{FR}\nabla^2\phi_{FR}(\underline{r}) + \Sigma_{RR}\,\phi_{FR}(\underline{r}) = 0 \qquad (4\text{-}17c)$$

$$-D_{TR} \nabla^2 \phi_{TR}(\underline{r}) + \Sigma_{a_{TR}} \phi_{FR}(\underline{r}) = \Sigma_{RR} \phi_{FR}(\underline{r}) \qquad (4\text{-}17d)$$

In introducing a boundary between the two regions, a need for four boundary conditions, two each for the fast and thermal fluxes, is introduced. These are readily supplied by the usual diffusion theory boundary conditions of continuity of flux and current:

$$\phi_{F,TC}(\underline{S}_1) = \phi_{F,TR}(\underline{S}_1) \qquad (4\text{-}18a)$$

$$D_{F,TC} \nabla \phi_{F,TC}(\underline{S}_1) = D_{F,TR} \nabla \phi_{F,TR}(\underline{r}) \qquad (4\text{-}18b)$$

at the core-reflector boundary $(\underline{S}_1)$. In addition, the usual extrapolated boundary conditions are applied at the outer surface of the reflector $(\underline{S}_2)$

$$\phi_{F,TR}(\underline{S}_2) = 0 \qquad (4\text{-}18c)$$

and the fluxes must be finite and non-negative everywhere within the system.

To solve the two group equations we shall attempt to find solutions in the core of the form:

$$\phi_{F,TC}(\underline{r}) = A_{F,T} e^{i\underline{k}\cdot\underline{r}}$$

(a sum of such solutions is also a solution, of course), and thus obtain the equations

$$[D_{FC} k^2 + \Sigma a_{FC} + \Sigma_{RC}] A_F - \nu \Sigma_{f_{TC}} A_T = 0 \qquad (4\text{-}19a)$$

$$[D_{TC} k^2 + \Sigma a_{TC}] \quad A_T - \Sigma_{RC} A_F = 0 \qquad (4\text{-}19b)$$

which have non-trivial solutions (non-zero fluxes) only if the determinant

$$\begin{vmatrix} D_{FC} k^2 + \Sigma_{aFC} + \Sigma_{RC} & -\nu\Sigma_{fTC} \\ -\Sigma_{RC} & D_{TC} k^2 + \Sigma_{aTC} \end{vmatrix}$$

vanishes. On expanding the determinant, one find that the critical condition to be:

$$\frac{\left(\frac{\nu\Sigma_{fTC}}{\Sigma_{aTC}}\right)\left(\frac{\Sigma_{RC}}{\Sigma_{RC}+\Sigma_{aFC}}\right)}{(1+L_T^2 k^2)(1+L_F^2 k^2)} = 1 \qquad (4\text{-}19c)$$

where the fast diffusion area, L_F^2, is defined in analogy to the earlier definition of L_T^2 (dropping the subscript "C" temporarily):

$$L_F^2 = \frac{D_F}{\Sigma_{aF}+\Sigma_R} = \frac{D_F}{\Sigma_{tF}} \qquad (4\text{-}19d)$$

Since its denominator is a monotonically increasing function of k^2, Equation (4-19c), considered as a function of k^2, can have at most one positive root and then only if:

$$\left(\frac{\nu\Sigma_{fT}}{\Sigma_{aT}}\right)\left(\frac{\Sigma_R}{\Sigma_R+\Sigma_{aF}}\right) > 1 \qquad (4\text{-}19e)$$

But, if the core were infinite, there would be no net neutron flow and critical condition would have the quantity (4-19e) set equal to unity. Therefore, this quantity must be the infinite medium multi-

plication factor k_∞ or

$$\eta f p = \left(\frac{\nu \Sigma_{fT}}{\Sigma_{aT}}\right)\left(\frac{\Sigma_R}{\Sigma_R + \Sigma_{aF}}\right) \qquad (4\text{-}19f)$$

since there is no fast fission in the present problem. Thus

$$p = \Sigma_R / (\Sigma_R + \Sigma_{aF}) \qquad (4\text{-}19g)$$

since from an earlier definition we had

$$\eta f = \nu \Sigma_{fT} / \Sigma_{aT} \qquad (4\text{-}19h)$$

This leads us to a very important point - <u>the group constants must be selected so as to yield the correct values of the thermal utilization and resonance escape probability</u> (and fast effect if fast fission is allowed) which may be computed by methods given earlier. In practice, absorption cross sections are obtained by insisting that the multigroup calculation predict the resonance integral correctly. Exactly how this is done will be shown in the next section.

Another result is that the material buckling is no longer a well defined quantity; the critical condition has more than one root for k^2. This is quite as one would expect, for if k^2 were unique, the results of Chapter I would obtain and the flux would obey the Helmholtz Equation with wave number B_m. Instead, denoting the real roots of Equation (4-19c) by $k = \pm B$, and the imaginary roots by $k = \pm i$, one sees that the flux shapes can generally be written a linear combination of $e^{\pm \underline{B} \cdot \underline{r}}$ and $e^{\pm i \underline{k} \cdot \underline{r}}$ or equivalently

$$\phi_{TC}(\underline{r}) = a_T \Psi_1(\underline{r}) + b_T \Psi_2(\underline{r}) \qquad (4\text{-}20a)$$

$$\phi_{FC}(\underline{r}) = a_F \Psi_1(\underline{r}) + b_F \Psi_2(\underline{r})$$

where $\Psi_1(\underline{r})$ and $\Psi_2(\underline{r})$ are the regular solutions of the Helmholtz Equation with wave numbers B and ik respectively. Quite generally, the Helmholtz Equation will have two solutions, but in three dimensions, one of these will always be irregular at the origin. In slab geometry, it will be seen that one solution can be removed by application of the condition that the flux be non-negative or equivalently, by imposing symmetry conditions.

The reflector equations are solved quite easily. Since Equation (4-17c) is homogeneous in $\phi_{FC}(\underline{r})$ and is the Helmholtz Equation with wave number $(1/L_{FR})$ where

$$L_{FR} = D_{FR} / \Sigma_{RR} \qquad (4\text{-}20c)$$

we can write:

$$\phi_{FR}(\underline{r}) = C_F \chi_1(\underline{r}) + d_F \chi_2(\underline{r}) \qquad (4\text{-}20d)$$

Here $\chi_1(\underline{r})$ and $\chi_2(\underline{r})$ are the two solutions of the Helmholtz Equation with wave numbers $(1/L_F)$, which may now be substituted into Equation (4-17d) to determine the thermal flux in the reflector. Once again, the solution can be written in terms of the solutions of the Helmholtz Equation

$$\phi_{TR}(\underline{r}) = C_T \chi_3(\underline{r}) + d_T \chi_4(\underline{r}) + \frac{\Sigma_{RR}}{\Sigma a_R + D_{TR}/L^2_{FR}} \phi_{FR} \qquad (4\text{-}20e)$$

where $\chi_3(\underline{r})$ and $\chi_4(\underline{r})$ are the two solutions of the Helmholtz Equation with wave numbers $(1/L_{TR})$.

$$L_{TR} = D_{TR}/\Sigma_{a_{TR}}$$

Eight constants of integration: a_T, a_F, b_T, b_F, c_T, c_F, d_T, d_F remain to be evaluated. Clearly, eight conditions are required. However, it is noticed that the four constants are not independent. For, on reinserting the expressions for the core flux in (4-17a) or (4-17b), and noting that $\Psi_1(\underline{r})$ and $\Psi_2(\underline{r})$ are linearly independent, we find that a_T and a_F are proportional and that b_T and b_F are likewise proportional:

$$a_T = \frac{D_{FC} B^2 + \Sigma a_{FC} + \Sigma_{RC}}{\nu \Sigma_{f_{TC}}} a_F = g_1 a_F \quad (4\text{-}21a)$$

$$b_T = \frac{D_{FC} K^2 + \Sigma a_{FC} + \Sigma_{RC}}{\nu \Sigma_{f_{TC}}} b_F = g_2 b_F \quad (4\text{-}21b)$$

Now, only six constants remain, and the four interface boundary conditions and the two extrapolated boundary conditions are just the conditions required to complete the solution. Applying them, one finds:

Continuity of flux:

$$a_F \Psi_1(\underline{S}_1) + b_F \Psi_2(\underline{S}_1) = c_F \chi_1(\underline{S}_1) + d_F \chi_2(\underline{S}_1)$$

$$g_1 a_F \Psi_1(\underline{S}_1) + g_2 b_F \Psi_2(\underline{S}_1) = c_T \chi_3(\underline{S}_1) + d_T \chi_4(\underline{S}_1) + \frac{\Sigma_{gR}}{\Sigma_{aR} + \frac{D_{TR}}{L_{TR}}} [c_F \chi_1(\underline{S}_1) + d_F \chi_2(\underline{S}_1)]$$

Continuity of current:

$$-D_{FC}\left[a_F \underline{\nabla} \Psi_1(\underline{s}_1)+b_F \underline{\nabla} \Psi_2(\underline{s}_1)\right] = -D_{FR}\left[c_F \underline{\nabla} \chi_1(\underline{s}_1)+d_F \underline{\nabla} \chi_2(\underline{s}_1)\right]$$

$$-D_{TC}\left[g_1 a_F \underline{\nabla} \Psi_1(\underline{s}_1)+g_2 b_F \underline{\nabla} \Psi_2(\underline{s}_1)\right] = -D_{TR}\left[c_T \underline{\nabla} \chi_3(\underline{s}_1)+d_T \underline{\nabla} \chi_4(\underline{s}_1)\right.$$

$$\left.+\frac{\Sigma_{RR}}{\Sigma_{aR}+\frac{D_{TR}}{L^2_{FR}}} c_F \underline{\nabla} \chi_1(\underline{s}_1)+\frac{\Sigma_{RR}}{\Sigma_{aR}+\frac{D_{TR}}{L^2_{FR}}} d_F \underline{\nabla} \chi_2(\underline{s}_1)\right]$$

Extrapolated boundary:

$$c_F \chi_1(\underline{s}_2)+d_F \chi_2(\underline{s}_2)=0$$

$$c_T \chi_3(\underline{s}_2)+d_T \chi_4(\underline{s}_2)=0$$

These are six homogeneous equations which are satisfied only if the six by six determinant

$$\begin{vmatrix}
\Psi_1(\underline{s}_1) & \Psi_2(\underline{s}_1) & \chi_1(\underline{s}_1) & \chi_2(\underline{s}_1) & 0 & 0 \\
g_1\Psi_1(\underline{s}_1) & g_2\Psi_2(\underline{s}_1) & \frac{\Sigma_{RR}}{D_{TR}+\Sigma a_R}\chi_1(\underline{s}_1) & \frac{\Sigma_{RR}}{D_{TR}+\Sigma a_R}\chi_2(\underline{s}_1) & \chi_3(\underline{s}_1) & \chi_4(\underline{s}_1) \\
-D_{FC}\underline{\nabla}\Psi_1(\underline{s}_1) & -D_{FC}\underline{\nabla}\Psi_2(\underline{s}_1) & -D_{FR}\underline{\nabla}\chi_1(\underline{s}_1) & -D_{FR}\underline{\nabla}\chi_2(\underline{s}_1) & 0 & 0 \\
-D_{TC}g_1\underline{\nabla}\Psi_1(\underline{s}_1) & -D_{TC}g_2\underline{\nabla}\Psi_2(\underline{s}_1) & \frac{-D_{TR}\Sigma_{RR}}{D_{TR}+\Sigma a_R}\underline{\nabla}\chi_1(\underline{s}_1) & -\frac{D_{TR}\Sigma_{RR}}{D_{TR}+\Sigma a_R}\underline{\nabla}\chi_2(\underline{s}_1) & -D_{TR}\underline{\nabla}\chi_3(\underline{s}_1) & -D_{TR}\underline{\nabla}\chi_4(\underline{s}_1) \\
0 & 0 & \chi_1(\underline{s}_2) & \chi_2(\underline{s}_2) & 0 & 0 \\
0 & 0 & 0 & 0 & \chi_3(\underline{s}_2) & \chi_4(\underline{s}_2)
\end{vmatrix}$$

is set equal to zero. This determinant arose from geometrical considerations through the boundary conditions on the fluxes and plays much the same role as did the definition of the geometric buckling in the simple one-region reactor considered in Chapter I. There, geometry determined an eigenvalue of the Helmholtz Equation (the geometric buckling) which, for criticality, had to be equal to the material buckling. In the present case, these quantities are not unique and a simple unified treatment is not possible. However, the condition (4-21) does give the relation between material composition and geometry required for criticality. Hence, Equation (4-21) is frequently called the criticality condition in the literature, but we prefer to call (4-19c) the criticality condition in analogy to the nomenclature of Chapter I. Equation (4-21) may then be taken as the condition which specifies the surfaces $\underline{S_1}$ and $\underline{S_2}$; the above development is possible only when these surfaces are the surfaces

$$\zeta = \text{constant}$$

in some coordinate system in which the Helmholtz Equation is separable, ζ being a coordinate of this system.[11] In other cases, exact solutions do not exist.

In many cases of interest, the reflector may be considered infinite. If the reflector is thicker than a few migration lengths ($M^2 = L^2 + \tau$) this is a good approximation. However, quite generally, one of the solutions of the Boltzmann Equation with wave number (1/L)

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[11] For a discussion of separable coordinate system, see, for example, P.M. Morse and H. Feshbach Methods of Theoretical Physics, New York: McGraw-Hill, 1953, Chapter VII.

increases exponentially at infinity and hence its coefficient must be zero. Then d_F and d_T drop out and the determinant (4-21) is only four by four.

In any case, the coefficients a_F, b_F, c_T, c_F, d_T, d_F are determined only to within an arbitrary multiplicative constant. This is a statement of the fact that a reactor operating without any feedback (temperature, xenon, control system, etc.) can have any power level, i.e., that criticality is independent of power level.

As an illustration we shall take the case of slab geometry. In the core the flux shapes are

$$\phi_{FC}^{(z)} = a_F \cos Bz + b_F \cosh \mathcal{H} z$$

$$\phi_{TC}^{(z)} = a_T \cos Bz + b_T \cosh \mathcal{H} z$$

where the origin is taken at the center of the core. Terms involving sin Bz and sinh $\mathcal{H}$z, which are solutions of the two group equations are eliminated by the condition that the flux be non-negative. In the reflector

$$\phi_{FR}^{(z)} = c_F e^{-z/L_{FR}} + d_F e^{z/L_{FR}}$$

$$\phi_{TR}^{(z)} = c_T e^{-z/L_{TR}} + d_T e^{z/L_{TR}}$$

and in an infinite system

$$d_F = d_T = 0$$

The solution leads to the well-known peak in the thermal flux in the reflector just outside the core (see Figure 1) and the thermal flux is flatter in the core than in the bare reactor case; the fast flux is also flattened somewhat by the presence of the reflector but the change in its shape is nowhere near so drastic. Physically, this peak arises from neutrons being slowed down in the reflector after having leaked out of the core as fast neutrons. Since the core is generally a much stronger absorber of thermal neutrons than is the reflector, the thermal flux dips near the core-reflector interface. Of course, the position and size of the peak are strongly affected by the reactor parameters.

An interesting limit is the bare reactor, i.e., one for which the reflector thickness goes to zero. Then the core flux must vanish on an extrapolated boundary, and, the coefficient of the hyperbolic cosines go to zero as one would expect. The interesting point is that the critical condition can then be written in the form

$$\frac{\eta f p}{(1+L_T^2 B^2)(1+L_F^2 B^2)} = 1 \quad (\epsilon = 1) \qquad (4\text{-}21a)$$

where $(1 + L_F^2 B^2)^{-1}$ can be recognized as the fast non-leakage probability. But if B^2 is small

$$\frac{1}{1+L_F^2 B^2} \approx e^{-B^2 L_F^2} \qquad (4\text{-}21b)$$

and on comparing this two group Age-Diffusion result with the non-leakage probability derived in Age-Diffusion Theory, $e^{-B^2\tau}$, one has

$$L_F^2 = \tau = D_F / \Sigma_R \qquad (4\text{-}21c)$$

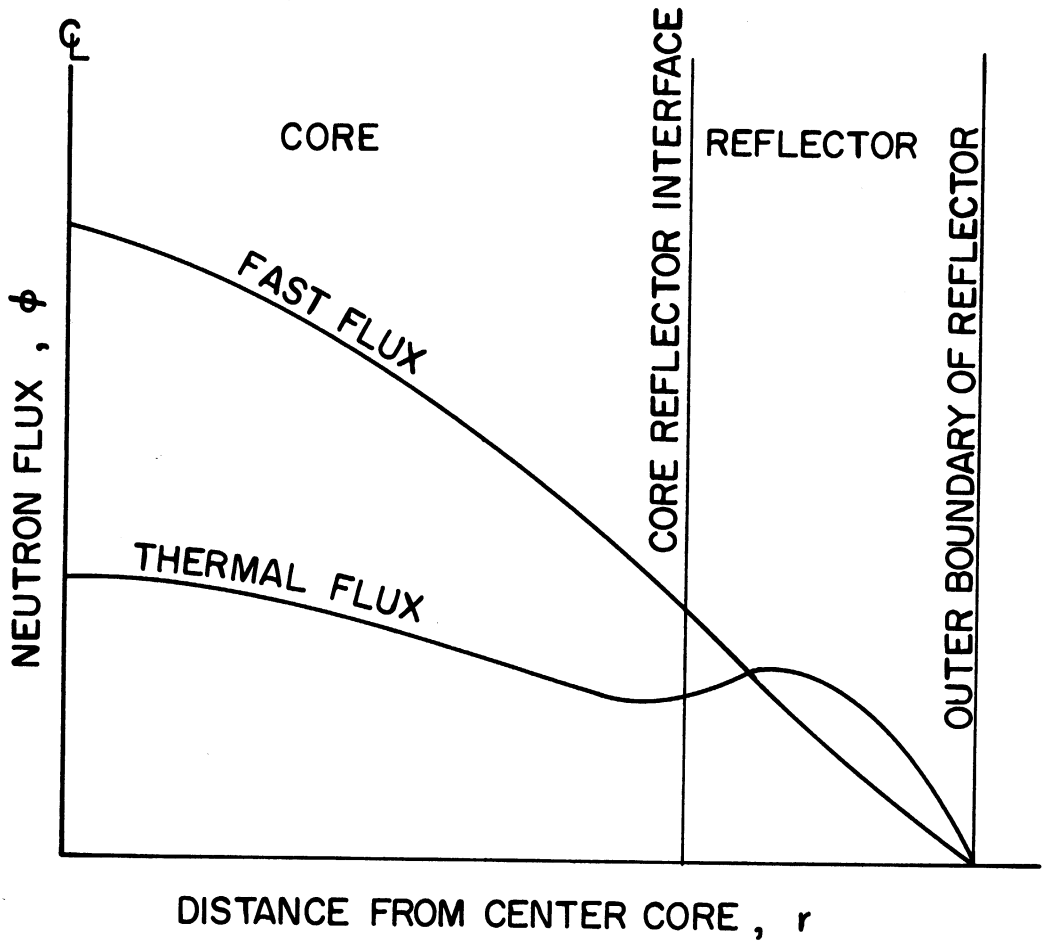

Figure IV-1 Fast and Thermal Neutron Flux Distributions as Derived from the Two Group - Two Region Model. The curves are qualitative but are typical of many existing thermal reactors.

This is another very important constraint on the choice of group constants. By demanding that the two-group calculation give the resonance escape probability, and neutron age correctly, one places two rigid constraints on the three fast group constants Σ_R, Σ_{aF}, and D_F. If fast fission is allowed Σ_{fF} will be determined by the fast fission factor. Thus, only one of the four fast group constants really needs to be obtained by other means.

6. Multigroup Age Theory

A check on the consistency of the multigroup equations derived from Age Diffusion Theory can be made by increasing the number of fast groups. As the number of groups increases and the size of each group decreases correspondingly, Age Diffusion Theory should again result. For simplicity, we shall assume that all fissions take place in the thermal groups and that all fission neutrons are born in the first (i.e., highest energy) group. (Generalization of these assumptions leads to no additional difficulty, other than an increase in the mathematical complexity.)

Since Age Diffusion Theory implicity assumes that the lethargy change by a neutron is small in any given collision, neutrons slowing down out of a given group should be scattered only to the next higher lethargy group. It is assumed that each group flux $\phi_j(\underline{r})$ is proportional to $\phi(\underline{r}, u_j)$ i.e., that ω_1 of Equation (4-15e) is zero. In the limit of many groups, it does not seriously matter how ω_1 and ω_2 are as chosen so long as they are consistent in the limit of an infinite number of groups, but by choosing them in this fashion, it is possible to write $\phi(r, u_j)$ or $q(r, u_j)$ in terms of $\phi_j(\underline{r})$ alone. Had ω_1

not been chosen as zero, this would not be possible. Then each equation contains only two $\phi_j(\underline{r})$, as was desired, and for a uniform reactor we can write

$$-D_1 \nabla^2 \phi_1(\underline{r}) + (\Sigma_{a_1} + \Sigma_{R_1})\phi_1(\underline{r}) = \nu\Sigma_{f_N} \phi_N(\underline{r}) \qquad (4\text{-}22a)$$

for the lowest lethargy group and

$$-D_j \nabla^2 \phi_j(\underline{r}) + (\Sigma_{a_j} + \Sigma_{R_j})\phi_j(\underline{r}) = \Sigma_{R_{j-1}} \phi_{j-1}(\underline{r}) \qquad (4\text{-}22b)$$

for the other fast groups with $2 \leq j \leq N - 1$. Here again the concept of removal cross section is employed: The thermal group equation (the subscript 'T' will be dropped in favor of 'N'), can be written

$$-D_N \nabla^2 \phi_N(\underline{r}) + \Sigma_{a_N} \phi_N(\underline{r}) = \Sigma_{R,N-1} \phi_{N-1}(\underline{r}) \qquad (4\text{-}22c)$$

On solving these equations by the method used in the two group case, one arrives at the critical condition

$$\frac{\eta f}{1 + L_N^2 k^2} \prod_{j=1}^{N-1} \frac{p_j}{1 + L_j^2 k^2} = 1 \qquad (4\text{-}23a)$$

where the group resonance escape probabilities p_j are defined in analogy to Equation (4-19g) as:

$$p_j = \frac{\Sigma_{R_j}}{\Sigma_{R_j} + \Sigma_{a_j}} \qquad (4\text{-}23b)$$

while the diffusion areas L_j^2 are

$$L_j^2 = \frac{D_j}{\Sigma_{R_j} + \Sigma_{a_j}} \qquad (4\text{-}23c)$$

Since we are dealing with a uniform bare reactor in the context of diffusion theory, the analysis of Chapter I applies and it is possible to identify:

$$\overline{P}_\infty(k^2) = \prod_{j=1}^{N-1} \frac{P_j}{1+L^2k^2} = p\lambda(k^2) \qquad (4\text{-}24)$$

as the Fourier Transform of the slowing down kernel. Inverting the Fourier Transform, the slowing down kernel itself is the convolution:

$$P_\infty(|\underline{r}-\underline{r}'|) = \int d^3r_{N-1} \int \cdots \int d^3r_1 \left[\prod_{j=1}^{N-2} P_j \frac{e^{-|r_j - r_{j-1}|/L_j}}{4\pi D_j |r_j - r_{j-1}|}\right] \frac{e^{-|r_{N-1} - r|/L_{N-1}}}{4\pi D_{N-1} |r_{N-1} - r|}$$

As the fast groups are narrowed uniformly one can approximate Equation (4-24) by

$$\lim_{N\to\infty} \overline{P}_\infty(k^2) = \lim_{N\to\infty} \prod_{j=1}^{N-1} \frac{P_j}{1+L_j^2k^2} = \lim_{N\to\infty} \prod P_j(1-L_j^2k^2)$$

$$\approx \lim_{N\to\infty} \left(1 - \sum_{j=1}^{N-1} L_j^2k^2\right) \prod_{j=1}^{N-1} P_j \approx e^{-k^2 \sum_{j=1}^{\infty} L_j^2} \prod_{j=1}^{N-1} P_j$$

(4-25a)

which one may readily recognize as the Fourier Transform of the Gaussian Age Diffusion kernel. Therefore, by comparison with the Age-Diffusion

result, it follows that

$$\tau = \sum_{j=1}^{\infty} L_j^2 = \sum_{j=1}^{\infty} \frac{D_j}{\Sigma_{R_j} + \Sigma_{a_j}} \approx \sum_{j=1}^{\infty} \frac{D_j}{\Sigma_{R_j}} \qquad (4\text{-}25b)$$

in the limit of small absorption. In actual practice, of course, the summation extends only over as many groups as are employed in the calculation. On the other hand, the Fermi Age Formula

$$\tau_{th} = \int_0^{u_T} \frac{D(u')}{\xi \Sigma_s(u')} du' \qquad (4\text{-}25c)$$

can be approximated by the sum

$$\tau_{th} \approx \sum_{j=1}^{\infty} \frac{D(u_j)}{\xi \Sigma_s(u_j)} \Delta u_j \qquad (4\text{-}25d)$$

if the Δu_j are small. Comparison of Equation (4-25d) with Equation (4-25b) leads to

$$\Sigma_{R_j} = \frac{\xi \Sigma_s(u_j)}{\Delta u_j} = \frac{\xi \Sigma_{s_j}}{\Delta u_j} \qquad (4\text{-}25e)$$

as a consistent definition of the removal cross section. If $\Sigma_s(u)$ is constant, as it frequently is to good approximation, the group constants are determined.

Returning to consideration of the resonance escape probability, we have in the limit on many groups:

$$p = \prod_{j=1}^{\infty} p_j = \prod_{j=1}^{\infty} \frac{\Sigma_{R_j}}{\Sigma_{R_j} + \Sigma_{a_j}} = \prod_{j=1}^{\infty} \left[1 - \frac{\Sigma_{a_j}}{\Sigma_{R_j} + \Sigma_{a_j}} \right] \approx 1 - \sum_{j=1}^{\infty} \frac{\Sigma_{a_j}}{\Sigma_{R_j}} \qquad (4\text{-}26a)$$

again, in the limit of small absorption. On the other hand, in the Age Diffusion Approximation we had

$$p = e^{-\int_0^{u_T} \frac{\Sigma_a(u')}{\xi \Sigma_s(u')} du'} \qquad (4\text{-}26b)$$

By approximating as before, we have

$$p \approx 1 - \int_0^{u_T} \frac{\Sigma_a(u')}{\xi \Sigma_s(u')} du' \approx 1 - \sum_{j=1}^{\infty} \frac{\Sigma_a(u_j)}{\xi \Sigma_s(u_j)} \Delta u_j \qquad (4\text{-}26c)$$

If Equation (4-25e) is used, we see that the two results [Equations (4-26a,-26b)] are consistent provided the group absorption cross sections are chosen as the averages of the absorption cross sections. Indeed the usual procedure is to choose Σ_{aj} so as to give the correct resonance escape probability across the group.

This analysis provides a very simple, but useful, set of group constants, which are valuable for hand calculations. In the next section, the subject of group constants will be studied in greater detail.

C. Group Constants

7. Fast Group-Analytical Methods

In the previous section it was shown how fast group constants could be obtained if the age and resonance escape probability are known. In the limit of many groups, it was shown that a reasonable estimate of the removal cross section is:

$$\Sigma_{Rj} = \frac{\xi \Sigma_{sj}}{\Delta u_j}$$

It is tempting to use this result for large group widths too, and this is indeed frequently done in preliminary reactor analysis.

An alternate, and somewhat intuitive, derivation of this result has been given by Wigner.[12] In crossing a lethargy interval of width Δu_j, a neutron can be expected to make approximately $\Delta u_j/\xi$ slowing down collisions. Now, since the scattering collision density in this lethargy interval is $\Sigma_{sj}\phi_j$,

$$\frac{\Sigma_{sj}\phi_j}{(\Delta u_j/\xi)} = \frac{\xi\Sigma_{sj}}{\Delta u_j}\phi_j \qquad (4\text{-}27a)$$

should be a resonable estimate of the number of neutrons leaving the lethargy interval Δu_j. Hence $\xi\Sigma_{sj}/\Delta u_j$ should be a reasonable estimate of the removal cross section, in agreement with our earlier results.

Using the removal cross section as just given, it was also shown that for the two group case, the remaining group constants could be obtained from

$$D_F = \Sigma_R \tau_{th} \qquad (4\text{-}27b)$$

$$\Sigma_{aF} = \Sigma_R \bar{P}_{th} \qquad (4\text{-}27c)$$

and one might infer

$$\Sigma_{fF} = (\epsilon - 1)\Sigma_{fT}$$

provided that fast absorption is small (which is a condition for the validity of Age Diffusion Theory). These group constants were obtained by insisting that the age, resonance escape probability and fast effect be predicted correctly.

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[12] A.M. Weinberg and E.P. Wigner, op.cit., p. 386.

Frequently, two group calculations are sufficient for preliminary calculations. However, they are insufficient for many other purposes. The choice of the number of groups rests on a combination of many factors, not the least of which is cost of computing machine time. In general, the time of running a calculation is proportional to the number of groups. There is further advantage, however, in keeping the group coupling to a minimum. If each group is coupled to all others, all of the spatial dependent group fluxes at lower lethargies must be used in calculation of any particular group flux. In turn, this entails having a machine with a large memory and the calculation of each group flux is showed considerably by the necessity of using all the other fluxes. Considerable advantage is thus gained in having each group coupled only to the ones immediately adjacent to it and in having fission neutrons born into only one group. All group widths should therefore be at least $\ell n\ 1/\alpha_m$ where α_m is the minimum value of $\alpha = (\frac{A-1}{A+1})^2$ for any moderator in the reactor.* If hydrogen is present this is clearly an impossibility; hence, water moderated reactor calculations rarely emply more than three or four groups, while calculations for other systems often use more than 20 groups. (These remarks do not necessarily apply to systems in which ineleastic scattering is important.)

In the onre-region multigroup problem, the resonance escape probability was found to be represented as a product

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* With the changes in scattering kernel that some of the approximations utilize (see Chapter III, Figure 4), there may be coupling between non-adjacent groups even if this criterion is met. This coupling will usually be small, however.

$$P = P_1 P_2 \cdots P_{N-1} = \left(\frac{\Sigma_{R1}}{\Sigma_{R1}+\Sigma_{a1}}\right)\left(\frac{\Sigma_{R2}}{\Sigma_{R_2}+\Sigma_{a_2}}\right)\cdots\left(\frac{\Sigma_{R\,N-1}}{\Sigma_{RN-1}+\Sigma_{aN-1}}\right) \qquad (4\text{-}28a)$$

a result which strongly suggests that multigroup absorption cross sections could be determined from

$$p(u_{j-1} \rightarrow u_j) = 1 - \frac{\Sigma_{aj}}{\Sigma_{Rj}}$$

or

$$\Sigma_{aj} = \left[1 - p(u_{j-1} \rightarrow u_j)\right] \Sigma_{Rj} \qquad (4\text{-}28b)$$

In a similar fashion, one would say that

$$\tau(u_{j-1} \rightarrow u_j) = \frac{D_j}{\Sigma_{Rj}}$$

or

$$D_j = \Sigma_{Rj}\, \tau(u_{j-1} \rightarrow u_j) \qquad (4\text{-}28c)$$

Estimates of the group fission cross sections can be obtained in a similar manner. Fast fission was neglected as a matter of convenience in the multigroup problem, but it is not to difficult to see that had it been included we would have had

$$\eta f \epsilon = \frac{\nu}{\Sigma_{aN}} \left[\Sigma_{fN} + \sum_{\delta=1}^{N-1} \Sigma_{f\delta} \right]$$

or

$$\epsilon - 1 = \sum_{\delta=1}^{N-1} \Sigma_{f\delta} \qquad (4\text{-}29a)$$

Then, if $(\epsilon - 1)_j$, the ratio of the number of fissions in the j^{th} group to the total number of fissions could be estimated, Σ_{fj} would be easily obtained

$$\Sigma_{f\delta} = \Sigma_{fT} (\epsilon - 1)_\delta \qquad (4\text{-}29b)$$

In general, $p(u_{j-1} \rightarrow u_j)$, $\tau(u_{j-1} \rightarrow u_j)$ and $(\epsilon-1)_j$ are not known but one could apply some of the formulae developed in Chapters II and III to determine them. For example, the Goertzel-Greuling calculations for the age and resonance escape probability could be applied to known cross sections and the fast effect could be calculated by methods of Chapter II.

As an alternative, it has been suggested by Wigner[13] that it would be simpler to average fast group constants over a 1/E spectrum rather than compute the age and resonance escape probability from the somewhat more complicated formulae suggested above. Thus, one would have

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13 Ibid.

$$\Sigma_{a_j} = \int_{\Delta u_j} \Sigma_a(u')du' \Big/ \Delta u_j \qquad (4\text{-}30a)$$

$$\Sigma_{f_j} = \int_{\Delta u_j} \Sigma_{f_j}(u')\,du' \Big/ \Delta u_j \qquad (4\text{-}30b)$$

which is equivalent to replacing the true resonance integral, I, by the infinitely dilute resonance integral I_∞ as given in Chapter II. The diffusion coefficient is simply

$$D_j = \int_{\Delta u_j} D(u')\,du' \Big/ \Delta u_j \qquad (4\text{-}30c)$$

in this approximation. In this scheme the age $\tau(u_{j-1}\rightarrow u_j)$ is represented by

$$\tau(u_{j-1}\rightarrow u_j) = \frac{\int_{\Delta u_j} D(u')du'}{\xi \Sigma_{s_j}} \qquad (4\text{-}30d)$$

which is equivalent to the approach used earlier in the Age Diffusion Approximation if $\xi\Sigma_s$ is constant in lethargy. If scattering resonances are important, however, an error may be introduced by using these approximations.

8. Fast Group - Numerical Methods

Group constants obtained by the methods just given are frequently useful for survey type calculations but they are generally unsatisfactory for more detailed calculations. For example, in a complex

reactor composed of many materials, cross sections vary considerably from point to point as a result of changes in material composition and temperature effects. Calculation of position-dependent cross sections by any but the simplest methods is nearly impossible. Furthermore, the cross sections given previously are based on an Age Diffusion approach; one cannot obtain reasonable results for hydrogen moderated systems by this method.

In much numerical work for obtaining group constants, use is made of the Fourier Transformed P_1 or B_1 equations, with modifications (AD, SG, GG, etc.) appropriate to the system under consideration. Although this is not strictly a legitimate procedure, it is frequently employed with considerable success. For the Fourier Transform variable k, one must then use some sort of a buckling. Since the terms containing the transform variable are those that arise out of the spatial dependence of the flux and are therefore those connected with the leakage, the buckling should be chosen so as correctly to represent the leakage.* As used in this manner, the buckling should be lethargy (or group) dependent. If, for example, one is interested in calculating the core group constants for a reflected reactor, the buckling should represent the net leakage from the core to the reflector in the group under consideration. It may turn out in some cases that the net leakage is into the core, as for example, at thermal energies in the two group - two region problem typified by Figure 1; a negative value of B^2 may then be indicated. Generally, it is difficult to actually calculate the net leakage so that one uses either a two group calculation and takes as a

* These arguments may also be obtained by averaging the P_1 equations over a region.

material buckling, the positive root of Equation (4-19c), or uses a bare reactor material buckling. This value is then applied to all fast groups.

For a calculation of this sort, the choice of the relation between q_j, $q(u_j)$ and $q(u_{j-1})$ (or between the corresponding η if the GG approximation is used) is not critical as many groups are usually used. However, Ehrlich and Hurwitz[14] have pointed out that for consistency one should choose $\omega_1 + \omega_2 = 1$ in Equation (4-15f) when the group widths become very small. Previously, we chose $\omega_1 = 0$, $\omega_2 = 1$, in order to reduce group coupling to a minimum. Here the choice $\omega_1 = \omega_2 = 1/2$ is also frequently made. For large groups, the above conclution on ω_1 and ω_2 will have to be greater or less than unity depending on whether absorption and leakage or sources are more important in the particular group.

Then, a many-group calculation (sometimes more than 200 groups are used) is made and the multigroup Fourier Transformed fluxes and currents are computed. Cross sections for this problem are usually obtained by numerical averaging of the true cross sections (which is acceptable because of the relatively small size of the groups) except for the case of resonance capture, for which the NR or NRIA resonance integral formulae are often applied. Inelastic scattering cross sections are again treated as described earlier.

Having obtained the spectrum, it is relatively simple to obtain the required group constants. From Fick's Law, written as

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[14] R. Ehrlich and H. Hurwitz, Jr., Nucleonics, 12, 23 (1954).

$$\phi_1(k,u) = \nu B D(u) \phi_0(k,u) \qquad (4\text{-}31a)$$

one obtains, quite simply

$$D_j = -\frac{i}{B} \frac{\int_{\Delta u_j} \phi_1(u')du'}{\int_{\Delta u_j} \phi_0(u')\,du'} \qquad (4\text{-}31b)$$

The indicated integrals are approximated by sums over many of the smaller lethargy groups. Removal cross sections are obtained from the definition

$$\Sigma_{Rj} \int_{\Delta u_j} \phi_0(u')du' = q(u_j) \qquad (4\text{-}31c)$$

which insures that $\Sigma_{Rj}\phi_j$ will be the slowing down density out of each group. Should the various groups be coupled to groups not adjacent to themselves, additional problems are raised, these may usually be avoided by selecting group limits carefully. If this is not possible, hydrogen (and possibly deuterium) cross sections may be treated as inelastic cross sections, thus circumventing the problem. Inelastic multigroup cross sections $\sigma_{mj\to k}$ are evaluated by simply calculating the source to group k from group j and dividing by ϕ_j. Absorption and/or fission cross sections are found by direct averaging.

$$\Sigma_{aj} = \frac{\int_{\Delta u_j} \Sigma_a(u')\phi_0(u')\,du'}{\int_{\Delta u_j} \phi_0(u')\,du'} \qquad (4\text{-}31d)$$

The scheme described here is similar to that employed in the MUFT[15] and other codes, which have been used quite successfully in reactor design. Although the physical basis of such codes is far from rigorous, the group constants obtained from then are generally more accurate than those obtained by the simple methods given in the previous section.

Group constants have been complied by Argonne National Laboratory[16] for single elements, in 30 groups. For few group problems, constants may be obtained by averaging these compiled results over an assumed flux energy spectrum, for example, an '1/E' spectrum. Results obtained in this way are not as accurate as those obtained numerically, but they have the obvious advantage of ease of use.

9. Thermal Group Constants

As was the case with the fast group, the greatest obstacle to obtaining thermal group constants is usually a lack of knowledge of the exact neutron energy spectrum. Considerable work in this field, called thermalization, has been done in recent years, but as Corngold[17] has written a book covering this material extensively, we shall only give a brief review here.

As explained in Chapter I, neutrons in equilibrium with the moderator would have the Maxwell-Boltzmann Spectrum (i.e., the canonical distribution) peculiar to the moderator temperature. However, the pres-

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15 H. Bohl, Jr., E.M. Gelbard, G.H. Ryan, "MUFT-4, Fast Neutron Spectrum Code," Report WAPD-TM-22, (1957).

16 "Reactor Physics Constants," ANL 5800, p. 60, et.seq.

17 N. Corngold, "Neutron Thermalization," to be published.

ence of sources and sinks means that the neutron distribution will not be canonical. In the language of statistical mechanics, the neutron distribution must be described in terms of a Grand Canonical Ensemble[18] which merely means that the statistical distribution function (density in phase space) involves not only the energy of the system byt the number of particles (neutrons in our case) as well. This, in general, leads to an energy spectrum which is shifted upwards in energy or "hardened."

Thus, to obtain the correct thermal energy spectrum over which to average the thermal cross sections, it is necessary to solve the Boltzmann Equation as a function of energy at thermal energies. This is usually done in the diffusion approximation with energy space separability assumed, the spatial part being taken as a fundamental mode of the Helmholtz equation. This merely modifies the infinite medium equation by adding a term DB^2 to the absorption cross section[19].

The solution of this equation is more complicated than is the case of the slowing down problem for three important reasons:

(1) In chemically bound moderators (e.g., water) the neutron energy may well be below the binding energy of the molecule, which is usually of the order of a few electron volts. Energy transferred from a neutron to a nucleus is then insufficient to break the chemical bond so that the neutron interacts with the whole molecule.

(2) In solids there are crystalline effects which are related to the effect mentioned above. At very low energies the wave properties of the neutron enter and diffraction effects come into play.[20]

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[18] See, e.g., T. Hill, "Statistical Mechanics," McGraw-Hill, 1956.

[19] See, e.g., D. Parks, Nuc. Sci. Eng., 9, 430 (1961).

[20] M. Nelkin, Nuc. Sci. Eng., 2, 199 (1957).

(3) The presence of up-scattering (scattering with increase in energy) complicates the equation considerably.

The simplest method of obtaining thermal group constants is simply to average the parameters over a Maxwellian spectrum corresponding to the physical temperature. Since tabulations of cross section are usually made for E = .025 ev (kT at 298°K - corresponding to a velocity of 2200 meters per second) the average absorption or fission cross sections are most often expressed in terms of σ_a (2200 m/s)

$$\sigma_{aT} = \sigma_a (2200\,m/s) \sqrt{\frac{\pi}{4}} \sqrt{\frac{T_0}{T}}\, g(T) \qquad (4\text{-}32)$$

where g is a factor which corrects for non-1/v behavior and is unity for pure 1/v cross sections. Values of g have been tabulated for various isotopes.[21] In Chapter I it was found that the best procedure for determining a thermal diffusion coefficient is to average the transport cross section over the current and set

$$D_T = \frac{1}{3\Sigma_{trT}} \qquad (4\text{-}33a)$$

At thermal energies scattering is elastic and isotropic in the center of mass system (again, ignoring crystalline effects), so we may write:

$$\Sigma_{tr} = \Sigma_a + \Sigma_s\left(1 - \frac{2}{3A}\right) \qquad (4\text{-}33b)$$

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[21] C.H. Westcott, "Effective Cross Section Values for Well Moderated Thermal Reactor Spectra" Atomic Energy of Canada Ltd. Report CRRP680 (1957).

But there is still another point to be considered, namely the chemical binding described earlier which makes both σ_s and A effectively energy dependent. In the first born approximation one can show that the scattering cross section is given by[22]

$$\sigma_s = \mu^2 \sigma_o = \left(\frac{A}{A+1}\right)^2 \sigma_o \qquad (4\text{-}34)$$

where μ is the reduced mass of the neutron-nuclear system and σ_o is the scattering cross section of the tightly bound atom. For bound hydrogen, this effect causes the scattering cross section to go to 80 barns at low energies whereas it is only 20 barns at high energies at which the hydrogen acts as if it is free. In heavier elements the effect is less dramatic. One may then use Equation (4-34) and empirical cross section data to calculate an effective mass A_{eff} which may be used in Equation (4-33b) for purposes of calculating Σ_{tr} as a function of energy even at low energies. Calculations using this prescription have been made and are compiled in the literature.[23]

The first study of the effect of the temperature on the thermal spectrum was made by Wigner and Wilkins,[24] who studied the effect of the thermal motion of the atoms of a moderator gas on the differential scattering cross section. They arrived at a linear integral equation for the spectrum which, unfortunately, is not generally soluable in closed form. We quote only the result. For $E < E'$:

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22 J.M. Blatt and V. Weiskopf, "Theoretical Nuclear Physics", (1952). The first application of this formula to the calculation of Σ_{trT} was by A. Radkowsky.

23 C.D. Petrie, M.L. Storm, and P.F. Zweifel, Nuc.Sci.Eng., 2, 728 (1957).

24 E.P. Wigner and J.E. Wilkins, Report AECD 2275.

$$\int F(E' \to E)\phi(E')\,dE' = \left[\chi(E) + \frac{\Delta}{2A}\right]\phi(E) \qquad (4-35)$$

where

$$F(E' \to E) = \frac{e^{-\beta(E-E')}}{\sqrt{2\alpha}}\left[I(\gamma S - \gamma A t) + I(\gamma A S + \gamma t)\right]$$

$$+ \frac{e^{\beta(E-E')}}{\sqrt{2\alpha}}\left[I(\gamma S - \gamma A t) - I(\gamma A S - \gamma t)\right] \qquad (4-35a)$$

I(x) is the error function

$$I(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-y^2}\,dy \qquad (4-35b)$$

and

$$S = \frac{1}{2}\left(\sqrt{E} + \sqrt{E'}\right) \qquad t = \frac{1}{2}\left(\sqrt{E'} - \sqrt{E}\right)$$

$$\beta = \frac{1}{kT} \qquad \gamma = (AkT)^{-1/2} \qquad (4-35c)$$

$$\Delta = 2A\,\frac{\Sigma_a(kT)}{\Sigma_s}$$

$$\chi(E) = \left[\sqrt{2E} + \frac{kT}{A\sqrt{2E}}\right] I(\gamma A\sqrt{E})$$

for $E > E'$ one can calculate the kernel from the principle of detailed balance

$$\sigma(E' \to E)\,M(E') = \sigma(E \to E')\,M(E)$$

For the case of hydrogen, or for heavy nuclei, this integral equation can be reduced to a differential equation which may be solved analytically. Of course, the advent of high speed digital computers has made possible the numerical solution of Equation (4-35). This leads to the possibility of obtaining thermal group constants by averaging over a "Wigner-Wilkins Spectrum." While this is not the true neutron spectrum, it is often a reasonable approximation to it. This is the basis of some of the codes frequently used in reactor design, e.g., the SOFOCATE Code.

For the case of small absorption, the Wigner Wilkins Spectrum must reduce to the Maxwell-Boltzmann Distribution. As an aid to hand calculation, it is useful to be able to fit this spectrum to a hardened Maxwellian, that is, a Maxwellian Boltzmann Distribution with a "neutron temperature" higher than the physical temperature. K. Cohen[26] suggested that a relation of the form

$$T_{eff} = T\left[1 + C\,\frac{\Sigma_a(kT)}{\xi\Sigma_s}\right]$$

might be used. Deutsch[27] suggests that a value of C = 0.75 be used whereas Coveyou, Bate, and Osborn[28], using Monte Carlo techniques and a least square fit find 0.46 as the best value of C.

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25 H. Amster and R. Suarez, "Description of the SOFOCATE Code." Report WAPD-TM-39.

26 "Research Reactors, Physics", New York: McGraw-Hill, p.375, (1955).

27 R.W. Deutsch, Nucleonics, 15, 47 (1957)

28 P.R. Coveyou, R.R. Bate, and R.K. Osborn, J.Nuc.Energ., 2, 153 (1956).

These simplified calculations are frequently valuable as an aid in hand calculation, especially in cases for which the use of computers is not justified.

D. Solution of the Multigroup Equations

10. A Formal Solution

In theory, the method applied to the solution of the two-group, two-region problem could be extended to any multiregion problem in which each region is homogeneous. However, the determinants encountered when this approach is used are too large to be evaluated even on a large computer. Other methods have been found to be faster.

As we shall be dealing with large sets of linear equations, it will be convenient to employ matrix notation in this section. A review of matrix analysis can be found in many standard texts. For applications to neutron problems see the report by Bilodeau and Hageman.[29]

Assuming now that the group constants are known, the multigroup equations can be written:

$$-\nabla\cdot D_j \nabla \phi_j(\underline{r}) + \Sigma_{t_j}(\underline{r})\phi_j(\underline{r}) = \sum_{i=1}^{j-1} \Sigma_{ij}(\underline{r})\phi_i(\underline{r}) + \chi_j \nu \sum_{i=1}^{N} \Sigma_{f_i}\phi_i \qquad (4\text{-}37)$$

where $\Sigma_{ij}(\underline{r})$ is the cross section for transfer from group i to group j as discussed earlier (inelastic scattering will be included in $\Sigma_{ij}(\underline{r})$ for the present, although it may prove more convenient in some cases to treat it as indicated earlier). The simplifying assumption of coupling

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[29] B. Bilodeau and L. Hageman, "A Survey of Numerical Methods in the Solution of Diffusion Problems", Report WAPD-TM-64 (1957).

only to adjacent groups is not made as yet, but will obtain if inelastic scattering is neglected or treated separately. Also, fission is allowed to occur in all groups; χ_j denotes the fraction of the fission spectrum which falls into the j^{th} group:

$$\chi_j = \int_{\Delta u_j} f(u')du'$$

where $f(u)$ is the fission spectrum discussed in Chapter I. It is assumed, however, that no up-scattering occurs, i.e., that thermal neutrons are treated as one group, denoted by the subscript N. By defining a flux vector* $\underline{\Phi}$ as

$$\underline{\underline{\Phi}}(\underline{r}) = \begin{pmatrix} \phi_1(\underline{r}) \\ \phi_2(\underline{r}) \\ \vdots \\ \phi_N(\underline{r}) \end{pmatrix} \qquad (4\text{-}38a)$$

and the operator matrices

$$\underline{\underline{M}} = \begin{pmatrix} -\underline{\nabla}\cdot D_1\underline{\nabla} + \Sigma_{t1} & 0 & 0 \\ 0 & -\underline{\nabla}\cdot D_2\underline{\nabla} + \Sigma_{t2} & \\ & 0 & \ddots \\ & & -\underline{\nabla}\cdot D_N\underline{\nabla} + \Sigma_{aN} \end{pmatrix} \qquad (4\text{-}38b)$$

$$\underline{\underline{\Pi}} = \begin{pmatrix} \chi_1\Sigma_{f1} & \chi_1\Sigma_{f2} & \cdots & \\ \chi_2\Sigma_{f2} & \chi_2\Sigma_{f2} & & \\ & \ddots & \ddots & \\ & & & \chi_N\Sigma_{fN} \end{pmatrix} \qquad (4\text{-}38c)$$

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* Again "vector" in the mathematical sense of an Nxl matrix.

and

$$\underline{\underline{\Sigma}} = \begin{pmatrix} 0 & 0 & 0 & & \\ \Sigma_{12} & 0 & & & \\ \Sigma_{13} & \Sigma_{23} & \ddots & 0 & 0 \\ \vdots & & & \Sigma_{N-1,N} & 0 \\ \Sigma_{1N} & & & & \end{pmatrix} \qquad (4\text{-}38d)$$

It is possible to write the multigroup equations in matrix form:

$$\underline{\underline{M}}\,\underline{\Phi} - \underline{\underline{\Sigma}}\,\underline{\Phi} - \nu\,\underline{\underline{F}}\,\underline{\Phi} = 0 \qquad (4\text{-}38e)$$

Proceeding formally, Equation (4-38e) can be written as

$$\frac{1}{\nu}\,\underline{\Phi} = (\underline{\underline{M-\Sigma}})^{-1}\,\underline{\underline{F}}\,\underline{\Phi} = \underline{\underline{L}}\,\underline{\Phi} \qquad (4\text{-}38f)$$

by operating with the matrix $(\underline{\underline{M - \Sigma}})^{-1}$, the inverse matrix to $(\underline{\underline{M - \Sigma}})$. That such a matrix exists can be shown and for the moment it is assumed to be a known matrix. Then one needs only to find the eigenvalues $(1/\nu)$ of the matrix $\underline{\underline{L}} = (\underline{\underline{M - \Sigma}})^{-1}\,\underline{\underline{F}}$. Again, formally, they may be obtained by setting the determinant of the matrix $(1/\nu\,\underline{\underline{I}} - \underline{\underline{L}})$ equal to zero. An algebraic equation of degree N in ν is thus obtained, yielding N values of ν. The largest of these, ν_c, will later be shown to be the significant one and k_{eff} is then determined as the ratio of the physical value of ν to this value. The eigenvector belonging to this eigenvalue, i.e., the function satisfying the relation

$$\underline{\underline{L}}\,\underline{\Phi} = \frac{1}{\nu_c}\,\underline{\Phi}$$

is then the steady state flux in the reactor.

All of this is quite formal, but the procedure may be used. In practice, the method is intractable because the problem of inverting the matrix $(\underline{\underline{M}} - \underline{\underline{\Sigma}})$ is quite a difficult one. Since $\underline{\underline{M}}$ involves the differential operator $\underline{\nabla} \cdot D \underline{\nabla}$ the inverse matrix $(\underline{\underline{M}} - \underline{\underline{\Sigma}})^{-1}$ will involve the inverse of this operator, which must be interpreted in terms of the Green's Function. That is

$$\left(-\underline{\nabla} \cdot D \underline{\nabla} + \Sigma_t\right)^{-1} \psi(\underline{r}) = \int_R G(\underline{r}, \underline{r}') \, \psi(\underline{r}') \, d^3 r' \qquad (4\text{-}39a)$$

where the Greens' Function $G(\underline{r}, \underline{r}')$ satisfies the equation

$$-\underline{\nabla} \cdot D \underline{\nabla} G(\underline{r}, \underline{r}') + \Sigma_t G(\underline{r}, \underline{r}') = -\delta(\underline{r} - \underline{r}') \qquad (4\text{-}39b)$$

with the boundary condition

$$G(\underline{r}, \underline{r}') = 0 \qquad (4\text{-}39c)$$

for $\underline{r}$ on the extrapolated boundary of the reactor. The problem of finding the inverse matrix $(\underline{\underline{M}} - \underline{\underline{\Sigma}})^{-1}$ is thus made extremely difficult and this approach has been found to be an extremely inefficient one. Other methods, which involve iterative procedures are used more frequently and will be described in succeeding sections.

11. Source Iteration

While the above method is simple and straight-forward in theory, it is quite impractical; other schemes must be found. In particular, one would like to have a series or iterative procedure that converges to the correct effective multiplication factor k_{eff} and the correct space-energy distribution of the flux.

Physically, if a reactor has a known neutron flux distribution in space and energy, at time $t = 0$, one expects that this flux will grow, die out, or stay constant according to whether the reactor is supercritical, subcritical, or just critical. Moreover, at much later times the neutron distribution in space and energy is expected to become independent of time; its magnitude may increase or decrease, but the space-energy distribution should remain the same. At this stage each neutron generation will have the same space-energy distribution as the one preceding it but will be multiplied or divided by a factor of k_{eff}. This is, in fact, an operational definition of k_{eff}.

Now one could use the multigroup equations to simulate this behavior. It is, however, somewhat inconvenient to work with the space-energy flux distribution itselfs this involves knowledge of a great many quantities. Rather, one notes that the neutron source for the i^{th} generation is

$$S^{i}(\underline{r}) = \nu \sum_{d=1}^{N} \Sigma_{fd} \phi_{d}^{(i-1)}(\underline{r}) \qquad (4\text{-}40a)$$

$\phi_j^{(i-1)}(\underline{r})$ being the (i-1)st generation flux in the j^{th} group, and that $S^i(\underline{r})$ becomes independent of i for large i. Since the spatial source shape is energy independent, a considerable saving in effort can be effected by using it rather than the flux itself; only one spatial distribution need be assumed.

Defining a source vector $\underline{S}$ as

$$\underline{S} = \begin{pmatrix} S_1 \\ S_2 \\ \vdots \\ S_N \end{pmatrix} \qquad (4\text{-}40b)$$

we note that the elements of this vector are

$$S_g(r) = \chi_g S(r) \qquad (4\text{-}40c)$$

and all have the same space dependence. Also by comparing Equation (4-40c) with the definition of the matrix $\underline{\underline{F}}$, Equation (4-38c), we have

$$\underline{S} = \nu \underline{\underline{F}} \underline{\Phi} \qquad (4\text{-}40d)$$

Operating on Equation (4-38f) with the matrix $\underline{\underline{F}}$, we find that the source vector $\underline{S}$ satisfies the matrix equation

$$\frac{1}{\nu}\underline{S} = \underline{\underline{F}}\underline{\underline{(M-\Sigma)}}^{-1}\underline{\underline{F}}\underline{\Phi} = \underline{\underline{F}}\underline{\underline{(M-\Sigma)}}^{-1}\underline{S} = \underline{\underline{P}}\underline{S} \qquad (4\text{-}40e)$$

where $\underline{\underline{P}}$ is the matrix

$$\underline{\underline{P}} = \underline{\underline{F}}\underline{\underline{(M-\Sigma)}}^{-1}$$

In particular, note that if $\underline{\Phi}$ is the eigenvector of $\underline{\underline{L}}$ corresponding to the eigenvalue ν_c then $\underline{\underline{F}}\,\underline{\Phi}$ is the eigenvector of $\underline{\underline{P}}$ with the same eigenvalue. Thus, the source and the multigroup fluxes can be used practically interchangably for obtaining the eigenvalues in a critical problem. This leads us to the following scheme.

A guess at the neutron source distribution is made, say $S_o(r)$, and inserted into the multigroup equations. Starting with the first group and working down to the thermal group, one calculates a set of multigroup fluxes, from which a new source can be calculated using Equation (4-40a). This is the source for the second generation; in carrying out this calculation, we have effectively followed the neutrons from the assumed source through one generation and found the distribution of fission events caused by them. This procedure is known as source iteration and it is physically reasonable that this procedure will converge. Mathematical proofs of the convergence of the method will be cited later. Within each group, iteration procedures are used to calculate the spatial distribution of the flux, i.e., to integrate numerically the group diffusion equation. Such iterations, to be described later, are known as inner iterations whereas the entire process of calculating a new source distribution from the previous one is known as an outer iteration. Hence, each outer iteration contains N inner iterations. In general, the procedures applied to the various iterations are different owing to the somewhat different nature of the two problems.

12. Outer Iterations

Outer iterations are, as explained above, used to calculate the eigenvalues of an equation of the type

$$\underline{\underline{L}}\,\underline{\Phi} = \lambda \underline{\Phi} \qquad (4\text{-}41a)$$

which is Equation (4-38f) written with $\lambda = 1/\nu$. An inner iteration is

really an attempt to solve a problem of the type

$$Q \phi_j(r) = T_j(r) \qquad (4-41b)$$

where Q is a space dependent operator, and $T_j(\underline{r})$ is the source (fission and slowing down) in the j^{th} group; $\phi_j(\underline{r})$ and $T_j(\underline{r})$ are to vanish on a boundary. Later, it will be shown how an equation of this type can be put into matrix form by means of finite difference techniques. The important point is that the source in the j^{th} group, is an inhomogeneous term in Equation (4-41b). The types of problems solved by inner and outer iterations are thus distinctly different; the former involves an inhomogeneous differential equation (or, in finite differences, a set of inhomogeneous linear algebraic equations) whereas the latter is an eigenvalue problem. It is to be expected, therefore, that the techniques applied to each of these types of iterations will be different. Outer iterations are considered first.

Before proceeding, a brief review of some of the more important properties of matrices will be given and a few mathematical theorems will be quoted.

It is known that an $N \times N$ matrix generally possesses N different linearly independent eigenvectors each with its own eigenvalue. That is, there are N different N-dimensional column vectors which satisfy the equations

$$\underline{\underline{A}}\ \underline{\psi}_n = \lambda_n \underline{\psi}_n$$

where $\underline{\underline{A}}$ is an $N \times N$ matrix, each eigenvector $\underline{\psi}_n$ corresponds to a definite eigenvalue λ_n (which may be complex and not necessarily

distinct). For a symmetric matrix, i.e., one which has the property

$$A_{ij} = A_{ji}$$

the eigenvalues are real and the eigenvectors are orthogonal, that is, the scalar product of two eigenvectors is zero for different eigenvectors. Normalization of the eigenvectors is possible, so that

$$(\underline{\psi}_n, \underline{\psi}_m) = \delta_{nm}$$

However, the multigroup matrix operator is certainly not symmetric. In this case it is possible to define a set of adjoint eigenvectors* by

$$\underline{\psi}_n^+ \underline{\underline{A}}^+ = \mu_n \underline{\psi}_n^+$$

with

$$\mu_n = \lambda_n^*$$

which, when the vectors are properly normalized, have the properties

$$(\underline{\psi}_n^+, \underline{\psi}_m) = \delta_{nm}$$

where the (*) denotes complex conjugation.

$\underline{\underline{A}}^+$ is the matrix adjoint to $\underline{\underline{A}}$. Finally, the eigenvectors of $\underline{\underline{A}}$ form a complete set (any vector with similar structure may be

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* The adjoint eigenvectors are N x 1 , i.e., row vectors.

expanded in terms of them).

Further results which apply specifically to the multigroup operators have been derived by Habetler and Martino[30]. They showed that the multigroup operator (the matrix $\underline{\underline{L}}$ here) possesses a real eigenvalue λ_o, which is larger in absolute value than any other eigenvalue. Moreover, this eigenvalue is non degenerate (only one eigenfunction is associated with it); its eigenvector which we shall call Ψ_o is the only one whose components (elements) are all non-negative throughout the reactor and its adjoint eigenvector, which satisfies the equation

$$\frac{1}{\nu_c}\,\underline{\Phi}_o^+ = \underline{\Phi}_o^+ \underline{\underline{L}}^+$$

is the only adjoint eigenvector whose elements are everywhere non-negative inside the reactor. These are the only eigenvectors which are acceptable on physical grounds as solutions to the reactor problem. Birkhoff and Varga[31] have proven similar results using the finite difference equations which will be given in the next section.

Having this knowledge and desiring to use an iterative procedure, all that one needs to do now is to show that a particular iteration scheme converges. The earlier discussion of iteration methods suggests the following iteration scheme known as the Power Method. Suppose that $\underline{S}^{(n+1)}$ is to be calculated from $\underline{S}^{(n)}$ by using the formula

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30 G.J. Habetler and M.A. Martino, "The Multigroup Diffusion Equations of Reactor Physics" Report KAPL-1886 (July 1958).

31 G. Birkhoff and R. Varga, "Reactor Criticality and Non-Negative Matrices", J. Soc. Ind. App. Math., 6, 354 (1959).

$$\underline{S}^{(n+1)} = \underline{\underline{P}}\,\underline{S}^{(n)} \qquad (4\text{-}43a)$$

Now one guesses an initial source, say $\underline{S}^{(0)}$, which can be expanded in terms of the eigenvectors of $\underline{\underline{P}}$:

$$\underline{S}^{(0)} = \sum_{n=1}^{N} \sigma_n \underline{\Psi}_n \qquad (4\text{-}43b)$$

where the $\underline{\Psi}_n$ satisfy

$$\underline{\underline{P}}\,\underline{\Psi}_n = \lambda_n \underline{\Psi}_n \qquad (4\text{-}43c)$$

Substituting this expansion into the iteration formula (4-43a) we have for the first iterate

$$\underline{S}^{(1)} = \sum_{n=1}^{N} \sigma_n \underline{\underline{P}}\,\underline{\Psi}_n = \sum_{n=1}^{N} \sigma_n \lambda_n \underline{\Psi}_n$$

Repeating this process k times, we have

$$\underline{S}^{(k)} = \sum_{n=1}^{N} \sigma_n \lambda_n^k \underline{\Psi}_n = \lambda_0^k \sum_{n=1}^{N} \sigma_n \left(\frac{\lambda_n}{\lambda_0}\right)^k \underline{\Psi}_n \qquad (4\text{-}44a)$$

where λ_0 is the real eigenvalue guaranteed by the work cited above. Since λ_0 is larger in absolute value than any of the other λ_n, the eigenfunction corresponding to it will become dominant after a sufficiently large number of iterations, provided that the original guess was such that $\sigma_0 \neq 0$. However, since $\underline{\Psi}_0$ is the only eigenvector whose elements are all non-negative within the reactor, this can be

guaranteed by making $\underline{S}^{(o)}$ non-negative throughout the reactor volume. Then, after a large number of iterations

$$\underline{S}^{(k)} \longrightarrow \lambda_o^k \sigma_o \underline{\psi}_o \qquad (4-44b)$$

and the eigenvalue λ_o (which is $1/\nu_c$) can be calculated quite simply, since we may now take the total source

$$S^{(k)}(\underline{r}) = \sum_{\mu=1}^{N} S_\mu^{(k)}(\underline{r}) \qquad (4-44c)$$

and find

$$\lambda_o = \frac{S^{(k+1)}(\underline{r})}{S^{(k)}(\underline{r})} \qquad (4-44d)$$

This scheme is a useful one and it is seen that the rate of convergence, i.e., the number of iterations required for dominance of the $\underline{\Psi}_o$ term, is related to (λ_1/λ_o) where λ_1 is the eigenvalue of $\underline{\underline{P}}$ with the second largest absolute value. It is also related to the ratio of the expansion coefficients σ_n so that there is considerable advantage in being able to supply an original source guess which is as accurate as possible. Such a guess might be obtained, for example, from a two group-two region problem.

There is still one major drawback in the above method. A scale factor λ_o^k, which may be quite different from unity is introduced and may cause the source iterate to grow to large (or small) for handling on a computer if many iterations are required. In turn, this poses a

difficult problem for computer applications.

This problem can be avoided by another choice of iteration scheme. Several variations of the above scheme have been suggested. After each iteration of the type described above, an estimate of the eigenvalue λ_o may be computed by some method. For example, by taking the scalar product of Equation (4-40c) with $\underline{S}$, one has:

$$\frac{1}{\nu} = \frac{(\underline{S}, \underline{\underline{P}}\,\underline{S})}{(\underline{S}, \underline{S})} \qquad (4\text{-}45a)$$

On the k^{th} iteration an estimate of ν is therefore:

$$\frac{1}{\nu^{(k)}} = \frac{(\underline{S}^{(k)}, \underline{\underline{P}}\,\underline{S}^{(k)})}{(\underline{S}^{(k)}, \underline{S}^{(k)})} \qquad (4\text{-}45b)$$

But, as we have seen in Equation (4-43a), $\underline{\underline{P}}\,\underline{S}^{(k)}$ is simply the source resulting from fissions induced by the multigroup fluxes generated with $\underline{S}^{(k)}$ as a source. Hence, each element of the vector $\underline{\underline{P}}\,\underline{S}^{(k)}$ has the same spatial dependence (although not the same spatial dependence as the elements of $\underline{S}^{(k)}$). Thus, one might as well compute

$$T^{(k)}(\underline{r}) = \sum_{i=1}^{N} (\underline{\underline{P}}\,\underline{S}^{(k)})_i \qquad (4\text{-}45c)$$

where the subscript "i" denotes the i^{th} element of the vector $\underline{\underline{P}}\,\underline{S}^{(k)}$ and calculate the eigenvalue from

$$\frac{1}{\nu^{(k)}} = \frac{\int_R T^{(k)}(\underline{r})\, S^{(k)}(\underline{r})\, d^3r}{\int_R [S(\underline{r})]^2 d^3r} \qquad (4\text{-}45d)$$

Having found an estimate of the eigenvalue, one may easily calculate the $(k+1)^{st}$ iterate of the source

$$S^{(k+1)}(\underline{r}) = \nu^{(k)} T^{(k)}(\underline{r}) \qquad (4\text{-}45e)$$

which is of the same magnitude as $S^{(k)}(\underline{r})$. No large scale factor is introduced when this iteration scheme is used and the eigenvalue, ν_c, which is generally as important a quantity as the flux itself, is obtained in the process. That this scheme converges to the desired eigenvalue and eigenvector can be shown; the proof is quite similar to that given for the earlier method but is omitted because of its length[32]. No improvement in the rate of convergence is obtained but the method does present the advantages enumerated above.

Another variation was suggested by Ehrlich and Hurwitz[33]. Instead of the straightforward method given above they make use of the adjoint multigroup equations. Instead of taking the scalar product of Equation (4-40c) with $\underline{S}$, they take the scalar product with the adjoint source $\underline{S}^+$ to obtain

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[32] A proof can be found in Bilodeau and Hageman, op.cit.

[33] R. Ehrlich and H. Hurwitz, Jr., Nucleonics, 12, 23 (1954).

$$\frac{1}{\nu} = \frac{(\underline{S}^+, \underline{\underline{P}}\,\underline{S})}{(\underline{S}^+, \underline{S})} = \frac{(\underline{\underline{P}}^+\underline{S}^+, \underline{S})}{(\underline{S}^+, \underline{S})} \qquad (4\text{-}46)$$

which is a variationally stationary and thus has the advantage of causing an error in ν_c to be the products of the relative errors in $\underline{S}$ and S^+. In using this method, a guess is made at both the source and its adjoint. Then one iterates, say first on $\underline{S}$ to find $\underline{\underline{P}}\,\underline{S}^{(o)}$. On substituting this into the first expression in Equation (4-46) an estimate of ν is obtained and the first iterate source may be found as in the previous cases. Then one can next follow a similar procedure with the adjoint source, using the guessed adjoint source in the adjoint multigroup equations to generate $\underline{\underline{P}}^+\,\underline{S}^{+(o)}$. In carrying out the inner iterations which comprise the outer iteration, one needs simply to use the group constants in a different order and to compute the group fluxes starting at thermal rather than at the highest energy group. This "adjoint" convergence scheme converges somewhat more rapidly than the methods previously discussed, and has the further advantage of yielding the adjoint flux which is a valuable quantity for carrying out perturbation calculations.

13. Extrapolation Methods

Many attempts have been made to improve the "non-adjoint" schemes[34]. The incentive for improvement lies, of course, in the fact that the power method and its variations require a great many iterations

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[34] Bilodeau and Hageman, op.cit.

for convergence. Most frequently, convergence of the eigenvalue is the criterion by which multigroup calculations are terminated; generally the criterion requires the eigenvalues for two successive iterations differ by less than some predetermined amount. In the power method one usually find that the eigenvalue is always to one side of the correct (converged) value and that the error decreases monotonically as the number of iterations increases.

This result is very helpful in formulating improved convergence schemes. Thus, if the last estimate of the eigenvalue is smaller than the one prior to it, it may be assumed that the current estimate is too high. It is then reasonable to choose a guess which is even lower than the last estimate -- one is practically guaranteed of being closer to the correct value. The danger in such a procedure is, of course, the possibility of "overshoot", i.e., of choosing a value which is lower than the correct result, since this may lead to oscillation in the estimated eigenvalue and accompanying increase in the number of iterations required. This difficulty may be overcome by the intuitive argument that the rate of convergence should be approximately the same on each iteration. Rationale for this argument for the flux is given by Equation (4-44a) in which it is seen that the coefficient of the second eigenfunction $\underline{\Psi}_1$, which is the major source of variation between $\underline{S}^{(n)}$ and the converged sources, decreases by a factor of (λ_1/λ_0) on each iteration. Thus, since one operates with the source, it might be reasonable to set

$$\underline{S}^{(n)\prime} = \underline{S}^{(n)} - (\underline{S}^{(n-1)} - \underline{S}^{(n)}) = 2\underline{S}^{(n)} - \underline{S}^{(n-1)} \qquad (4\text{-}47a)$$

where $\underline{S}^{(n)'}$ is now the source guess to be used in the $(n+1)^{st}$ iteration. However, this may lead to overshoot and oscillation so that one generally introduces an "extrapolation factor" α :

$$\underline{S}^{(n)'} = \underline{S}^{(n)} - \alpha(\underline{S}^{(n-1)} - \underline{S}^{(n)}) = (1+\alpha)\underline{S}^{(n)} - \alpha \underline{S}^{(n-1)}$$

$$= [(1+\alpha)\underline{\underline{P}} - \alpha \underline{\underline{I}}]\, \underline{S}^{(n-1)} \qquad (4\text{-}47b)$$

where $\underline{\underline{I}}$ is the unit matrix

$$I_{ij} = \delta_{ij}$$

Generally, in order to avoid overshoot one chooses α to be less than unity. This results in the extrapolation method. Clearly, for $\alpha = 0$ the extrapolation method is identical to the power method.

In this procedure the additional question of the choice of the extrapolation factor α arises. Usually α will be different for each iteration and the optimum choice will be that which minimizes the number of iterations required. Means of choosing optimum values for α will be given after the next paragraph.

Having decided that an extrapolation scheme can lead to an improved rate of convergence, one can then generalize the technique. Instead of choosing as the $(n+1)^{st}$ iteration source $\underline{S}^{(n)'}$ of Equation (4-47b) one might attempt to employ the sources calculated on several

previous iterations:

$$\underline{S}^{(n)'} = \sum_{i=1}^{n} \beta_i \underline{S}^{(i)} \qquad (4-48a)$$

or, since

$$\underline{S}^{(i)} = \underline{\underline{P}}^{i} \underline{S}^{(0)}$$

$$\underline{S}^{(n)'} = \sum_{i=1}^{n} \beta_i \underline{\underline{P}}^{i} \underline{S}^{(0)} \qquad (4-48b)$$

If the initial source guess $\underline{S}^{(0)}$ is again expanded in terms of the eigenfunctions Ψ_k of $\underline{\underline{P}}$ as in Equation (4-43b)

$$\underline{S}^{(0)} = \sum_{k=0}^{N-1} \sigma_k \underline{\Psi}_k$$

and inserted into Equation (4-48b), one has

$$\underline{S}^{(n)'} = \sum_{i=1}^{n} \sum_{k=0}^{N-1} \beta_i \sigma_k \lambda_k^i \underline{\Psi}_k$$

$$= \sum_{k=0}^{N-1} \sigma_k \underline{\Psi}_k \left(\sum_{i=1}^{n} \beta_i \lambda_k^i \right)$$

From Equation (4-48c) it is seen that to obtain the maximum dominance of Ψ_0 one should select the β_i such that the ratio of

$$\sum_{i=1}^{n} \beta_i \lambda_k^i$$

for $k = 0$ is a maximal with respect to this sum for all $k \neq 0$.

Here a theorem of Flanders and Shortley[35] proves extremely useful. It states that of all polynomials of degree n having the value $+1$ at a given point, say $x = x_o (x_o > 1)$, the polynomial

$$Q_n(x) = \frac{T_n(x)}{T_n(x_o)} \qquad (4\text{-}49a)$$

where $T_k(x)$ is the Tschebycheff Polynomial of degree n, has the minimum maximum absolute value in the range $|x| < x_o$. That is, any polynomial of degree n will in general have maxima (in its absolute value) in the range under consideration; the Tschebycheff Polynomial has the property that it has the lowest value at any of these points. Note that the point $x = -x_o$ may be considered as one of these points if the function is increasing (in absolute value) at x_o.

This theorem provides exactly the recipe required for choosing the β_i of Equation (4-48a) as it proves that if the β_i are taken to be the coefficients of x^i in the polynomial $Q_k(x)$ of Equation (4-49a), the dominance of $\underline{\Psi}_o$ is maximized, i.e., its coefficient is greatest relative to any of the coefficients of the other $\underline{\Psi}_k$. (Note $\lambda_k < \lambda_o$ for $k > 0$). In practice, the use of this method is severely restricted by the fact that it requires all previous source iterates in forming the

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35 D.A. Flanders and G. Shortley, J. Appl. Phys., 21, 132 (1950).

current source guess. Again, this requires a larger computer memory than the earlier techniques.

Thus, a logical step would be to attempt to modify the extrapolation method in such a way that it acts essentially as the Tschebycheff Polynomial Method. Use of the iteration scheme suggested by Equation (4-47b) leads to the result

$$\underline{S}^{(n)'} = \prod_{\mu=1}^{n} \left[(1+\alpha_i)\underline{\underline{P}} + \alpha_i \underline{\underline{I}} \right] \underline{S}^{(0)} \qquad (4-49b)$$

after n iterations if the scale factor introduced by dividing each source by $\nu^{(i)}$ is omitted for the sake of this argument. Then it is seen that after n iterations it is possible to have

$$\underline{S}^{(n)'} = Q_n(\underline{\underline{P}})\,\underline{S}^{(0)} \qquad (4-49c)$$

provided only that the α_i are selected so as to generate Q_n after n iterations. Furthermore, this can always be done as the roots of the Tschebycheff Polynomials are all real and one can therefore always write

$$Q_n(x) = \prod_{\mu=1}^{n} \left[(1+\alpha_i)x - \alpha_i \right] \qquad (4-49d)$$

with a suitable choice of α_i . Bilodeau[36] has shown that the proper

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[36] G.G. Bilodeau, "Extraploation Techniques for Real Symmetric Matrices," WAPD-TM-52 (1957).

choice of the α_i are:

$$\alpha_i^{(n)} = \frac{\lambda_1 + \lambda_{N-1} + (\lambda_1 - \lambda_{N-1}) \cos \frac{2i+1}{2n} \pi}{2\lambda_o^{(n)} - \lambda_1 - \lambda_{N-1} - (\lambda_1 - \lambda_{N-1}) \cos \frac{2i+1}{2n} \pi} \qquad (4-49e)$$

where $\lambda_o^{(n)}$ is the n^{th} estimate of the eigenvalue λ_o, λ_{N-1} is smallest eigenvalue of $\underline{\underline{P}}$ and λ_1 is the second largest eigenvalue of $\underline{\underline{P}}$. Thus, having selected a number of iterations n, one can always make the extrapolation method and the Tschebycheff Polynomial method coincide.

14. The Finite Difference Equations

Within each outer iteration, it is necessary to find the spatial dependence of the N group fluxes. Given the fission source, one may begin with the highest energy group and calculate the spatial dependence of the flux in this group. When this flux is known, the source for the next higher energy group is also determined as

$$\Sigma_{R1} \phi_1(\underline{r}) + \chi_2 S(\underline{r})$$

where the subscript "1" refers to the highest energy group. From this source, the spatial dependence of the flux in group "2" may be determined. Repetition of the procedure yields all N of the group fluxes and finally a new source

$$\sum_{J=1}^{N} \Sigma_{f_J}(\underline{r})\,\phi_J(\underline{r})$$

which completes one outer iteration. Within each group the problem of calculating the individual group fluxes must be solved.

Basically the problem can be stated as one of solving the equation

$$-\nabla \cdot D_j(\underline{r})\nabla\phi_j(\underline{r}) + \Sigma_j(\underline{r})\phi_j(\underline{r}) = S_j(\underline{r}) \qquad (4\text{-}50a)$$

where we have written

$$\Sigma_j(\underline{r}) = \Sigma_{a_j}(\underline{r}) + \Sigma_{R_j}(\underline{r}) \qquad (4\text{-}50b)$$

and $S_j(\underline{r})$ represents the sum of the slowing down and fission source terms. The boundary conditions that the flux $\phi_j(\underline{r})$ and the current

$$-D_j(\underline{r})\nabla\phi_j(\underline{r})$$

are continuous at all points in the reactor and that the flux obey a given outer boundary condition are to be applied. Generally, for reactor problem the outer boundary condition is that the flux vanish on some surface, but frequently one wishes to apply multigroup calculations to the calculation of group constants for a cell. For example, in a periodic lattice, a cell of the repeating structure may be chosen and it is assumed that the cell is placed in the lattice such that there is no net

flow of neutrons into or out of this cell. Such a condition is accurate provided that the cell is in a region in which the spatial variation of the flux (ignoring details within a cell) is nearly flat (such as would obtain, for example, near the center of a large reactor). Then one must solve the (4-50a) subject to the condition that

$$\underline{\nabla}\, \phi_g(\underline{r}) = 0 \qquad (4\text{-}50c)$$

on the outer boundary.

In any case, the important point is that a boundary value problem must be solved. Generally, such problems are considerably more difficult than similar initial value problems; the latter are much simplified by the fact that it is generally possible to begin at the initial value and solve for the value of the desired function at each successive point. For boundary value problems the procedure is more likely to be one of guessing the solution and then using the differential equation to correct (relax) the guess in such a fashion that the differential equation is satisfied everywhere and the correct boundary values are assumed on the boundary.

Since all of this work will require finite difference approximations, the operator $\underline{\nabla} \cdot D\, \underline{\nabla}$ is first reduced to difference form. First, we note that in Cartesian Coordinates

$$\underline{\nabla} \cdot D \nabla \phi = \frac{\partial}{\partial x}\left(D \frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(D \frac{\partial \phi}{\partial y}\right) + \frac{\partial}{\partial z}\left(D \frac{\partial \phi}{\partial z}\right) \qquad (4\text{-}51a)$$

(all of the follwing may be carried out in any coordinate system with little added difficulty). Now a three dimensional mesh of points is laid

on the reactor and one can approximate, for a point midway between i, j, k and i + 1, j, k

$$D\frac{\partial}{\partial x} \simeq \frac{\left[\phi_{i+1,j,k} - \phi_{i,j,k}\right]}{\Delta X_{ijk}} D^{x}_{ijk} \qquad (4\text{-}51b)$$

where

$$\Delta X_{ijk} = X_{i+1} - X_i$$

$$D^{x}_{ijk} = \frac{\left[D_{i+1,j,k} + D_{i,j,k}\right]}{2}$$

with similar approximations in the y and z directions (indices j and k). Note that the mesh spacings ΔX need not be all the same size. Naturally, it is advantageous to use finer spacings in regions in which there is a need for more detailed knowledge of the spatial variation of the flux. Approximating further, one can write

$$\frac{\partial}{\partial x} D \frac{\partial \phi}{\partial x} = \left[D^{x}_{ijk} \frac{\phi_{i+1,j,k} - \phi_{ijk}}{\Delta X_i} - D^{x}_{i-1,j,k} \frac{\phi_{i,j,k} - \phi_{i-1,j,k}}{\Delta X_{i-1}}\right] \cdot \frac{2}{\Delta X_i + \Delta X_{i-1}}$$

which, using the abbreviations

$$a^{+}_{ijk} = \frac{D^{x}_{ij,k}}{\Delta x_i} \quad \frac{2}{\Delta x_i + \Delta x_{i-1}}$$

$$a^{-}_{ijk} = \frac{D^{x}_{i-1,j,k}}{\Delta x_{i-1}} \quad \frac{2}{\Delta x_i + \Delta x_{i-1}}$$

$$a_{ijk} = \left[\frac{D^{x}_{i,j,k}}{\Delta x_i} + \frac{D^{x}_{i-1,j,k}}{\Delta x_i} \right] \frac{2}{\Delta x_i + \Delta x_{i-1}}$$

can be rewritten as

$$\left. \frac{\partial}{\partial x} D \frac{\partial \phi}{\partial x} \right]_{i,j,k} = a^{+}_{i,j,k} \phi_{i+1,j,k} + a^{-}_{i,j,k} \phi_{i-1,j,k} - a_{i,j,k} \phi_{i,j,k} \qquad (4\text{-}51e)$$

One can make a similar analysis in the y and z directions to arrive at the result:

$$\begin{aligned} \left. \nabla \cdot D \nabla \phi \right]_{ijk} = {} & a^{+}_{ijk} \phi_{i+1,j,k} + a^{-}_{ijk} \phi_{i-1,j,k} \\ & + b^{+}_{ijk} \phi_{i,j+1,k} + b^{-}_{ijk} \phi_{i,j-1,k} \\ & + c^{+}_{ijk} \phi_{ij,k+1} + c^{-}_{i,j,k} \phi_{i,j,k-1} \\ & + d_{i,j,k} \phi_{i,j,k} \end{aligned} \qquad (4\text{-}51f)$$

where by analogy to the quantities defined earlier we have defined:

$$b^{\pm}_{i,j,k} = \frac{2}{\Delta y_j + \Delta y_{j-1}} \frac{D^{y}_{i\{j,j-1\}k}}{\Delta y_{\{j,j-1\}}}$$

$$C^{\pm}_{i,j,k} = \frac{2}{\Delta z_k + \Delta z_{k-1}} \frac{D^{z}_{ij\{k,k-1\}}}{\Delta z_{\{k,k-1\}}} \qquad (4\text{-}51g)$$

with

$$D^{y}_{i,j,k} = \frac{D_{i,j+1,k} + D_{i,j,k}}{2}$$

$$D^{z}_{i,j,k} = \frac{D_{i,j,k+1} + D_{i,j,k}}{2}$$

and

$$\Delta y_j = y_{i,j+1,k} - y_{i,j,k}$$
$$\Delta z_k = z_{i,j,k+1} - z_{i,j,k}$$

$$d_{i,j,k} = a_{i,j,k} + b_{i,j,k} + c_{i,j,k}$$

$$b_{i,j,k} = \left[\frac{D^{y}_{i,j,k}}{\Delta y_j} + \frac{D^{y}_{i,j-1,k}}{\Delta y_{j-1}} \right] \frac{2}{\Delta y_j + \Delta y_{j-1}}$$

$$C_{i,j,k} = \left[\frac{D^{z}_{i,j,k}}{\Delta z_k} + \frac{D^{z}_{i,j,k-1}}{\Delta z_{k-1}} \right] \frac{2}{\Delta z_k + \Delta z_{k-1}}$$

Equation (4-51f) is frequently referred to as the seven point difference formula. In one and two dimensions the difference formulae are, of course, three and five point formulae.

The difference equations are thus

$$a^{+}_{i,j,k}\,\phi_{i+1,j,k} + a^{-}_{i,j,k}\,\phi_{i-1,j,k} + b^{+}_{i,j,k}\,\phi_{i,j-1,k} + b^{-}_{i,j,k}\,\phi_{i,j+1,k}$$

$$+ c^{+}_{i,j,k}\,\phi_{i,j,k+1} + c_{i,j,k}\,\phi_{i,j,k-1} + (d_{i,j,k} + \Sigma_{i,j,k})\,\phi_{i,j,k} = S_{i,j,k} \qquad (4\text{-}51h)$$

Equations (4-51h) are a set of linear inhomogeneous algebraic equations for the unknown ϕ_{ijk}, the number of equations and unkowns being equal to the number of mesh points.

In the usual calculation, in which the flux is zero at the boundary, the boundary points are left unnumbered and the appropriate ϕ are set equal to zero. However, should the boundary condition require zero current at the boundary, the condition can be simulated by adding a fictitious row of additional mesh points outside the boundary and requiring the flux to be the same at these points as at the internal points of which they are images. The symmetry introduced then gives rise to the desired result. However, the boundary points must then be included in the mesh and the equations at the boundary are somewhat different. In Equation (4-51f) one must make the substitution for a boundary parallel to the x - y plane:

$$a^{+}_{i,j,k}\,\phi_{i,j,k+1} + a^{-}_{i,j,k}\,\phi_{i,j,k-1} \rightarrow 2a^{+}_{i,j,k}\;\phi_{i,j,k+1} \qquad (4\text{-}52a)$$

with an appropriate change in D_{ijk} also:

$$\left[\frac{D_{i,j,k}}{\Delta z_k} + \frac{D_{i,j,k-1}}{\Delta z_{k-1}}\right]\frac{2}{\Delta z_k + \Delta z_{k-1}} \rightarrow \frac{2\,D_{i,j,k}}{[\Delta z_k]^2}$$

In order to deal with Equations (4-51h) in a neat fashion it is desirable to cast them into matrix form, for which it is, in turn, necessary to relable the ϕ such that they have only one index. If there are N_x intervals in the x direction, N_y in the y direction, and N_z in the z direction, this is conveniently done by setting

$$\ell(i,j,k) = N_y N_z (i-1) + N_z (j-1) + k \qquad (4\text{-}53a)$$

and

$$\Psi_\ell = \phi_{i,j,k}$$

so that the index ℓ of Ψ runs from 1 to $N_x N_y N_z = N$. This then allows one to form an N-dimensional vector:

$$\underline{\Psi} = \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_N \end{pmatrix} \qquad (4\text{-}53b)$$

Now, we set

$$\Sigma'_{i,j,k} = c_{i,j,k} + \Sigma_{i,j,k} \qquad (4\text{-}53c)$$

where Σ_{ijk} is the cross section (removal and absorption) at the point i, j, k. Further, we set

$$\Sigma'_{i,j,k} = A_{\ell\ell}$$

with ℓ given by Equation (4-52a). Finally, we set

$$a^{+}_{i,j,k} = A_{\ell\ell'} \qquad (4\text{-}53d)$$

where ℓ' is given be Equation (4-53a) with i replaced by i + 1 :

$$\ell' = N_y N_z (i) + N_z (j+1) + k$$
$$= \ell + N_y N_z$$

Similarly, one sets a^{-}, $b^{\pm}$, $c^{\pm}$ equal to $A_{\ell\ell'}$ where the ℓ' are again obtained from Equation (4-53a) by setting i = i+1, j=j-1, j=j+1, k=k-1, and k=k+1 respectively. In this way, a matrix $\underline{\underline{A}}$ can be formed from the coefficients of the difference equations. This allows the difference equations to be rewritten as

$$\underline{\underline{A}}\ \underline{\Psi} = \underline{S} \qquad (4\text{-}53e)$$

where $\underline{S}$ is the source vector formed from the

$$S_\ell = S_{i,j,k} \qquad (4\text{-}53f)$$

and

$$S = \begin{pmatrix} S_1 \\ \vdots \\ S_{N_x N_y N_z} \end{pmatrix} \qquad (4\text{-}53g)$$

In this manner, the equations for inner iterations are cast into matrix form. Necessarily, the means of solving this matrix problem will differ considerably from those employed in the outer iteration problem. Rather than a set of homogeneous linear equations, which leads to an eigenvalue problem, we have an inhomogeneous set of linear equations, which can be expected to possess a unique solution.

15. Inner Iterations - Solution of the Finite Difference Equations

Again, the most obvious means of solution involves straightforward matrix methods. Formally the solution to Equation (4-53e) can be written:

$$\underline{\Psi} = \underline{\underline{A}}^{-1} \underline{S} \qquad (4\text{-}54a)$$

where $\underline{\underline{A}}^{-1}$ is the inverse matrix of $\underline{\underline{A}}$. A problem will, however, generally require of the order of a hundred mesh lines in each dimension so that $\underline{\underline{A}}$ may be the order of thousands by thousands. Even with the great number of zero elements, inversion of a matrix of this magnitude is an overwhelming task, except, possibly, in the one-dimensional case. Thus, we must again resort to iteration methods in problems involving two or three dimensions.

Equation (4-53e) is not in a suitable form for iteration as it stands, for on inserting a guess at $\underline{\Psi}$, there is no means for

obtaining an iterated guess. Hence, some simple transformations are usually applied. The simplest is probably to decompose $\underline{\underline{A}}$ into the sum of two matrices, one of which is diagonal (i.e., it has no non-zero elements with different indices). That is, a matrix $\underline{\underline{\Sigma}}$ is formed whose elements are

$$\begin{aligned} \Sigma_{ij} &= A_{ij} \qquad i = j \\ &= 0 \qquad\quad i \neq j \end{aligned} \tag{4-54b}$$

and a matrix $\underline{\underline{B}}$ is formed

$$\begin{aligned} B_{ij} &= A_{ij} \qquad i \neq j \\ &= 0 \qquad\quad i = j \end{aligned} \tag{4-54c}$$

Then clearly

$$\underline{\underline{A}} = \underline{\underline{\Sigma}} + \underline{\underline{B}} \tag{4-54d}$$

Now the inverse of $\underline{\underline{\Sigma}}$ is simply

$$\underline{\underline{\Sigma}}^{-1} = \begin{pmatrix} 1/A_{11} & 0 & 0 \\ 0 & 1/A_{22} & \cdots\cdots \\ 0 & & 1/A_{NN} \end{pmatrix} \tag{4-54e}$$

Rewriting Equation (4-53e) as

$$\underline{\underline{\Sigma}}\ \underline{\Psi} = \underline{S} - \underline{\underline{B}}\ \underline{\Psi} \tag{4-54f}$$

and operating on it with $\underline{\underline{\Sigma}}^{-1}$

$$\underline{\Psi} = \underline{\underline{\Sigma}}^{-1}\ \underline{S} - \underline{\underline{\Sigma}}^{-1}\ \underline{\underline{B}}\ \underline{\Psi} \tag{4-54g}$$

or denoting

$$\underline{\underline{\Sigma}}^{-1}\ \underline{\underline{B}} = -\underline{\underline{M}}$$

$$\underline{\underline{\Sigma}}^{-1}\ \underline{S} = \underline{S}' \qquad (4\text{-}54h)$$

we obtain a set of equations which is amenable to iteration:

$$\underline{\Psi} = \underline{\underline{M}}\ \underline{\Psi} + \underline{S}' \qquad (4\text{-}54j)$$

which is really only the set of difference equations with each equation divided by the coefficient of ϕ_{ijk}. Here, an iteration scheme immediately suggests itself. After guessing an initial flux $\underline{\Psi}^{(o)}$, successive iterates are calculated from:

$$\underline{\Psi}^{(m+1)} = \underline{\underline{M}}\ \underline{\Psi}^{(m)} + \underline{S}' \qquad (4\text{-}55a)$$

This, the <u>simultaneous relaxation</u> method (also known as the Gauss or Richardson Method) is a simple method which will be shown to converge, but it is not very rapidly convergent compared to methods to be given later. It should be noted that what this iteration scheme really does is to substitute a set of previous values of the flux $\phi_{ijk}^{(m)}$ at the neighboring points into the difference Equations (4-51h) to arrive at a new set of fluxes $\phi_{ijk}^{(m+1)}$.

To demonstrate convergence, we define an error vector $\underline{E}^{(m)}$ as

$$\underline{E}^{(m)} = \underline{\Psi} - \underline{\Psi}^{(m)} \qquad (4\text{-}55b)$$

i.e., the difference between the correct flux and a given iterate.

Subtracting Equation (4-55a) from

$$\underline{\Psi} = \underline{\underline{M}}\ \underline{\Psi} + \underline{S}' \qquad (4\text{-}55c)$$

we find the error vectors $\underline{E}^{(k)}$ obey the equation:

$$\underline{E}^{(m+1)} = \underline{\underline{M}}\ \underline{E}^{(m)} \qquad (4\text{-}55d)$$

Now, the error vectors can be expanded in terms of the eigenvectors of the matrix $\underline{\underline{M}}$, which satisfy the equation:

$$\underline{\underline{M}}\ \underline{\chi}_n = \lambda_n \underline{\chi}_n \qquad (4\text{-}55e)$$

$$\underline{E}^{(m)} = \sum_{n=1}^{N} a_n^{(m)}\ \underline{\chi}_n \qquad (4\text{-}55f)$$

Inserting the expansion into Equation (4-55d) we have:

$$\underline{E}^{(m+1)} = \sum_{n=1}^{N} a_n^{(m+1)}\ \underline{\chi}_n = \sum_{n=1}^{N} a_n^{(m)}\ \lambda_n\ \underline{\chi}_n \qquad (4\text{-}55g)$$

or, in terms of the error in the original guess:

$$\underline{E}^{(m+1)} = \sum_{n=1}^{N} a_n^{(0)}\ \lambda_n^m\ \underline{\chi}_n \qquad (4\text{-}55h)$$

Thus, the error vector will become zero after many iterations provided that all of the eigenvalues are less than unity in absolute value. In fact, it can be seen that the rate of convergence depends solely on the degree to which the absolute value of the largest eigenvalue (called the

spectral norm) is less than unity. In general, matrices do not possess this property but Young[37] has shown that the properties of the matrix $\underline{\underline{M}}$ are such that it does in fact have the desired properties. Indeed, Young has discovered many useful properties of this type of matrix (said to possess Property A) which will be introduced as required. Space does not permit the inclusion of some rather lengthy proofs here.

As was the case with outer iterations, the most obvious iteration procedure is not the one which converges most rapidly. An easy means of improving the convergence rate is suggested by a rather simple argument. In the Simultaneous Relaxation method the m^{th} iterate flux is obtained by substituting the $(m-1)^{st}$ iterate flux into the difference equations. In so doing an orderly procedure would be to start at once corner of the mesh and then step point by point along an edge and then continue along an adjacent parallel line. In so doing, we are not taking full advantage of the material at hand. For example, if the second line is chosen adjacent to the first, in the calculation of the fluxes along the second line the fluxes on the first line are required. Thus, the Simultaneous Relaxation method does not take advantage of the fact that the m^{th} iterate fluxes on the first line have already been calculated. Furthermore, the computer memory requirement is increased in this method (e.g., doubled). Thus, it will be advantageous to use the already computed m^{th} iterate fluxes wherever they are available.

To establish this method in the matrix formulation we note that the simultaneous relaxation method calculates the elements Ψ_ℓ of the flux vector in increasing order (i.e., $\ell = 0, 1, 2$ ----) and that the

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[37] D. Young, Trans. Amer. Math. Soc., 76, 92 (1954).

terms of the matrix $\underline{\underline{M}}$ (say $M_{\ell\ell'}$) which connect an element Ψ_ℓ with those calculated previously (i.e., with $\ell' < \ell$) are those which lie below the diagonal. Hence, it is natural to define two new matrices, $\underline{\underline{L}}$ and $\underline{\underline{U}}$ as the upper and lower halves of $\underline{\underline{M}}$.

$$\begin{aligned} L_{ij} &= M_{ij} && \text{if} \quad i > j \\ &= 0 && \quad\ i < j \end{aligned} \qquad (4\text{-}56a)$$

$$\begin{aligned} u_{ij} &= M_{ij} && \text{if} \quad i < j \\ &= 0 && \quad\ i > j \end{aligned}$$

so that

$$\underline{\underline{M}} = \underline{\underline{L}} + \underline{\underline{u}}$$

In terms of the new matrices, the Simultaneous Relaxation Method can be written

$$\underline{\Psi}^{(m+1)} = \underline{\underline{L}}\ \underline{\Psi}^{(m)} + \underline{\underline{u}}\ \underline{\Psi}^{(m)} + \underline{S}$$

The iteration scheme for the new method we are seeking, called the Successive Relaxation (or Seidel-Young or Leibman) method, can then be written

$$\underline{\Psi}^{(m+1)} = \underline{\underline{L}}\ \underline{\Psi}^{(m+1)} + \underline{\underline{u}}\ \underline{\Psi}^{(m)} + \underline{S} \qquad (4\text{-}56b)$$

or

$$\begin{aligned} \underline{\Psi}^{(m+1)} &= \left(\underline{\underline{I}} - \underline{\underline{L}}\right)^{-1} \underline{\underline{u}}\ \underline{\Psi}^{(m)} + \left(\underline{\underline{I}} - \underline{\underline{L}}\right)^{-1} \underline{S} \\ &= \underline{\underline{P}}\ \underline{\Psi}^{(m)} + \left(\underline{\underline{I}} - \underline{\underline{L}}\right)^{-1} \underline{S} \end{aligned}$$

The convergence of this method was demonstrated by Geiringer[38] who also showed that the eigenvalues of $(\underline{\underline{I}} - \underline{\underline{L}})^{-1}\,\underline{\underline{U}} = \underline{\underline{P}}$ are the squares of the eigenvalues of $\underline{\underline{M}}$. Hence, the spectral norm of $\underline{\underline{P}}$ is the square of the spectral norm of $\underline{\underline{M}}$ and the Successive Method converges twice as fast as the simultaneous method.

It is also natural to inquire as to whether the extrapolation method used in the outer iteration problem may be applied to the solution of the set of inhomogeneous equations using in the inner iterations. Intuitively, it is clear that the procedure is again valid and it may in fact be applied to either of the methods already developed. As the Simultaneous Method does not converge as rapidly as the Successive Method, it is natural to work only with the latter; the method can, of course, be applied to the Simultaneous Method if desired. This leads then to the Successive Overrelaxation (or Extrapolated Leibman) Method.

As with the extrapolation procedure for the solution of homogeneous equations, we let the m^{th} iterate flux $\underline{\Psi}^{(m)}$ be a linear combination of

$$(\underline{\underline{I}} - \underline{\underline{L}})^{-1}\,\underline{\underline{U}}\;\Psi^{(m-1)} + (\underline{\underline{I}} - \underline{\underline{L}})\,\underline{S}$$

and $\underline{\Psi}^{(m-1)}$ itself, i.e., we choose

$$\underline{\Psi}^{(m)'} = \left\{(\underline{\underline{I}} - \underline{\underline{L}})^{-1}\,\underline{\underline{U}}\;\underline{\Psi}^{(m-1)} + (\underline{\underline{I}} - \underline{\underline{L}})^{-1}\,\underline{S}\right\}(1+\alpha) - \alpha\,\underline{\Psi}^{(m-1)} \qquad (4\text{-}57)$$

In practice, this simply means that one carries out the Successive

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[38] H. Geiringer, Reisner Anniversary Volume, p.360 (1950).

Relaxation scheme as outlined earlier and then forms $\underline{\Psi}^{(m)'}$ from the result of that calculation and the earlier one.

Finally, it is possible to carry over the Tschebycheff Polynomial method to inner iterations. That is, after m iterations, one selects as the m^{th} guess:

$$\underline{\Psi}^{(m)'} = \sum_{j=1}^{m} B_j \, \underline{\Psi}^{(j)} \qquad (4\text{-}58a)$$

with

$$\sum B_j = 1$$

On writing this in terms of the error vector, we have

$$\underline{E}^{(m)'} = \sum_{j=1}^{m} B_j \, \underline{E}^{(j)} \qquad (4\text{-}58b)$$

But, subtracting Equation (4-56b) from

$$\underline{\Psi} = \underline{\underline{P}} \, \underline{\Psi} - \left(\underline{\underline{I}} - \underline{\underline{L}}\right)^{-1} \underline{S}$$

we have

$$\underline{\underline{E}}^{(m+1)} = \underline{\underline{P}} \, \underline{E}^{(m)}$$

So that

$$\underline{E}^{(m)'} = \sum_{j=1}^{m} B_j \, \underline{\underline{P}}^{j} \, \underline{\underline{E}}^{(0)}$$

Expanding $\underline{E}^{(o)}$ in terms of the eigenfunctions $\underline{\chi}_n$ of $\underline{\underline{P}}$ where

$$\underline{\underline{P}}\ \underline{\chi}_n = \lambda_n \chi_n \qquad (4\text{-}58f)$$

$$\underline{E}^{(m)} = \sum_{n=1}^{N} e_n^{(m)}\ \underline{\chi}_n \qquad (4\text{-}58g)$$

we have

$$e_n^{(m)'} = \sum_{j=1}^{N} \beta_j\ \lambda_n^j\ e_n^{(o)} \qquad (4\text{-}58h)$$

where the linear independence of the $\underline{\chi}_n$ has been applied. Again to minimize $e_n^{(m)'}$ for all $\lambda_n < 1$ (note that the λ_n all satisfy this condition as a result of Young's work) we must again choose the β_j as the coefficients of χ^j in $Q_j(\chi)$ $\chi/\chi/$ of Equation.(4.49a).

APPENDIX A

TIME DEPENDENT ASYMPTOTIC REACTOR THEORY*

In this appendix we shall treat the time dependent problems alluded to in Chapter I. For the sake of brevity the asymptotic (bare homogeneous thermal) reactor model is adhered to. The rationale for so doing lies in the fact that all the basic principles may be discovered within the framework of the asymptotic theory; the development for more complex models yields essentially the same information, albeit in a more rigorous form.** We shall also make the further, and more serious, approximation of ignoring the effets of delayed neutrons.

Within the framework of the diffusion approximation to asymptotic reactor theory, it was shown in Chapter I that the time-dependent thermal flux obeys the following equation:

$$\frac{1}{v}\frac{\partial \phi(\underline{r},t)}{\partial t} - D\nabla^2\phi(\underline{r},t) + \Sigma_a\phi(\underline{r},t) = S(\underline{r},t) + \nu\Sigma_f\int_0^t dt'\int_{\text{all space}} d^3r'\,\phi(\underline{r}',t')P(|\underline{r}-\underline{r}'|,t-t') \tag{A-1}$$

where $P(|\underline{r}|, t)$ is the time-dependent slowing down kernel of Chapter I and $S(\underline{r}, t)$ is to represent only non-fission sources.

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* This appendix closely follows T.J. Krieger and P.F. Zweifel, Nuc. Sci. Eng., 5, 21 (1959).

** For more complex discussions of time dependent reactor problems, the reader is referred to A. Henry, PICG P/ (1955); A. Ussacheff, PICG P/ (1955).

As in Chapter I, the flux and source are expanded in terms of the eigenfunctions of the wave Equation (1-26):

$$\phi(\underline{r},t) = \sum_{n=0}^{\infty} a_n(t)\,\chi_n(\underline{r}) \qquad (A\text{-}2a)$$

$$S(\underline{r},t) = \sum_{n=0}^{\infty} \sigma_n(t)\,\chi_n(\underline{r}) \qquad (A\text{-}2b)$$

On substituting the expansions (A-2) into Equation (A-1), applying lemma (1-34), and equating the coefficients of each of the $\chi_n(\underline{r})$, we have the following equation for the $a_n(t)$:

$$\frac{1}{v}\frac{da_n(t)}{dt} + (\Sigma_a + DB_n^2)\,a_n(t) = \sigma_n(t) + \nu\Sigma_f \int_0^t a_n(t')\,\bar{P}(B_n^2, t-t')\,dt' \qquad (A\text{-}3)$$

In general, the source $S(\underline{r}, t)$ may be one of either fast of thermal neutrons. Of course, in practice all sources emit only fast neutrons so that it is sufficient to consider only that case. Furthermore, one need only consider a pulsed source

$$\sigma_n(t) = \sigma_n\,\delta(t)$$

since the solution for this case is the Green's Function for the general case. However, this type of source gives rise to a source

$$\sum_{n=0}^{\infty}\sigma_n\int_{\text{all space}}\chi_n(\underline{r})\int_0^t\delta(t)\,P(|\underline{r}-\underline{r}'|,t-t')\,dt'\,d^3r' = \sum_{n=0}^{\infty}\sigma_n\,\bar{P}(B_n^2,t)$$

of the thermal neutrons. Finally, since the solution for this source can be written in terms of the solution for a pulsed thermal source, one need consider a source of this type. Hence, Equation (A-3) becomes

$$\frac{1}{v}\frac{da_n(t)}{dt} + (\Sigma_a + DB_n^2)\,a_n(t) = C_n\delta(t) + \int_0^t a_n(t')\,\bar{P}(B_n^2,t-t')\,dt' \qquad (A-4)$$

Equation (A-4) may be solved by any of the standard techniques for solving Volterra Integral equations, but we shall choose the Laplace Transform method. Since $a_n(t) = 0$, $t<0$, we have, on taking the Laplace Transform of (A-4):

$$\left(\frac{s}{v} + \Sigma_a + DB_n^2\right)\bar{a}_n(s) = \nu\Sigma_f\,\bar{\bar{P}}(B_n^2,s) + C_n \qquad (A-5)$$

where

$$\bar{a}_n(s) = \int_0^{\infty} dt\, e^{-st}a_n(t) \qquad (A-6a)$$

$$\bar{\bar{P}}(B_n^2,s) = \int_0^{\infty} dt\, e^{-st}\,\bar{P}(B_n^2,t) \qquad (A-6b)$$

It is noteworthy that the calculation of $\bar{\bar{P}}(B^2, s)$ is simply that of calculating $\bar{P}(B^2)$ (as in Chapter I) with Σ_a replaced by $\Sigma_a + S/v$. On solving for $\bar{a}_n(s)$ we have

$$\bar{a}_n(s) = \frac{v c_n}{s + v(\Sigma_a + DB_n^2) + v\nu\Sigma_f \bar{\bar{P}}(B_n^2, s)} \qquad (A-7)$$

which may be inverted formally to yield

$$a_n(t) = \frac{c_n v}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{e^{st}\, ds}{s + v(\Sigma_a + DB_n^2) + v\nu\Sigma_f \bar{\bar{P}}(B_n^2, s)} \qquad (A-8)$$

The only singularities of the integrand are the roots of

$$s + v(\Sigma_a + DB_n^2) + v\nu\Sigma_f \bar{\bar{P}}(B_n^2, s) = 0 \qquad (A-9)$$

In a critical reactor it was shown in Chapter I that the neutron flux is all in the first mode and is constant in time. This solution arises from the fact that Equation (A-9) then has a root $s = 0$, which then makes Equation (A-9) the criticality condition (1-25b). For a reactor not far from critical, this root can be expected to move only slightly from zero and since it is a single root it is reasonable to expect that the asymptotic solution will be due to the pole arising from this zero. For small s we may expand

$$\bar{\bar{P}}(B_n^2, s) = \bar{\bar{P}}(B_n^2, 0) + s \left.\frac{\partial \bar{\bar{P}}(B_n^2, s)}{\partial s}\right)_{s=0} \qquad (A-10)$$

so that the solution of Equation (A-9) becomes

$$s_{n_0} = \frac{\nu\Sigma_f \bar{\bar{P}}(B_n^2, 0) - (\Sigma_a + DB_n^2)}{\frac{1}{v} - \nu\Sigma_f \left(\frac{\partial \bar{\bar{P}}(B_n^2, s)}{\partial s}\right)_{s=0}}$$

$$= \frac{k_n - 1}{l_n - \langle t \rangle_n k_n} \qquad (A\text{-}11)$$

Here we have defined

$$\langle t \rangle_n = \frac{\left(\frac{\partial \bar{\bar{P}}(B_n^2, s)}{\partial s}\right)_{s=0}}{\bar{\bar{P}}(B_n^2, 0)} = \frac{\int_0^\infty t\, \bar{P}(B_n^2, t)\, dt}{\int_0^\infty \bar{P}(B_n^2, t)\, dt} \qquad (A\text{-}12)$$

which is the mean slowing down time for a neutron in the n^{th} mode; and in accord with the results of Chapter I

$$k_n = \frac{\nu\Sigma_f \bar{\bar{P}}(B_n^2, 0)}{\Sigma_a + DB_n^2} \qquad (A\text{-}13a)$$

$$l_n = \frac{1}{v(\Sigma_a + DB_n^2)} \qquad (A\text{-}13b)$$

are the multiplication constant and lifetime for the n^{th} mode respectively. The condition for the expansion (A-10) to be valid is that the second term be much smaller in magnitude that the first, i.e.,

that

$$|k_n - 1| \langle t \rangle_n \ll \ell_n + \langle t \rangle_n k_n \qquad (A-14)$$

Since k_n falls off rapidly with increasing n, this approximation is clearly valid only for small n.

The asymptotic behavior of $a_n(t)$ is then

$$a_n(t) \simeq \alpha_n e^{s_{n_0} t} \qquad (A-15)$$

where α_n is the residue to the integrand of Equation (A-5) at $s = s_{n_0}$:

$$\alpha_n = c_n \upsilon \left(1 - \upsilon \nu \Sigma_f \left(\frac{\partial \bar{\bar{P}}(B_n^2, s)}{\partial s} \right)_{s=0} \right)^{-1} \qquad (A-16)$$

APPENDIX B

VECTOR IDENTITIES

In Chapter I five vector identities were used which are proved here.

$$(1)\int d\underline{\Omega} = 4\pi$$

Proof: Note that $d\underline{\Omega}$ is just a differential area on a unit sphere (see Figure B1).

$$d\underline{\Omega} = \sin\theta\, d\theta\, d\varphi = d(\cos\theta)\, d\varphi$$

or with

$$\mu = \cos\theta$$

$$d\underline{\Omega} = d\mu\, d\varphi$$

The azimuthal angle runs from 0 to 2π while θ runs from $-\pi$ to 0 (or -1 to 1 in μ) in covering the sphere. Hence

$$\int d\underline{\Omega} = \int_{-1}^{1} d\mu \int_{0}^{2\pi} d\varphi = 4\pi$$

$$(2)\quad \int \underline{A}\cdot\underline{\Omega}\, d\Omega = 0$$

Choose as the polar axis in Figure B1 a vector in the $\underline{A}$ direction. Then

$$\underline{A}\cdot\underline{\Omega} = |A|\cos\theta = |A|\mu$$

$$\int \underline{A}\cdot\underline{\Omega}\, d\underline{\Omega} = |A|\int_{-1}^{1} \mu\, d\mu \int_{0}^{2\pi} d\varphi = 0$$

(3) $$\int \underline{\Omega}\, d\underline{\Omega} = 0$$

The proof of this identity is readily obained by a symmetry argument. For each of the three components of $\underline{\Omega}$ ($\Omega_x, \Omega_y, \Omega_z$ denoted by Ω_i) one can write

$$\int_0^1 \Omega_i\, d\mu \int_0^{2\pi} d\varphi = -\int_{-1}^0 \Omega_i\, d\mu \int_0^{2\pi} d\varphi$$

by changing the integration variable from $\underline{\Omega}$ to $-\underline{\Omega}$. Then

$$\int_{-1}^1 \Omega_i\, d\mu \int_0^{2\pi} d\varphi = \int_{-1}^0 \Omega_i\, d\mu \int_0^{2\pi} d\varphi + \int_0^1 \Omega_i\, d\mu \int_0^{2\pi} d\varphi = 0$$

The same result is more easily obtained by arguing that the result of the integration must be a vector. The only vector in the problem is $\underline{\Omega}$ which is integrated over. Thus, the result must be zero.

(4) $$\int \underline{A}\cdot\underline{\Omega}\,\underline{\Omega}\, d\underline{\Omega} = \frac{4\pi}{3}\,\underline{A}$$

This integral is readily evaluated by noting that the only vector not integrated over is $\underline{A}$. Hence, the result must be proportional to $\underline{A}$.

$$\int \underline{A}\cdot\underline{\Omega}\,\underline{\Omega}\, d\underline{\Omega} = C\underline{A}$$

To evaluate C one takes the scalar product of this equation with $\underline{A}$ to get

$$|A|^2 C = \int (\underline{A} \cdot \underline{\Omega})^2 \, d\underline{\Omega}$$

and again choosing $\underline{A}$ as the polar axis

$$|A|^2 C = |A^2| \int_{-1}^{1} \mu^2 d\mu \int_0^{2\pi} d\varphi = \frac{4\pi}{3} |A^2|$$

or

$$C = \frac{4\pi}{3}$$

(5) $$\int (\underline{A} \cdot \underline{\Omega})(\underline{B} \cdot \underline{\Omega}) d\underline{\Omega} = \frac{4\pi}{3} \underline{A} \cdot \underline{B}$$

This is easily proved by taking the scalar product of (4) with $\underline{B}$.

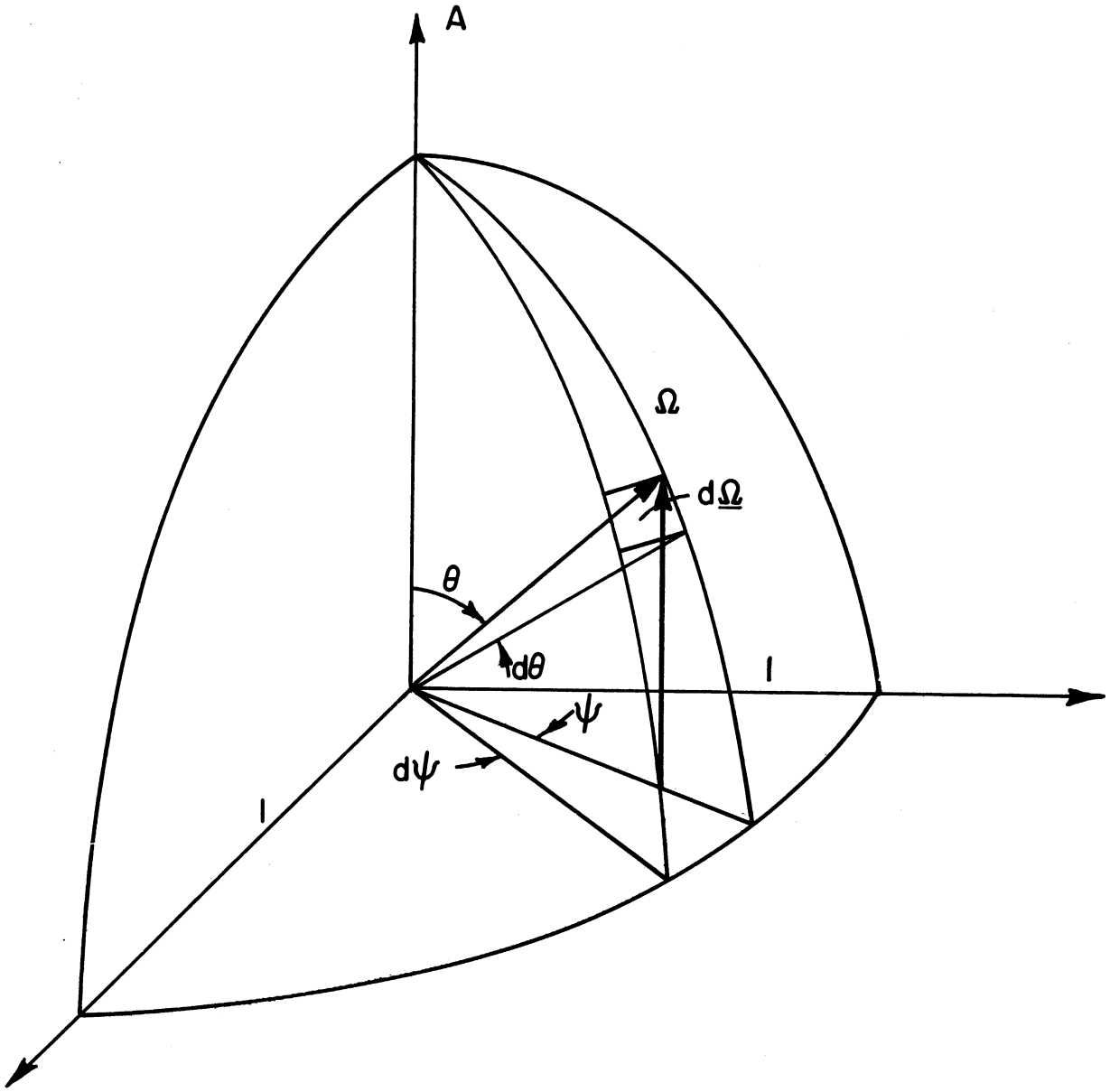

Figure B-1.

APPENDIX C

THE VALIDITY OF ASYMPTOTIC REACTOR THEORY*

In Chapter I it was shown how the major results of bare reactor theory could be derived quite simply by means of asymptotic reactor theory. However, the development of asymptotic reactor theory presented was at best highly intuitive and the limitations inherent in the theory were not at all obvious. In this appendix a set of sufficient conditions for the validity of asymptotic reactor theory are determined.

In essence, asymptotic reactor theory is the following. The criticality problem is that of solving the thermal diffusion equation

$$D\nabla^2\phi(\underline{r}) + \Sigma_a\phi(\underline{r}) = \nu\Sigma_f\int_R \phi(\underline{r}')\,P(\underline{r}'\to\underline{r})\,d^3r' \qquad (C-1)$$

together with the boundary condition

$$\phi(\underline{r}) = 0 \qquad \underline{r}\in S \qquad (C-2)$$

where R is the reactor surface bounded by S. Asymptotic reactor theory claims that the solution to this problem is identical to that of the equation

$$D\nabla^2\phi'(\underline{r}) + \Sigma_a\phi'(\underline{r}') = \int_{\text{allspace}} \phi'(\underline{r}')\,K(|\underline{r}-\underline{r}'|)\,d^3r' \qquad (C-3)$$

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* The development closely follows K.M. Case, J.H. Ferziger and P.F. Zweifel, Nuc. Sci. Eng., 10, 352 (1961).

with the boundary condition (C-2) . That is, for $\underline{r}\epsilon R$

$$\phi'(\underline{r}) = \phi(\underline{r})$$

If it is possible to find a kernel K which makes these statements true, and if K is indeed the infinite medium kernel $P_{\infty}(|\underline{r} - \underline{r}'|)$ then the results derived in Chapter I follow.

The proof is as follows. If the above statements are true then the left-hand sides of Equations (C-1) and (C-3) are equal for $\underline{r}\epsilon R$. Then

$$\int_R \phi(\underline{r}') P(\underline{r}' \to \underline{r}) d^3r' = \int_{\text{all space}} \phi'(\underline{r}') K(|\underline{r}-\underline{r}'|) d^3r' \qquad (C-4)$$

Now $\phi(\underline{r})$ may be expanded in terms of the eigenfunctions $\chi_n(\underline{r})$ which satisfy the Helmholtz equation

$$\nabla^2 \chi_n(\underline{r}) + B_n^2 \chi_n(\underline{r}) = 0 \qquad (C-5)$$

and vanish on $\underline{S}$; the set so defined is complete and orthogonal in R^* . Thus formally

$$\phi(\underline{r}) = \sum_n \left[\int_R \phi(\underline{r}') \chi_n(\underline{r}') \, d^3r' \right] \chi_n(\underline{r}) \qquad \underline{r} \in R \qquad (C-6)$$

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* R. Courant and D. Hilbert, "Methods of Mathematical Physics," Interscience, (1953).

Since $\phi' = \phi$ for $\underline{r} \epsilon R$ and ϕ' is assumed to have no singular points on the real line, $\phi'(\underline{r})$ must be the unique analytic continuation of $\phi(\underline{r})$ to all space. The $\chi_n(\underline{r})$ are readily continued to all space and these continuations are, in fact, just the solutions of Equation (C-5) in all space with the boundary condition that they vanish on S. Hence

$$\phi'(\underline{r}) = \sum_n \left[\int_R \chi_n(\underline{r}') \phi(\underline{r}') d^3r' \right] \chi_n(\underline{r}) \qquad (C-7)$$

Substituting Equation (C-7) into Equation (C-4) we have, after interchanging the order of the operations:

$$\int_R \phi(\underline{r}') P(\underline{r}' \to \underline{r}) d^3r' =$$

$$\int_R \sum_n \chi_n(\underline{r}'') \phi(\underline{r}'') d^3r'' \int_{\text{all space}} \chi_n(\underline{r}') K(|\underline{r}-\underline{r}'|) d^3r' \qquad (C-8)$$

Application of the lemma (1-34) yields

$$\int_R \phi(\underline{r}') P(\underline{r}' \to \underline{r}) d^3r' = \int_R \phi(\underline{r}'') \sum_n \chi_n(\underline{r}'') \chi_n(\underline{r}) \bar{K}(B_n^2) d^3r'' \qquad (C-9)$$

Hence

$$P(\underline{r}' \to \underline{r}) = \sum \chi_n(\underline{r}) \chi_n(\underline{r}') \bar{K}(B_n^2) \qquad (C-10)$$

Equation (C-10) yields much important information. First, it allows calculation of $P(\underline{r}' \to \underline{r})$ once $K(|\underline{r}-\underline{r}'|)$ is known; it also shows

that the kernel $P(\underline{r}' \to \underline{r})$ is symmetric and that if the kernel P can be written in this form, asymptotic reactor theory is valid.

Now $P(\underline{r}' \to \underline{r})$ is the slowing down density of neutrons at $\underline{r}$ at the thermal cutoff energy E_T due to a unit source of fission neutrons at $\underline{r}'$. Thus, it is related to the flux $\phi(\underline{r}' \to \underline{r}, E)$ by Equation (1-32b).

$$P(\underline{r}' \to \underline{r}) = \int_0^{E_T} dE \int_{E_T}^{\infty} dE' \, \Sigma_{s_0}(E' \to E) \phi(\underline{r}' \to \underline{r}, E) \qquad (C\text{-}11)$$

Since the relationship between $\phi(\underline{r}' \to \underline{r}, E)$ and $P(\underline{r}' \to \underline{r})$ does not involve the spatial variable, Equation (C-10) will be satisfied if

$$\phi(\underline{r}' \to \underline{r}, E) = \sum_n \bar{h}(B_n^2, E) \chi_n(r) \chi_n(r') \qquad (C\text{-}12)$$

where $\bar{h}(B_r^2, E)$ is a function such that

$$\bar{K}(B_n^2) = \int_0^{E_T} dE \int_{E_T}^{\infty} dE' \, \Sigma_{s_0}(E' \to E) \bar{h}(B_n^2, E) \qquad (C\text{-}13)$$

The flux $\phi(\underline{r}' \to \underline{r}, E)$ is the total flux at point $\underline{r}$ at energy E due to a unit fission source at $\underline{r}'$ and may therefore be obtained from the solution of the Boltzmann Equation with a source of this type. But, Davison* has shown that for the one speed case in the P_L approximation, with L odd, the total flux obeys an equation of

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* B. Davison, "Neutron Transport Theory," Oxford (1955).

the form

$$F_{(L+1)/2}(\nabla^2)\,\phi(\underline{r},E) = G_{(L-1)/2}(\nabla^2)\,S(\underline{r},E) \qquad (C-14)$$

where F_N and G_M are polynomials of degree N and M respectively. For the multispeed case the "coefficients" become operators with respect to energy, i.e., integrals containing the kernels $\Sigma_{sj}(E'\rightarrow E)$. For $\phi(\underline{r}'\rightarrow\underline{r}, E)$ Equation (C-14) becomes

$$F_{(L+1)/2}(\nabla^2)\,\phi(\underline{r}'\rightarrow\underline{r},E) = G_{(L-1)/2}(\nabla^2)\,\delta(\underline{r}-\underline{r}')\,f(E) \qquad (C-15)$$

Now if we attempt to find a solution of the form

$$\phi(\underline{r}'\rightarrow\underline{r},E) = \sum \alpha_n(\underline{r}',E)\,\chi_n(\underline{r}) \qquad (C-16)$$

and note that

$$\delta(\underline{r}'-\underline{r}) = \sum \chi_n(\underline{r})\,\chi_n(\underline{r}') \qquad (C-17)$$

we have

$$F_{(L+1)/2}(-B_n^2)\,\alpha_n(\underline{r}',E) = G_{(L-1)/2}(-B_n^2)\,f(E)\,\chi_n(\underline{r}') \qquad (C-18)$$

From this equation it is seen that

$$\alpha_n(\underline{r}',E) = \bar{\phi}_\infty(B_n^2,E)\,\chi_n(\underline{r}') \qquad (C-19)$$

and where $\bar{\phi}_\infty(B_n^2, E)$ is seen to be the solution the Fourier Transform

of Equation (C-15) evaluated at $-B_n^2$. Hence,

$$\phi(\underline{r}' \to \underline{r}, E) = \sum_n \bar{\phi}_\infty(B_n^2, E) \chi_n(\underline{r}) \chi_n(\underline{r}') \quad (C\text{-}20)$$

which, when inserted into Equation (C-11) shows that $P(\underline{r}' \to \underline{r})$ does indeed have the form (C-10). Furthermore, the fact that $\bar{\phi}_\infty(B_n^2, E)$ is the Fourier Transform of the flux in an infinite medium shows that $K(|\underline{r}-\underline{r}'|)$ is the infinite medium slowing down kernel as asserted earlier.

To recapitulate, it has been shown that if the expansion (C-6) is a legitimate representation of the neutron flux in a reactor, then the slowing down kernel does have the form predicted for it asymptotic reactor theory. Hence the proof of the validity of asymptotic reactor theory is complete provided an interpretation of the expansion (C-6) [or (C-16)] can be given. This interpretation is most readily obtained by an investigation of the rigorous solution of the Milne problem, i.e., the problem of a half space bounded by a plane that contains a source in the deep interior. In the Milne problem it is found that the flux far from the boundary has an asymptotic exponential shape and that this flux extrapolates to zero a short distance from the physical boundary of the system. Near the surface, however, there is a large non-asymptotic component of the flux which tends toward zero in the interior. Since the asymptotic flux obeys the boundary condition implied by an expansion of the type (C-6), namely Equation (C-2), it must be this flux which the asymptotic theory calculates; this, in fact, must be the origin of the term "asymptotic reactor theory."

Asymptotic reactor theory is therefore a sensible approach so long as the asymptotic flux from a point source is a reasonable approximation to the actual flux. In general, this condition obtains for systems larger than a mean free path and asymptotic reactor theory can therefore be applied even to relatively small systems.*

Finally, it may be noted that the asymptotic theory has meaning not only in diffusion theory but in higher order approximations as well. For, while diffusion theory does not correctly predict the asymptotic behavior of the flux from a point source (i.e., it gives the wrong exponential), asymptotic reactor theory does predict this exponent correctly.

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* For an application of asymptotic reactor theory, see S. Yip and P.F. Zweifel, Nuc.Sci.Eng., 10, 361 (1961).

APPENDIX D

EXTENSIONS OF ASYMPTOTIC REACTOR THEORY

Although the development of asymptotic reactor theory has heretofore generally been restricted to completely thermal reactors and to diffusion theory (Appendix C shows that this restriction is not necessary), the same methods may be applied to any model for a homogeneous reactor. Thus we may take as a starting point the Boltzmann Equation (1-11):

$$\underline{\Omega} \cdot \underline{\nabla} \Phi (\underline{r}, E, \underline{\Omega}) + \Sigma_t(E) \Phi(\underline{r}, E, \underline{\Omega}) = \frac{\nu}{4\pi} \int dE' f(E') \int P(\underline{r}' \rightarrow \underline{r}, E' \rightarrow E, \underline{\Omega}) d^3r' \cdot \int dE'' \Sigma_f(E'') \int \Phi(\underline{r}', E', \underline{\Omega}') d\underline{\Omega}' \qquad (D-1)$$

$$+ \frac{\nu f(E)}{4\pi} \int \Sigma_f(E') dE' \int \Phi (r, E', \underline{\Omega}') d\underline{\Omega}'$$

For convenience, thermal neutrons will not be treated separately, but their behavior is to be included in the details of calculation of the kernel P appearing on the right-hand side of Equation (D-1). As in Chapter I, the asymptotic reactor model is now invoked: all cross sections are independent of position, the kernel $P(\underline{r}' \rightarrow \underline{r}, E' \rightarrow E; \underline{\Omega})$ is replaced by the infinite medium kernel $P_\infty(\underline{r}' \rightarrow \underline{r}, E' \rightarrow E, \underline{\Omega})$ and the integral over

$\underline{r}'$ is extended to all space. Then denoting

$$P_\infty(\underline{r}'-\underline{r}, E, \underline{\Omega}) = \int f(E') P(\underline{r}'-\underline{r}, E' \to E, \underline{\Omega}) dE' \qquad (D-2)$$

Equation (D-1) becomes

$$\underline{\Omega} \cdot \nabla \Phi(\underline{r}, E, \underline{\Omega}) + \Sigma_t(E) \Phi(\underline{r}, E, \underline{\Omega}) =$$

$$\frac{\chi}{4\pi} \int_{\text{all space}} P_\infty(\underline{r}'-\underline{r}, E, \underline{\Omega}) d^3r' \cdot \qquad (D-3)$$

$$\cdot \int \Sigma_f(E') dE' \int \Phi(\underline{r}', E', \underline{\Omega}') d\Omega' + \frac{\nu f(E)}{4\pi} \int \Sigma_f(E') \int \Phi(\underline{r}, E, \underline{\Omega}') d\Omega'$$

The symmetry properties of P_∞ need not be applied at this point but will be useful later: P_∞ is a function only of the source to field point distance $|\underline{r} - \underline{r}'|$ and the cosine of the angle between $(\underline{r} - \underline{r}')$ and $\underline{\Omega}$, i.e., of $(\underline{r} - \underline{r}') \cdot \underline{\Omega}$. As before, the use of the asymptotic model renders the Boltzmann Equation amenable to Fourier Transformation.

On taking the Fourier Transform of Equation (D-3) we have

$$\left(\Sigma_t(E) + i\underline{\Omega} \cdot \underline{k}\right) \bar{\Phi}(\underline{k}, E, \underline{\Omega}) = \frac{\nu P_\infty}{4\pi}(\underline{k}, E, \underline{\Omega}) \int \Sigma_f(E') dE' \int \bar{\Phi}(\underline{k}, E, \underline{\Omega}') d\underline{\Omega}' \qquad (D-4)$$

$$+ \frac{\nu f(E)}{4\pi} \int \Sigma_f(E') dE' \int \Phi(\underline{k}, E', \underline{\Omega}') d\underline{\Omega}'$$

The critical condition is now easily derived by dividing Equation (D-4) by $\Sigma_t + i\,\underline{\Omega} \cdot \underline{k}$, multiplying by $\Sigma_f(E)$ and integrating over energy and angle:

$$\int \Sigma_f(E)dE \int \bar{\Phi}(\underline{k},E,\underline{\Omega})d\underline{\Omega} = \left[\frac{\nu}{4\pi}\int \Sigma_f(E)\frac{\bar{P}_0(\underline{k},E,\underline{\Omega})}{\Sigma_t(E)+\iota\,\underline{\Omega}\cdot\underline{k}}d\Omega\,dE + \frac{\nu}{4\pi}\int\frac{f(E)\Sigma_f(E)dE}{\Sigma_t(E)+\iota\,\underline{\Omega}\cdot\underline{k}}d\underline{\Omega}\right]\int\Sigma_f(E')dE'\int\bar{\Phi}(\underline{k},E,\underline{\Omega}')d\Omega' \quad (D-5)$$

so that $\bar{\Phi}(k, E, \Omega) = 0$ unless

$$1 = \frac{\nu}{4\pi}\int\Sigma_f(E)dE\int\frac{\bar{P}_0(\underline{k},E,\underline{\Omega})}{\Sigma_t(E)+\iota\,\underline{\Omega}\cdot\underline{k}}d\Omega + \frac{\nu}{4\pi}\int\frac{f(E)\Sigma_f(E)}{\Sigma_t(E)+\iota\,\underline{\Omega}\cdot\underline{k}}dE\,d\underline{\Omega} \quad (D-6)$$

which is the desired critical condition. It still remains to show that the critical condition depends only on k^2 and has only one positive real root for k^2. Now since $P(\underline{r}, E, \underline{\Omega}) = P(r, E, \underline{r}\cdot\underline{\Omega})$, its Fourier Transform can be written $P(\underline{k}, E, \underline{\Omega}) = P(k, E, \underline{k}\cdot\underline{\Omega})$ so that by choosing the axis for the integration over $\underline{\Omega}$ in the direction of $\underline{k}$, the integration over azimuthal angle can be performed immediately.

$$1 = \frac{\nu}{2}\int\Sigma_f(E)dE\int\frac{\bar{P}_0(k,E,\mu)}{\Sigma_t+\iota k\mu}d\mu + \frac{\nu}{2}\int f(E)\Sigma_f(E)dE\int\frac{d\mu}{\Sigma_t(E)+\iota k\mu} \quad (D-7)$$

where

$$\mu = \frac{\underline{\Omega}\cdot\underline{k}}{k}$$

Now the slowing down kernel may be expanded in Legendre Polynomials:

$$\bar{P}_0(\underline{k},E,\underline{\Omega}) = \sum(2l+1)P_l(\underline{k},E)\,P_l(\mu) \quad (D-8)$$

Upon inserting this expansion into Equation (D-7) we see immediately that the μ integrals are just the definitions of the $A_o(\eta)$ (see Equation

(3-69a)), so that Equation (D-7) becomes

$$1 = \nu \sum_{\ell=0}^{\infty} (2\ell+1) \int \Sigma_f(E) P_\ell(k, E) A_{0\ell}(\eta)\, dE + \nu \int \Sigma_f(E) f(E) A_{00}(\eta)\, dE \qquad (D\text{-}9)$$

But the slowing down kernel is really the degradation integral in the Boltzmann in a problem involving a point source of fission neutrons, so that the $P_\ell(\underline{k}, E)$ are identical to the Legendre moments $J_\ell(k, E)$ of the degradation integral for this problem. Hence, using the basic equation (3-68) of the B_L method, Equation (D-9) becomes:

$$1 = \nu \int \Sigma_f(E) \phi_0(\underline{k}, E)\, dE \qquad (D\text{-}10)$$

where $\phi_0(\underline{k}, E)$ is the Fourier Transform of the total flux generated by a point source of fission neutrons in an infinite medium. However, in an infinite medium the flux $\phi_0(\underline{r}, E)$ depends only on the distance $|\underline{r}|$ so that $\phi(\underline{k}, E)$ depends only on the magnitude of $\underline{k}$, i.e., only on k^2. Finally, since $\phi_0(\underline{k}, E)$ is related to the slowing down kernel $\overline{P}_0(k^2, E)$ by an operator that acts only on the energy variable, it will have the same behavior as a function of k^2 as $\overline{P}_0(k^2 E)$. As a consequence of the "Second Fundamental Theorem" discussed in Chapter III, $\overline{P}_0(k^2, E)$ must be a monotonically decreasing function of k^2. Hence $\phi_0(k^2, E)$ is a monotonically decreasing function of k^2 and Equation (D-10) can have only one root with $k^2 > 0$. All of the results of asymptotic reactor theory follow from this result.

APPENDIX E

IMPROVEMENTS IN CRITICALITY CALCULATIONS

Most criticality calculations performed by reactor designers are done within the framework of diffusion theory, generally in the multigroup approximation. The reasons for the choice of diffusion theory as a basis for calculations are, as pointed out in Chapter IV, the simplicity of the equations involved, the short computation time required, and, to a lesser extent, a lack of fundamental data. Frequently the justification lies no deeper than the reasons given above, and several ill-evaluated approximations inherent in the theory are often invoked. In this appendix we shall derive simple formulae by means of which one can test whether a consistent P1 calculation will yield a significant improvement over diffusion theory insofar as the multiplication constant is concerned.

In the previous appendix a critical condition was derived by applying the asymptotic reactor model to a general bare homogeneous system. Although the use of an angular dependent kernel, i.e., $P(\underline{r}' - \underline{r}, E, \underline{\Omega})$, in asymptotic reactor theory has not been justified, we shall assume that the critical condition (D-9) is a reasonable approximation to the true critical condition. The proof of this follows the argument given in Appendix C.

We start by rewriting Equation (D-9)

$$\int \Sigma_f(E)\,dE \sum_{l=0}^{\infty}(2l+1)\,A_{0l}\left(\frac{\Sigma_t}{k}\right)\left[P_l(\underline{k},E)+f(E)\delta_{l0}\right] \qquad \text{(E-1)}$$

For simplicity, first collision fission shall be neglected, i.e., we shall drop the second term in the bracket. Within the framework of diffusion theory, slowing down collisions are assumed isotropic in the laboratory system, so that diffusion theory results from retaining only the first term of the series in Equation (E-1). Diffusion theory also requires that $A_{00}(\eta)$ be approximated by an expansion in powers of η up to η^2. Thus, a measure of the change in the multiplication constant obtained by considering anisotropic slowing down is:

$$\left|\frac{A_{10}(\eta)\,P_1(\underline{k},E)}{A_{00}(\eta)\,P_0(\underline{k},E)}\right| \qquad \text{(E-2)}$$

In order to evaluate (E-2) we note that to order η^2

$$A_{00}(\eta) = 1+\frac{\eta^2}{3} \qquad \text{(E-3)}$$

and that

$$A_{01}(\eta) = \frac{A_{00}(\eta)-1}{\eta} = \frac{\eta}{3} \qquad \text{(E-4)}$$

Now, from the definitions of the expansion coefficients $P_l(\underline{r}, E)$ we have at energies above thermal:

$$P_0(\underline{r},E) = \int \Sigma_{s_0}(E' \to E)\,\phi_0(\underline{r},E')\,dE' \simeq \Sigma_s(E)\,\phi_0(\underline{r},E) \quad \text{(E-5)}$$

and

$$P_1(\underline{r},E) = \int \Sigma_{s_1}(E' \to E)\,\phi_1(\underline{r},E')\,dE' \simeq \Sigma_s(E)\,\bar{\mu}(E)\,\phi_1(\underline{r},E)$$
$$\simeq -\Sigma_s\,\bar{\mu}\,D\,\nabla\phi_0$$

Hence,

$$|P_1(\underline{k},E)| \simeq \Sigma_s\,\bar{\mu}\,k\,D\phi_0 \simeq D\bar{\mu}\,k\,|P_0(k,E)| \quad \text{(E-6)}$$

Substituting the values into the expression (E-2) we have

$$\left|\frac{A_{01}P_1}{A_{00}P_0}\right| \simeq \left|\frac{ik}{3\Sigma_t}\,D\bar{\mu}\,k\right| = \frac{D\bar{\mu}k^2}{3\Sigma_t} \simeq \left(\frac{k}{\Sigma_t}\right)^2 \frac{\bar{\mu}}{9} \quad \text{(E-7)}$$
$$\simeq D^2k^2\bar{\mu}$$

which is the desired result to the lowest order of approximation. In a criticality expression, k^2 would have the significance of a geometric buckling B_g^2 and the criterion (E-7) then states that $D^2B_g^2\bar{\mu}$ (or $\frac{\bar{\mu}}{9}\,\frac{B_g^2}{\Sigma_t^2}$) must be small. This in turn implies that for the P_1 approximations to have any advantage over diffusion theory, the system must be small or scattering must be quite anisotropic in the laboratory system.

The above argument (i.e., the approximations (E-5) and (E-6)),

is valid only at energies above thermal. At thermal energies use of the slowing down kernel employed in Appendix D becomes rather clumsy and it is somewhat easier to use the one group approximation. Instead, a thermal Boltzmann Equation could be written

$$\underline{\Omega} \cdot \underline{\nabla} \phi_T(\underline{r}, \underline{\Omega}) + \Sigma_{t_T} \phi_T(\underline{r}, \underline{\Omega}) = \int \Sigma_s(\underline{\Omega} \cdot \underline{\Omega}') \phi_T(\underline{r}, \underline{\Omega}') d\underline{\Omega}' + \nu \Sigma_{f_T} \int d^3r' \phi_{T_0}(\underline{r}') P(\underline{r}' - \underline{r}, \underline{\Omega}) \quad \text{(E-8)}$$

where $P(\underline{r}' - \underline{r}, \underline{\Omega})$ is the thermalization, or angular dependent slowing down density, kernel (see Chapter III, Section) at the thermal cutoff energy. Now, proceeding as in Appendix D, the thermal flux $\phi_T(\underline{r}, \underline{\Omega})$ and the thermalization kernel can be expanded in Legendre Polynomials, the Fourier Transform taken and a critical condition extracted.* Since we are interested only in the first term beyond diffusion theory we quote only the P1 result.

$$\nu \Sigma_{f_T} \frac{\left[\overline{P}_0(k^2) - 3D \underline{k} \cdot \underline{\nabla}_k \overline{P}_1(k^2) \right]}{1 + L^2 k^2} = 1 \quad \text{(E-9)}$$

where **D** and L^2 retain the meanings ascribed to them in Chapter III and $\overline{P}_0(k^2)$ and $\overline{P}_1(k^2)$ are the Fourier Transforms of the first two Legendre moments of $P(\underline{r} - \underline{r}', \underline{\Omega})$, i.e., the first two moments of the slowing

* The details of this calculation are given in P. F. Zweifel and J. H. Ferziger, Nuc. Sci. Eng., 10 , 357 (1961).

down density at the thermal cutoff energy. To simplify Equation (E-9) somewhat we will use the expansions given in Chapter III, Section and additionally Fick's Rule:

$$P_0(\underline{r}' \to \underline{r}) = \xi \Sigma_s \phi_0(\underline{r}' \to \underline{r})$$
$$P_1(\underline{r}' \to \underline{r}) = -D\eta\Sigma_s \left| \underline{\nabla} \phi_0(\underline{r}' \to \underline{r}) \right| \qquad \text{(E-10)}$$

Finally a Gaussian kernel is assumed for ϕ_0.

$$\xi \Sigma_s \phi_0(\underline{r}' \to \underline{r}) = \frac{e^{-|\underline{r}-\underline{r}'|^2/4\tau}}{(4\pi\tau)^{3/2}} \qquad \text{(E-11)}$$

Under these approximations Equation (E-9) becomes (with $k^2 = B^2$)

$$k_{eff} = \frac{\nu\Sigma_{fT}}{\Sigma_{aT}} \frac{e^{-B^2\tau}}{1 + L^2B^2} \left[1 - \frac{3\eta}{\xi} D^2 B^2 \right] \qquad \text{(E-12)}$$

The corrections for some common moderators are given below:

Element	$\frac{3\eta}{\xi} D^2$
H	+.0435
D	-.140
Be	-.310
C	-.754

APPENDIX F

EQUIVALENCE OF THE B_L AND P_L APPROXIMATIONS

In Section 17 of Chapter III it was stated without proof that the P_L approximation is equivalent to the B_L approximation if the $A_{j\ell}(\eta)$ of the latter are evaluated by the $L+1$ point Gauss Quadrature scheme. That is, if the statement is true, the P_L equations can be written in the form:

$$\Sigma_t \phi_j = \sum_{\ell=0}^{L} (2\ell+1) A'_{j\ell} [J_\ell + S\delta_{0\ell}] \qquad (F\text{-}1)$$

where

$$A'_{j\ell} = \frac{1}{2} \int_{G_{L+1}}^{1} \frac{d\mu}{1-\eta\mu} P_\ell(\mu) P_j(\mu) \qquad A'_{L+1,\ell} = A'_{\ell,L+1} = 0$$

However, the P_L equations are already of the form

$$J_\ell = \sum_{m=0}^{L} B_{\ell m} \phi_m - S\delta_{0\ell} \qquad (F\text{-}2)$$

where the B_{lm} may be read from Equations (3-10a)

$$B_{\ell m} = \Sigma_t \delta_{\ell m} - \frac{\imath k \ell}{2\ell+1} \delta_{m,\ell-1} - \frac{\imath k(\ell+1)}{2\ell+1} \delta_{m,\ell+1}(1-\delta_{mL}) \qquad (F\text{-}3)$$

Substituting Equation (F-2) into Equation (F-1) we have

$$\Sigma_t \phi_j = \sum_{\ell=0}^{L} (2\ell+1) A'_{j\ell} \left[\sum_{m=0}^{L} B_{\ell m} \phi_m - S\delta_{0\ell} + S\delta_{0\ell} \right]$$

$$= \sum_{m=0}^{L} \phi_m \sum_{\ell=0}^{L} A'_{j\ell} B_{\ell m} (2\ell+1) \qquad (F\text{-}4)$$

However, this equation holds only if

$$\sum_{\ell=0}^{L} (2\ell+1)\, A'_{j\ell}\, B_{\ell m} = \delta_{jm}\, \Sigma_t \qquad (F-5)$$

and, on inserting the expression (F-3) for B_{l_m}, we have for $m \leq L$

$$(2m+1)\,\frac{A'_{jm}}{\eta} - m\, A'_{j,m-1} - (m+1)\, A'_{j,m+1} = \delta_{jm} \qquad (F-6)$$

But it is simple to show that the $A'_{j\ell}$ do obey the recursion relation (F-6). The proof is identical with the proof that

$$A_{j\ell} = \int_{-1}^{1} \frac{P_j(\mu)\, P_\ell(\mu)}{1-\eta\mu}\, d\mu$$

satisfies the similar recursion relation Equation (3-69a); we write the recursion relation for Legendre Polynomials

$$(2m+1)\,\mu\, P_m(\mu) - (m+1)\, P_{m+1}(\mu) - m\, P_{m-1}(\mu) = 0 \qquad (F-7)$$

multiply through by

$$\frac{1}{2}\,\frac{P_j(\mu)}{1-\eta\mu}$$

to obtain

$$(2m+1)\, P_m P_j \frac{\mu}{1-\eta\mu} - (m+1)\,\frac{P_{m+1} P_j}{1-\eta\mu} - m\,\frac{P_{m-1} P_j}{1-\eta\mu} = 0 \qquad (F-8)$$

Now

$$\frac{\mu}{1-\eta\mu} = -\frac{1}{\eta}\left[1 - \frac{1}{1-\eta\mu}\right]$$

Thus, Equation (F-8) becomes

$$\frac{2m+1}{2}\frac{P_m P_j}{\eta(1-\eta\mu)} - \frac{(m+1)}{2}\frac{P_{m+1}P_j}{1-\eta\mu} - \frac{m}{2}\frac{P_{m-1}P_j}{1-\eta\mu} = \frac{2m+1}{2}\frac{P_m P_j}{\eta} \qquad (F-9)$$

If we now integrate over μ, we obtain Equation (3-69a), the recursion relation for the A_{jm}. However, if we integrate over μ by the (L+1) Gauss Quadrature formula we obtain

$$(2m+1)\frac{A'_{mj}}{\eta} - (m+1)A'_{m+1,j} - m A'_{m-1,j} = \int_{G_{L+1}} \frac{2m+1}{2}\frac{P_m P_j}{\eta}\, d\mu$$

$$= \frac{\delta_{mj}}{\eta} \qquad (F-10)$$

For $m<L$ and $j \leq L$. The last equality in Equation (F-10) follows from the fact that $P_m P_j$ is a polynomial μ of degree $(m+j)$ and is thus integrated rigorously for $m+j \leq 2(L+1) - 1 = 2L + 1$. For $m = L$, this equality still holds for $j \leq L$ (actually $j \leq L + 1$), but the term $A'_{m+1,\,j} = 0$ because the integral is evaluated at the zeroes of $P_{L+1}(\mu)$ which means the factor $P_{m+1}(\mu)$ is identically zero at each discrete ordinate. Since no values of A'_{jm} enter the P_L approximation if either index is greater than L, this proves the recursion relation. This also completes the proof because the recursion relation

(F - 3) defines a unique set of functions A'_{jm} for any given value of L since two of the A'_{jm} have been defined (i.e., $A'_{j,\,-1} = A'_{j,\,L+1} = 0$).

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