ANL-6227
Physics and Mathematics
(TID-4500, 15th Ed.)
AEC Research and
Development Report

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois

SPECIAL LECTURES ON THE PHYSICAL
FOUNDATION OF REACTOR ANALYSIS*

by

Paul J. Persiani
Reactor Engineering Division

October 1960

*This series of lectures was delivered at the
AEC-ASEE-Purdue University 1960 Summer Institute
July 5-7, 1960

Operated by The University of Chicago
under
Contract W-31-109-eng-38

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

TABLE OF CONTENTS

	<u>Page</u>
1. Introduction	3
2. Boltzmann Transport Equation	4
3. Velocity and Angular Moments of the Boltzmann Transport Equation.	10
4. Eigenvalue Problem	16
5. Kinematics of Scattering	17
6. Diffusion-Age Approximation	24
7. Method of Groups	28
8. Adjoint Equations	34
9. Perturbation Theory	38

SPECIAL LECTURES ON THE PHYSICAL FOUNDATION OF REACTOR ANALYSIS

by

Paul J. Persiani

1. Introduction

This introductory treatise on the physical foundation of reactor analysis is the result of a series of lectures designed to present reactor physics in a systematic and somewhat rigorous manner. The time limitation under which these lectures were given (six one-hour lecture periods), necessarily reduced the number of important topics pertinent to actual reactor calculations. It is hoped, however, that the selection of the subject matter represents an adequate initial sampling of reactor physics.

The starting point is the Boltzmann transport equation. Since neutron transport theory is essentially concerned with a statistical problem, the behavior of neutrons in a medium is described in terms of measurable macroscopic (averaged) dynamical quantities such as velocity, energy density tensor, energy flow tensor, flux, etc., rather than the distribution function itself. These quantities are generated by the technique of taking velocity or angular moments of the Boltzmann equation. This avoids the usual procedure of discussing transport phenomenon in terms of spherical harmonics or of any other harmonic.

Although in the notes only the flux, zeroth moment in angle, and the current, first moment in angle, are used, the higher moments are also defined, so that this set of lectures may easily be extended to include a study of the thermodynamics of the neutrons in a medium.

Physical quantities and relations, such as Fick's law and average logarithmic energy loss, are developed systematically and are shown to result from the various approximations leading to the diffusion-age equations and the group equations.

2. The Boltzmann Equation

The behavior of a system of interacting particles (neutron-nucleus; neutron-nucleon) may be described by the Boltzmann equation. This equation is a continuity equation in phase space for the distribution function $f(\underline{r}, \underline{v}, t)$, which may be defined as the number density function, i.e., the number of particles per unit volume at $\underline{r}$ per unit velocity volume at $\underline{v}$ and per unit time at t . With this interpretation of the density function, integration over phase space then yields the total number of particles at time t :

$$N(t) = \int_{\underline{v}} d\underline{v} \int_{\underline{r}} d\underline{r} f(\underline{r}, \underline{v}, t) ,$$

where $d\underline{v}$ and $d\underline{r}$ are volume elements in velocity and coordinate space, respectively.

The continuity equation for the neutron density function $f_n(\underline{r}, \underline{v}, t)$ is

$$\frac{\partial f_n(\underline{r}, \underline{v}, t)}{\partial t} + \text{div}_{\underline{r}} f_n(\underline{r}, \underline{v}, t) \underline{v} = \left. \frac{\partial f_n}{\partial t} \right|_{\text{col}} .$$

The second term on the left-hand side of the above equation is essentially the time rate of change of the distribution function due to drift. The right-hand side is the time rate of change due to collisions (scattering, absorption, source). For particles in general, the drift term should include the net outflow of particles in velocity space due to external forces (gravitational, electric and magnetic fields). In the case of neutrons, the effects of these forces are negligible and the term is not included.

The time rate of change of $f_n(\underline{r}, \underline{v}, t)$ due to scattering is obtained by considering a particle balance in phase space. The total number of particles leaving and entering the elemental volume $d\underline{r} d\underline{v}$ in phase space in time dt is

$$\left. \frac{\partial f_n(\underline{r}, \underline{v}, t)}{\partial t} \right|_{\text{scat}} d\underline{r} d\underline{v} dt .$$

During a collision the spatial coordinates of the two interacting particles do not change appreciably, so that only the change in velocity need be considered.

To ease notation, the velocity of the neutron [or particle of interest specified by $f_n(\underline{r}, \underline{v}, t)$] is designated by $\underline{v}$ and that of the scattering particle by $\underline{u}$.

The number of neutrons leaving the volume element in velocity space $d\underline{v}$ is equal to the number of neutrons in $d\underline{v}$ multiplied by the probability of a neutron leaving this element. The number of neutrons in $d\underline{v}$ per cc in time interval dt is $f_n(\underline{r}, \underline{v}, t) d\underline{v} dt$. The probability of scattering out of $\underline{v}$ into $\underline{v}'$ is

$$\int_{\underline{u}} d\underline{u} f_{\beta}(\underline{r}, \underline{u}, t) \int_{\underline{u}'} d\underline{u}' W \sigma_s(\underline{v} \rightarrow \underline{v}'; \underline{u} \rightarrow \underline{u}') ,$$

where $f_{\beta}(\underline{r}, \underline{u}, t)$ is the density function for the β -type (n = neutrons, a = nuclei) particle, $W = |\underline{v} - \underline{u}|$ is the relative speed before collision, and $\sigma_s(\underline{v} \rightarrow \underline{v}'; \underline{u} \rightarrow \underline{u}')$ is the scattering cross section in which the particle of interest is scattered from $\underline{v}$ to $\underline{v}'$ and the scattering particle from $\underline{u}$ to $\underline{u}'$. The number of neutrons scattered out of $d\underline{v}$ about $\underline{v}$ into $d\underline{v}'$ about $\underline{v}'$ is then

$$f_n(\underline{r}, \underline{v}, t) d\underline{v} dt d\underline{v}' \int_{\underline{u}} d\underline{u} f_{\beta}(\underline{r}, \underline{u}, t) \int_{\underline{u}'} d\underline{u}' W \sigma_s(\underline{v} \rightarrow \underline{v}'; \underline{u} \rightarrow \underline{u}') ,$$

and the number scattered out of $d\underline{v}$ about $\underline{v}$ regardless of final energy is then obtained by integrating over all velocities $\underline{v}'$:

$$N_{s_{out}} = f_n(\underline{r}, \underline{v}, t) d\underline{v} dt \int_{\underline{v}'} d\underline{v}' \int_{\underline{u}} d\underline{u} f_{\beta}(\underline{r}, \underline{u}, t) \times \\ \int_{\underline{u}'} d\underline{u}' W \sigma_s(\underline{v} \rightarrow \underline{v}'; \underline{u} \rightarrow \underline{u}') .$$

The number of neutrons scattered into $d\underline{v}$ about $\underline{v}$ is obtained in an analogous manner. The number of neutrons scattered out of $d\underline{v}'$ about $\underline{v}'$ into $d\underline{v}$ about $\underline{v}$ is

$$f_n(\underline{r}, \underline{v}', t) d\underline{v}' dt d\underline{v} \int_{\underline{u}'} d\underline{u}' f_{\beta}(\underline{r}, \underline{u}', t) \int_{\underline{u}} d\underline{u} W' \sigma_s(\underline{v}' \rightarrow \underline{v}; \underline{u}' \rightarrow \underline{u}) ,$$

so that the number of neutrons scattered into $d\underline{v}$ about $\underline{v}$ from all $\underline{v}'$ is

$$N_{s_{in}} = d\underline{v} dt \int_{\underline{v}'} d\underline{v}' f_n(\underline{r}, \underline{v}', t) \int_{\underline{u}'} d\underline{u}' f_{\beta}(\underline{r}, \underline{u}', t) \times \\ \int_{\underline{u}} d\underline{u} W' \sigma_s(\underline{v}' \rightarrow \underline{v}; \underline{u}' \rightarrow \underline{u}) .$$

The time rate of change of $f_n(\underline{r}, \underline{v}, t)$ due to scattering collisions is then

$$\left. \frac{\partial f_n(\underline{r}, \underline{v}, t)}{\partial t} \right|_{scat} d\underline{v} dt = N_{s_{in}} - N_{s_{out}} ,$$

giving

$$\begin{aligned} \left. \frac{\partial f_n(\underline{r}, \underline{v}, t)}{\partial t} \right|_{\text{scat}} &= \int_{\underline{v}'} d\underline{v}' f_n(\underline{r}, \underline{v}', t) \int_{\underline{u}'} d\underline{u}' f_\beta(\underline{r}, \underline{u}', t) \times \\ &\quad \int_{\underline{u}} d\underline{u} W' \sigma_s(\underline{v}' \rightarrow \underline{v}; \underline{u}' \rightarrow \underline{u}) - f_n(\underline{r}, \underline{v}, t) \int_{\underline{v}'} d\underline{v}' \times \\ &\quad \int_{\underline{u}} d\underline{u} f_\beta(\underline{r}, \underline{u}, t) \int_{\underline{u}'} d\underline{u}' W \sigma_s(\underline{v} \rightarrow \underline{v}'; \underline{u} \rightarrow \underline{u}') \quad . \end{aligned}$$

For a system of particles comprised of two or more components, the scattering term is to be summed over all components. The neutron-neutron interactions may be neglected since the density of neutrons is much lower than that of the material nuclei. The term remaining involves the distribution function, $f_a(\underline{r}, \underline{u}, t)$, of the nuclei. The products of the relative speeds and the microscopic cross sections when integrated over the distribution function of the nuclei are called the macroscopic reaction rates per incident neutron and are defined as follows:

$$\begin{aligned} v' \Sigma_s(\underline{r}, \underline{v}' \rightarrow \underline{v}) &= \int_{\underline{u}'} d\underline{u}' f_a(\underline{r}, \underline{u}', t) \int_{\underline{u}} d\underline{u} W' \sigma_s(\underline{v}' \rightarrow \underline{v}; \underline{u}' \rightarrow \underline{u}) \quad , \\ v \Sigma_s(\underline{r}, \underline{v} \rightarrow \underline{v}') &= \int_{\underline{u}} d\underline{u} f_a(\underline{r}, \underline{u}, t) \int_{\underline{u}'} d\underline{u}' W \sigma_s(\underline{v} \rightarrow \underline{v}'; \underline{u} \rightarrow \underline{u}') \quad , \end{aligned}$$

where the distribution function for the nuclei is assumed to be time independent.

That the reaction rates may be written in this form can be expected by considering the simple case in which the nuclei are assumed to be initially at rest in the laboratory system of coordinates. The distribution function may be represented in terms of the Dirac delta function as

$$f_a(\underline{r}, \underline{u}, t) = N_a(\underline{r}) \delta(\underline{u} - \underline{o}) \quad ,$$

where N_a is the number of nuclei per cc and $\delta(\underline{u} - \underline{o})$ is the Dirac delta function having the property that

$$\int dx \delta(x - b) f(x) = f(b) \quad .$$

Substituting the above distribution and changing the order of integration in the latter equation gives

$$\begin{aligned}
 N_a(\underline{r}) \int_{\underline{u}'} d\underline{u}' \int_{\underline{u}} d\underline{u} \delta(\underline{u}-\underline{u}') |\underline{v}-\underline{u}| \sigma_s(\underline{v} \rightarrow \underline{v}'; \underline{u} \rightarrow \underline{u}') \\
 = N_a(\underline{r}) v \int_{\underline{u}'} d\underline{u}' \sigma_s(\underline{v} \rightarrow \underline{v}'; \underline{u}') = N_a(\underline{r}) v \sigma_s(\underline{v} \rightarrow \underline{v}') \\
 = v \Sigma_s(\underline{r}, \underline{v} \rightarrow \underline{v}') ,
 \end{aligned}$$

which is of the form stated.

The rate of change due to scattering becomes

$$\begin{aligned}
 \left. \frac{\partial f_n(\underline{r}, \underline{v}, t)}{\partial t} \right|_{\text{scat}} &= \int_{\underline{v}'} d\underline{v}' f_n(\underline{r}, \underline{v}', t) v' \Sigma_s(\underline{r}, \underline{v}' \rightarrow \underline{v}) \\
 &\quad - f_n(\underline{r}, \underline{v}, t) v \int_{\underline{v}'} d\underline{v}' \Sigma_s(\underline{r}, \underline{v} \rightarrow \underline{v}').
 \end{aligned}$$

The last term may be further reduced by considering the general form of the scattering cross section. This cross section does not depend on the initial and final direction of the scattered particle but only on the incident and final speeds ($|\underline{v}|$, $|\underline{v}'|$) and the angle through which it has scattered: $\cos \Theta = \underline{\Omega} \cdot \underline{\Omega}'$, where $\underline{\Omega}$ and $\underline{\Omega}'$ are unit directional vectors in velocity space ($\underline{v} = v \underline{\Omega}$; $d\underline{v} = v^2 dv d\underline{\Omega}$), $\Sigma_s(\underline{v} \rightarrow \underline{v}') = \Sigma_s(v \rightarrow v'; \underline{\Omega} \cdot \underline{\Omega}')$. Integrating the last term over v' and $\underline{\Omega}'$,

$$\Sigma_s(\underline{r}, v) = \int_{\underline{v}'} d\underline{v}' \Sigma_s(\underline{r}, \underline{v} \rightarrow \underline{v}') .$$

The time rate of change of the number density function due to scattering collisions is finally

$$\begin{aligned}
 \left. \frac{\partial f_n(\underline{r}, \underline{v}, t)}{\partial t} \right|_{\text{scat}} &= \int_{\underline{v}'} d\underline{v}' f_n(\underline{r}, \underline{v}', t) v' \Sigma_s(\underline{r}, \underline{v}' \rightarrow \underline{v}) \\
 &\quad - v \Sigma_s(\underline{r}, v) f_n(\underline{r}, \underline{v}, t) .
 \end{aligned}$$

For the collisions which result in the absorption of a neutron, in an analogous manner as in the scattering out of the velocity range $d\underline{v}$ about $\underline{v}$, the number of neutrons in $d\underline{v}$ about $\underline{v}$ being absorbed is

$$\left. \frac{\partial f_n(\underline{r}, \underline{v}, t)}{\partial t} \right|_{\text{abs}} d\underline{v} dt = - f_n(\underline{r}, \underline{v}, t) d\underline{v} dt \int_{\underline{u}} d\underline{u} f_a(\underline{r}, \underline{u}, t) W \sigma_a(\underline{v}, \underline{u}) .$$

Taking the absorption to be just a function of the relative speeds,

$$v \Sigma_a(\underline{r}, v) = \int_{\underline{u}} d\underline{u} f_a(\underline{r}, \underline{u}, t) W \sigma_a(v, u) ,$$

and the time rate of change of $f_n(\underline{r}, \underline{v}, t)$ due to absorption becomes

$$\left. \frac{\partial f_n(\underline{r}, \underline{v}, t)}{\partial t} \right|_{\text{abs}} = - v \Sigma_a(\underline{r}, v) f_n(\underline{r}, \underline{v}, t) .$$

Neutrons, in the range $d\underline{v}$ about $\underline{v}$, are generated by absorptions which result in the emission of one or more neutrons at various energies (fission process). The number of neutrons having the velocity $\underline{v}$ being absorbed and emitting ν_f neutrons, of which a fraction $\chi(\underline{v})$ have the velocity $\underline{v}$, is

$$\chi(\underline{v}) \nu_f v \Sigma_f(\underline{r}, v) f_n(\underline{r}, \underline{v}, t) ,$$

where $\Sigma_f(\underline{r}, v)$ is the macroscopic fission cross section per unit solid angle.

The total number of neutrons being generated in the range $d\underline{v}$ about $\underline{v}$ due to absorptions occurring at all energies of the incident neutron is then obtained by integrating the above expression over all neutron velocities. The time rate of change of $f_n(\underline{r}, \underline{v}, t)$ due to fissions is then

$$\left. \frac{\partial f_n(\underline{r}, \underline{v}, t)}{\partial t} \right|_{\text{fiss}} = \chi(v) \nu_f \int_{\underline{v}'} d\underline{v}' f_n(\underline{r}, \underline{v}', t) v' \Sigma_f(\underline{r}, v') ,$$

where it has been assumed that the fraction of neutrons, $\chi(v)$, is independent of direction and ν_f is independent of the neutron energy.

Collecting all the collisional terms, the continuity or number-density balance equation for neutrons is

$$\begin{aligned} \frac{\partial f(\underline{r}, \underline{v}, t)}{\partial t} + \text{div}_{\underline{r}} \underline{v} f(\underline{r}, \underline{v}, t) &= \int_{\underline{v}'} d\underline{v}' f(\underline{r}, \underline{v}', t) v' \Sigma_s(\underline{r}, \underline{v}' \rightarrow \underline{v}) - v \Sigma_t(\underline{r}, v) f(\underline{r}, \underline{v}, t) \\ &+ \chi(v) \nu_f \int_{\underline{v}'} d\underline{v}' f(\underline{r}, \underline{v}', t) v' \Sigma_f(\underline{r}, v') , \end{aligned}$$

where

$$\Sigma_t(\underline{r}, v) = \Sigma_s(\underline{r}, v) + \Sigma_a(\underline{r}, v) \quad .$$

The subscript n denoting the distribution function for the neutrons is now not necessary.

3. Velocity Moments of the Boltzmann Transport Equation

The problem is now to solve for the distribution function and, using this function, to derive quantities which may be observed experimentally. Except for very simple systems, the solution of the Boltzmann equation is rather complicated. Since the experimental instruments generally used do not measure the distribution function directly, even for the simple systems, the detailed knowledge of the distribution function may be avoided. For example, in the study of the behavior of neutrons in a medium, the quantity measured is the reaction rate (scattering, absorption, fission, etc.). If the behavior of the detector is known as a function of position, velocity and time, then the distribution function is inferred from the observed reaction rates. Usually detectors are used in a manner insensitive to direction so that the flux (i.e., the distribution function averaged over the angles) is inferred rather than the distribution function $f(\underline{r}, \underline{v}, t)$ itself.

The Boltzmann equation may be transformed to give relations between averaged quantities which may be readily measured. The resulting equations for certain systems may be handled more easily than the Boltzmann equation for the distribution function itself.

The usual method is to introduce quantities involving the velocity of the particles. The Boltzmann equation is multiplied by some function of velocity $Q(\underline{v}) = \underline{v}^n$ ($n = 0, 1, \dots$) and integrated over velocity space. The zeroth moment, $n = 0$, gives the number-density balance; the first moment $n = 1$, gives the momentum-density balance; the second moment, $n = 2$ ($\underline{v}\underline{v}$ a dyad) gives the energy-density-tensor balance; and the third moment gives the energy-density-tensor flow (heat flow). These interpretations are obtained from the property of $f(\underline{r}, \underline{v}, t)$ in defining macroscopic (averaged) quantities:

$$\begin{aligned}
 n(\underline{r}, t) &= \int_{\underline{v}} d\underline{v} f(\underline{r}, \underline{v}, t) && \text{particle density} && \text{(zeroth moment)} \\
 \underline{J}(\underline{r}, t) &= \int_{\underline{v}} d\underline{v} \underline{v} f(\underline{r}, \underline{v}, t) = n(\underline{r}, t) \langle \underline{v} \rangle && \text{current density} && \text{(first moment)} \\
 \tilde{\underline{P}}(\underline{r}, t) &= \int_{\underline{v}} d\underline{v} \underline{v}\underline{v} f(\underline{r}, \underline{v}, t) = n(\underline{r}, t) \langle \underline{v}\underline{v} \rangle && \text{energy density tensor} && \text{(second moment)} \\
 \tilde{\underline{P}}(\underline{r}, t) &= \int_{\underline{v}} d\underline{v} \underline{v}\underline{v}\underline{v} f(\underline{r}, \underline{v}, t) = n(\underline{r}, t) \langle \underline{v}\underline{v}\underline{v} \rangle && \text{energy density tensor} && \text{flow (third moment)}
 \end{aligned}$$

The tilde on $\underline{P}$ is used to denote a dyad quantity.

The transformed Boltzmann equation for a general function $Q(\underline{v})$ is

$$\begin{aligned} \frac{\partial}{\partial t} n(\underline{r}, t) \langle Q(\underline{v}) \rangle + \text{div}_{\underline{r}} n(\underline{r}, t) \langle Q(\underline{v}) \underline{v} \rangle + n(\underline{r}, t) \langle \underline{v} \Sigma_t(\underline{r}, \underline{v}) Q(\underline{v}) \rangle \\ = \int_{\underline{v}} d\underline{v} \int_{\underline{v}'} d\underline{v}' f(\underline{r}, \underline{v}', t) \underline{v}' \Sigma_s(\underline{v}' \rightarrow \underline{v}) Q(\underline{v}) + \int_{\underline{v}} d\underline{v} Q(\underline{v}) S(\underline{r}, \underline{v}, t), \end{aligned}$$

with the source

$$S(\underline{r}, \underline{v}, t) = \chi(\underline{v}) \nu_f \int_{\underline{v}'} d\underline{v}' f(\underline{r}, \underline{v}', t) \underline{v}' \Sigma_f(\underline{r}, \underline{v}').$$

The zeroth moment equation, $n = 0$, $Q(\underline{v}) = 1$, is

$$\frac{\partial}{\partial t} n(\underline{r}, t) + \text{div}_{\underline{r}} \underline{J}(\underline{r}, t) + n(\underline{r}, t) \langle \underline{v} \Sigma_a(\underline{v}) \rangle = \int_{\underline{v}} d\underline{v} S(\underline{r}, \underline{v}, t),$$

where the scattering terms cancel since on the right-hand side changing the order of integration in the scattering term gives

$$\int_{\underline{v}} d\underline{v} \Sigma_s(\underline{v}' \rightarrow \underline{v}) = \Sigma_s(\underline{v}').$$

This is the well-known number-density continuity equation for any system in which the time rate of change of the number of particles per cc in a finite system is a balance between leakage, sinks and sources.

The first moment equation, $n = 1$, $Q(\underline{v}) = \underline{v}$, is

$$\begin{aligned} \frac{\partial}{\partial t} \underline{J}(\underline{r}, t) + \text{div}_{\underline{r}} \tilde{\underline{P}}(\underline{r}, t) + n(\underline{r}, t) \langle \underline{v} \underline{v} \Sigma_t(\underline{v}) \rangle \\ = \int_{\underline{v}} d\underline{v} \int_{\underline{v}'} d\underline{v}' f(\underline{r}, \underline{v}', t) \underline{v}' \Sigma_s(\underline{v}' \rightarrow \underline{v}) \underline{v}, \end{aligned}$$

where the source term drops out since for an isotropic source

$$\int_{\underline{v}} d\underline{v} \underline{v} S(\underline{r}, \underline{v}, t) = 0.$$

The equations for higher moments may be obtained in an analogous manner. For moments greater than $n = 3$, the physical interpretation of the averaged or macroscopic quantity becomes obscure; nevertheless, the hierarchy of equations must be solved simultaneously. The reason for this is that equation for the n^{th} moment contains a leakage term which involves the quantity defined for the next highest moment ($n' = n + 1$). If the number density is required, then the outflow of particles ($\text{div}_{\underline{r}} \underline{J}$) must be known. To get the current density the equation for the energy density tensor must be solved, and so on. However, when the Boltzmann equation is transformed into relations involving macroscopic quantities, physics commensurate with

the problem usually indicates where the higher moments equation may be cut off. For example, there may be a known equation of state for the system, or, as will be shown in the case of neutrons, the energy density tensor may be diagonalized (scalar pressure).

As was previously stated in the case of neutrons, a useful macroscopic quantity is the flux, which is the number density at a given speed multiplied by that speed:

$$\phi(\underline{r}, v, t) = n(\underline{r}, v, t) v = \int_{\underline{\Omega}} d\underline{\Omega} v f(\underline{r}, \underline{v}, t) .$$

The current density at speed v is defined as

$$\underline{J}(\underline{r}, v, t) = n(\underline{r}, v, t) \langle \underline{v} \rangle_{\underline{\Omega}} = \int_{\underline{\Omega}} d\underline{\Omega} \underline{\Omega} v f(\underline{r}, \underline{v}, t) .$$

These quantities are averages over direction in velocity space, and the transport equations are obtained as before except for neglecting the integration over speed.

The zeroth moment of angle in velocity space is

$$\begin{aligned} \frac{1}{v} \frac{\partial}{\partial t} \phi(\underline{r}, v, t) + \text{div}_{\underline{r}} \underline{J}(\underline{r}, v, t) + \Sigma_t(\underline{r}, v) \phi(\underline{r}, v, t) \\ = \int_{\underline{\Omega}} d\underline{\Omega} \int_{\underline{v}'} d\underline{v}' f(\underline{r}, \underline{v}', t) v' \Sigma_s(\underline{r}, \underline{v}' \rightarrow \underline{v}) + 4\pi S(\underline{r}, v, t) . \end{aligned}$$

Note that since the integration over speed is neglected, the scattering terms do not cancel. The scattering term on the right-hand side may be further reduced by integrating $\Sigma_s(\underline{r}, \underline{v}' \rightarrow \underline{v})$ over $d\underline{\Omega}$ and, as before, with the scattering dependent on scattering angle only,

$$\int d\underline{\Omega} \Sigma_s(\underline{r}, \underline{v}' \rightarrow \underline{v}) = \int d\underline{\Omega} \Sigma_s(\underline{r}, v' \rightarrow v; \underline{\Omega} \cdot \underline{\Omega}') = \Sigma_s(\underline{r}, v' \rightarrow v) ,$$

the term reduces to

$$\begin{aligned} \int_{\underline{\Omega}} d\underline{\Omega} \int_{\underline{v}'} d\underline{v}' f(\underline{r}, \underline{v}', t) v' \Sigma_s(\underline{r}, \underline{v}' \rightarrow \underline{v}) \\ = \int_0^\infty dv' v'^2 \int_{\underline{\Omega}'} d\underline{\Omega}' f(\underline{r}, \underline{v}', t) \Sigma_s(\underline{r}, v' \rightarrow v) \\ = \int_0^\infty dv' v'^2 \phi(\underline{r}, v', t) \Sigma_s(\underline{r}, v' \rightarrow v) . \end{aligned}$$

In the source term the 4π may be absorbed in the definition of $\Sigma_f(\underline{r}, v)$, which is now the total (with respect to angle) macroscopic fission cross section. The zeroth moment transport equation is then

$$\begin{aligned} \frac{1}{v} \frac{\partial \phi(\underline{r}, v, t)}{\partial t} + \text{div}_{\underline{r}} \underline{J}(\underline{r}, v, t) + \Sigma_t(\underline{r}, v) \phi(\underline{r}, v, t) \\ = \int_0^\infty dv' v'^2 \phi(\underline{r}, v', t) \Sigma_s(\underline{r}, v' \rightarrow v) + S(\underline{r}, v, t) \end{aligned}$$

The first moment of angle in velocity space is

$$\begin{aligned} \frac{1}{v} \frac{\partial \underline{J}(\underline{r}, v, t)}{\partial t} + \int_{\underline{\Omega}} d\underline{\Omega} \underline{\Omega} \text{div}_{\underline{r}} \left\{ f(\underline{r}, \underline{v}, t) \underline{v} \right\} + \Sigma_t(\underline{r}, v) \underline{J}(\underline{r}, v, t) \\ = \int_{\underline{\Omega}} d\underline{\Omega} \underline{\Omega} \int_{\underline{v}'} d\underline{v}' f(\underline{r}, \underline{v}', t) \underline{v}' \Sigma_s(\underline{r}, \underline{v}' \rightarrow \underline{v}) \end{aligned}$$

where the term for an isotropic source is zero. The second and fourth terms of the above equation may be reduced further.

Consider the fourth term, which can be written as

$$\int_{\underline{v}'} d\underline{v}' f(\underline{r}, \underline{v}', t) \underline{v}' \int_{\underline{\Omega}} d\underline{\Omega} \underline{\Omega} \Sigma_s(\underline{r}, \underline{v}' \rightarrow \underline{v})$$

The integration of the term $\underline{\Omega} \Sigma_s(\underline{r}, \underline{v}' \rightarrow \underline{v})$ over angle takes the form (this will be shown later)

$$\int_{\underline{\Omega}} d\underline{\Omega} \underline{\Omega} \Sigma_s(\underline{r}, \underline{v}' \rightarrow \underline{v}; \underline{\Omega} \cdot \underline{\Omega}') = \mu_L \Sigma_s(\underline{r}, \underline{v}' \rightarrow \underline{v}) \underline{\Omega}'$$

where $\mu_L = \cos \theta = \cos$ of the scattering angle in the laboratory system. The fourth term then becomes

$$\begin{aligned} \int_0^\infty dv' v'^2 \mu_L \Sigma_s(\underline{r}, v' \rightarrow v) \int_{\underline{\Omega}'} d\underline{\Omega}' \underline{\Omega}' v' f(\underline{r}, \underline{v}', t) \\ = \int_0^\infty dv' v'^2 \underline{J}(\underline{r}, v', t) \mu_L \Sigma_s(\underline{r}, v' \rightarrow v) \end{aligned}$$

Before reducing the second term in the above transport equation, consider the corresponding term (energy density tensor) in the first moment of the velocity equation:

$$\text{div}_{\underline{r}} \tilde{\mathbf{P}}(\underline{r}, t) = \text{div}_{\underline{r}} \int_{\underline{v}} d\underline{v} \underline{v} \underline{v} f(\underline{r}, \underline{v}, t) = \int_{\underline{v}} d\underline{v} \text{div}_{\underline{r}} \underline{v} \underline{v} f(\underline{r}, \underline{v}, t)$$

Expanding the dyad $\underline{v}\underline{v}$ and performing the divergence operation, this term becomes

$$\operatorname{div}_{\underline{r}} \tilde{P}(\underline{r}, t) = \int_{\underline{v}} d\underline{v} \left(\begin{aligned} & \underline{i} \frac{\partial}{\partial x} v_x^2 + \underline{j} \frac{\partial}{\partial x} v_x v_y + \underline{k} \frac{\partial}{\partial x} v_x v_z \\ & + \underline{i} \frac{\partial}{\partial y} v_y v_x + \underline{j} \frac{\partial}{\partial y} v_y^2 + \underline{k} \frac{\partial}{\partial y} v_y v_z \\ & + \underline{i} \frac{\partial}{\partial z} v_z v_x + \underline{j} \frac{\partial}{\partial z} v_z v_y + \underline{k} \frac{\partial}{\partial z} v_z^2 \end{aligned} \right) f(\underline{r}, \underline{v}, t) .$$

Collecting the diagonal and off-diagonal terms (O.D.T.),

$$\operatorname{div}_{\underline{r}} \tilde{P}(\underline{r}, t) = \int_{\underline{v}} d\underline{v} \left[\underline{i} \frac{\partial}{\partial x} v_x^2 + \underline{j} \frac{\partial}{\partial y} v_y^2 + \underline{k} \frac{\partial}{\partial z} v_z^2 \right] f(\underline{r}, \underline{v}, t) + \text{O.D.T.}$$

The neutrons in the medium may be considered as a neutron gas and the O.D.T. are neglected, that is, the energy density tensor (pressure tensor) is diagonalized, which means that the pressure is assumed to be a scalar. This is not a bad approximation for the neutron gas.

From the equipartition of kinetic energy,

$$\langle v_x^2 \rangle = \langle v_y^2 \rangle = \langle v_z^2 \rangle = \frac{1}{3} \langle v^2 \rangle ;$$

the divergence term is then

$$\frac{1}{3} \operatorname{grad}_{\underline{r}} P(\underline{r}, t) ,$$

where

$$P(\underline{r}, t) = \int_{\underline{v}} d\underline{v} v^2 f(\underline{r}, \underline{v}, t) = \text{scalar pressure.}$$

It is this condition that will be used to truncate the system of moments in angle equations. The second term in the first moment transport equation is

$$\int_{\underline{\Omega}} d\underline{\Omega} \underline{\Omega} \operatorname{div}_{\underline{r}} \underline{v} f(\underline{r}, \underline{v}, t) = \int_{\underline{\Omega}} d\underline{\Omega} \operatorname{div}_{\underline{r}} \underline{\Omega} \underline{v} f(\underline{r}, \underline{v}, t) ,$$

and with (in cartesian coordinates)

$$\underline{\Omega} = \underline{i} \frac{v_x}{v} + \underline{j} \frac{v_y}{v} + \underline{k} \frac{v_z}{v} , \quad \underline{v} = v \underline{\Omega} ,$$

becomes equal to

$$\int_{\underline{\Omega}} d\underline{\Omega} \left[v_x \underline{\Omega} \frac{\partial}{\partial x} + v_y \underline{\Omega} \frac{\partial}{\partial y} + v_z \underline{\Omega} \frac{\partial}{\partial z} \right] f(\underline{r}, \underline{v}, t) ,$$

and, retaining only the diagonal terms, becomes equal to

$$\frac{1}{3} \text{grad}_{\underline{r}} \int_{\underline{\Omega}} d\underline{\Omega} v f(\underline{r}, \underline{v}, t) = \frac{1}{3} \text{grad}_{\underline{r}} \phi(\underline{r}, v, t) .$$

The first moment in angle transport equation is finally

$$\begin{aligned} \frac{1}{v} \frac{\partial}{\partial t} \underline{J}(\underline{r}, v, t) + \frac{1}{3} \text{grad}_{\underline{r}} \phi(\underline{r}, v, t) + \Sigma_t(\underline{r}, v) \underline{J}(\underline{r}, v, t) \\ = \int_0^\infty dv' v'^2 \underline{J}(\underline{r}, v', t) \mu_L \Sigma_s(\underline{r}, v' \rightarrow v) . \end{aligned}$$

The zeroth and first moment equations comprise the complete set necessary to describe the behavior of neutrons in a medium, that is, the two quantities, flux and current density, are obtained by solving the zeroth and first moment transport equations simultaneously.

The steady-state reactor equations are then

$$\text{div}_{\underline{r}} \underline{J}(\underline{r}, v) + \Sigma_t(v) \phi(\underline{r}, v) = \int_0^\infty dv' v'^2 \phi(\underline{r}, v') \Sigma_s(\underline{r}, v' \rightarrow v) + S(\underline{r}, v) ,$$

$$\frac{1}{3} \text{grad}_{\underline{r}} \phi(\underline{r}, v) + \Sigma_t(v) \underline{J}(\underline{r}, v) = \int_0^\infty dv' v'^2 \underline{J}(\underline{r}, v') \mu_L \Sigma_s(\underline{r}, v' \rightarrow v) ,$$

with

$$S(\underline{r}, v) = \chi(v) \nu_f \int_0^\infty dv' v'^2 \phi(\underline{r}, v') \Sigma_f(\underline{r}, v') .$$

The time-independent reactor equations may be cast in terms of energy rather than speed v by the normalization of the flux:

$$\int_0^\infty dv' v'^2 \phi(\underline{r}, v') = \phi(\underline{r}) = \int_0^\infty dE' \phi(\underline{r}, E') ,$$

so that

$$\text{div}_{\underline{r}} \underline{J}(\underline{r}, E) + \Sigma_t(\underline{r}, E) \phi(\underline{r}, E) = \int_0^\infty dE' \phi(\underline{r}, E') \Sigma_s(\underline{r}, E' \rightarrow E) + S(\underline{r}, E) ,$$

$$\frac{1}{3} \text{grad}_{\underline{r}} \phi(\underline{r}, E) + \Sigma_t(\underline{r}, E) \underline{J}(\underline{r}, E) = \int_0^\infty dE' \underline{J}(\underline{r}, E') \Sigma_s(\underline{r}, E' \rightarrow E) \mu_L ,$$

where

$$S(\underline{r}, E) = \chi(E) \frac{\nu_f}{k_{\text{eff}}} \int_0^\infty dE' \phi(\underline{r}, E') \Sigma_f(\underline{r}, E') .$$

4. Eigenvalue Problem

In a finite system, the flux $\phi(\underline{r}, E, t)$ must satisfy certain boundary conditions, e.g., the flux is zero at the surface of the bounded domain (reactor). This means that the solutions of the spatial part of the equations are eigenfunctions, and the solutions exist for certain values of a parameter, say λ (the eigenvalue).

Of all the parameters in the above equations, only ν_f indicates whether enough neutrons are being produced for this balance. The problem is then to find those certain values of λ , say $\lambda_1, \lambda_2, \dots$, which will satisfy the above equations. Consider that of all the λ 's only one, say $\lambda_1 = \lambda$, gives an eigenfunction which is non-negative (e.g., in the case of trigonometric functions this would be the positive part of the fundamental mode). This function will then describe the flux in a reactor, which is critical when

$$\lambda_1 = \lambda$$

The value of λ_1 , which may be taken as ν_f , is a function of the material only, whereas λ is a function of the geometry.

The quantity ν_f appears in the source term and to make this an eigenvalue problem ν_f is replaced by λ . Then, defining

$$k_{\text{eff}} = \lambda_1 / \lambda = \nu_f / \lambda$$

or

$$\lambda = \nu_f / k_{\text{eff}}$$

the source term becomes

$$S(\underline{r}, E) = \lambda(E) \frac{\nu_f}{k_{\text{eff}}} \int_0^\infty dE' \phi(\underline{r}, E') \Sigma_f(\underline{r}, E')$$

When $k_{\text{eff}} = 1$ ($\lambda_1 = \lambda$), then the neutron-balance equation is satisfied and the reactor is said to be critical.

5. Kinematics of Scattering

A neutron-nucleus interaction (scattering and absorption) varies as a function of neutron energy and the energy state of the nucleus. At neutron energies greater than 1 kev for light nuclei and greater than 1 ev for heavy nuclei, the reactions involve resonance absorption, direct absorption, resonance scattering, and direct scattering phenomenon. Below these energies, for which nuclei excitation levels are absent, neutrons may be scattered by direct interaction phenomena. However, the low-energy range in which this occurs is rather limited since nuclei are bound in some sort of lattice or aggregate and do not act as free nuclei.

The scattering probabilities or cross sections as functions of initial and final energies are rather complex expressions and make further analytical analysis cumbersome, if not impossible. In most cases one has to resort to numerical methods. There are scattering models which are simple and can be handled analytically. In such a model the nucleus is represented as a hard sphere having no initial motion in the laboratory system. This model, however, does not properly account for the energy exchange between the interacting particles. If the scattering nuclei were given an initial velocity (thermal motion) in the laboratory system, then processes in which the neutron may gain energy (scattering up in energy) would be included. However, this latter model, called the "free gas" model, necessitates the use of numerical methods in solving the transport equations.

The hard-sphere model, with zero velocity in the laboratory system, does give an order-of-magnitude effect from which a critical system may be designed with some degree of confidence.

The scattering angles and energy relations in both the center-of-mass and laboratory systems are obtained from momentum and energy considerations for elastic collisions between neutrons (of mass m) and nuclei (of mass $M = mA$, where A is the mass number).

Using primed and unprimed quantities to denote the state before and after collisions, respectively, and designating the quantities in the center-of-mass system with a subscript c , the following relations are derived:

$$\underline{v}' = (1 + A)\underline{v}_c$$

$$\underline{u}' = 0$$

$$\underline{v}_c' = \underline{v}' - \underline{v}_c = \frac{A}{1 + A} \underline{v}'$$

$$\underline{u}_c' = \frac{-1}{(1 + A)} \underline{v}'$$

where

$\underline{v}_c$ is the velocity of the center of mass.

From momentum and energy conditions, the relations between neutron energy in the laboratory system and the cosine of the scattering angles in the center-of-mass and laboratory system are as follows:

$$\begin{aligned} \frac{\mathbf{v}_c \cdot \mathbf{v}_c'}{v_c v_c'} = \cos \phi = \mu_c &= 1 - \frac{(1+A)^2}{2A} \left(1 - \frac{E}{E'}\right) \\ &= \frac{(A^2 - 1 + \mu_L^2)^{1/2} \mu_L - 1 + \mu_L^2}{A} , \end{aligned}$$

$$\begin{aligned} \frac{\mathbf{v} \cdot \mathbf{v}'}{vv'} = \cos \Theta = \mu_L &= \frac{(1+A)}{2} \left(\frac{E}{E'}\right)^{1/2} - \frac{(A-1)}{2} \left(\frac{E'}{E}\right)^{1/2} \\ &= \frac{1 + A \mu_c}{(1 + 2A \mu_c + A^2)^{1/2}} \end{aligned}$$

$$\frac{E}{E'} = 1 - \frac{2A}{(A+1)^2} (1 - \mu_c) = \frac{\left\{ \mu_L + (A^2 - 1 + \mu_L^2)^{1/2} \right\}^2}{(A+1)^2}$$

If the scattering in the center-of-mass system is forward,

$$\phi = 0,$$

$$\mu_c = 1,$$

$$\mu_L = 1,$$

and

$$E/E' = 1,$$

so that there is no energy loss.

If the scattering is head-on in the center-of-mass system,

$$\phi = \pi ,$$

$$\mu_c = -1,$$

$$\mu_L = -1,$$

and

$$E/E' = 1 - \frac{4A}{(A+1)^2} = 1 - \alpha ,$$

where

$$\alpha = 4A/(A+1)^2 .$$

The range of final energy E is

$$(1 - \alpha)E' \leq E \leq E' \text{ (scattering down only).}$$

The scattering cross section for changing the energy E' and direction $\underline{\Omega}'$ into a unit energy interval about E and unit solid angle about $\underline{\Omega}$ has been written as (spatial dependence is to be understood)

$$\Sigma_s(E' \rightarrow E; \underline{\Omega}' \rightarrow \underline{\Omega}) = \Sigma_s(E' \rightarrow E; \underline{\Omega}' \cdot \underline{\Omega}) = \Sigma_s(E' \rightarrow E; \mu_L) ,$$

where $\mu_L = \underline{\Omega}' \cdot \underline{\Omega} = \cos \Theta$, since the scattering is dependent only on the angle through which it is scattered. A way in which the angular dependence may be analyzed is to expand the cross section in Legendre polynomials:

$$\Sigma_s(E' \rightarrow E, \mu_L) = \sum_{\ell} S_{\ell}(E' \rightarrow E) P_{\ell}(\cos \Theta) .$$

The coefficient $S_{\ell}(E' \rightarrow E)$ is obtained by utilizing the orthogonality relation of Legendre polynomials:

$$\int_{\underline{\Omega}} P_{\ell'}(\mu_L) P_{\ell}(\mu_L) d\underline{\Omega} = 2\pi \int_{-1}^{+1} P_{\ell'}(\mu_L) P_{\ell}(\mu_L) d\mu_L = \frac{4\pi}{2\ell+1} \delta_{\ell\ell'} ,$$

where $\delta_{\ell\ell'}$ is the Kronecker delta function: $\delta_{\ell\ell'} = 1$ for $\ell = \ell'$ and zero otherwise; further $d\underline{\Omega} = 2\pi \sin \Theta d\Theta = -2\pi d\mu_L$. Multiplying the cross section by $P_{\ell'}(\mu_L)$, integrating over $d\underline{\Omega}$, and summing over ℓ , there is obtained

$$\begin{aligned} S_{\ell}(E' \rightarrow E) &= \frac{2\ell+1}{4\pi} \int_{\underline{\Omega}} \Sigma_s(E' \rightarrow E; \mu_L) P_{\ell}(\mu_L) d\underline{\Omega} , \\ &= \frac{2\ell+1}{2} \int_{-1}^{+1} \Sigma_s(E' \rightarrow E; \mu_L) P_{\ell}(\mu_L) d\mu_L . \end{aligned}$$

The energy condition for elastic scattering, given by the relation E/E' , is introduced into the cross section as a Dirac delta function:

$$\Sigma_s(E' \rightarrow E, \mu_L) = \Sigma_s(E', \mu_L) \delta \left\{ E - E' + \frac{2AE'}{(A+1)^2} (1 - \mu_C) \right\} .$$

The relation in the center-of-mass system is chosen because it facilitates subsequent analysis. In the study of nuclear reactions, the incident neutrons having energies in the kev region (p,d-wave neutrons) give rise to a strong forward bias in the center-of-mass system. To account for this, the component $\Sigma_s(E', \mu_L)$ of the above cross section is

expressed in terms of the cross section in the center-of-mass system and, in turn, is then expanded in Legendre polynomials. Starting with the condition that

$$\int d\mu_L \Sigma_s(E', \mu_L) = \Sigma_s(E') = \int d\mu_C \Sigma_s(E', \mu_C) \quad ,$$

the relation between the cross sections is

$$\Sigma_s(E', \mu_L) = \Sigma_s(E', \mu_C) \frac{d\mu_C}{d\mu_L} \quad ,$$

and, expanding $\Sigma_s(E', \mu_C)$ in Legendre polynomials,

$$\Sigma_s(E', \mu_C) = \sum_{\ell'} S_{\ell'}(E') P_{\ell'}(\mu_C) \quad .$$

Substituting all these terms in the expression for $S_{\ell}(E' \rightarrow E)$, the result is

$$S_{\ell}(E' \rightarrow E) = \frac{2\ell + 1}{2} \sum_{\ell'} S_{\ell'}(E') \times \\ \int_{-1}^{+1} d\mu_C P_{\ell'}(\mu_C) P_{\ell}(\mu_L) \delta \left\{ E - E' + \frac{\alpha E'}{2} (1 - \mu_C) \right\} \quad .$$

The integral is evaluated by making a change of variables. Let

$$\xi = - \frac{\alpha E'}{2} (1 - \mu_C);$$

$$d\xi = \frac{\alpha E'}{2} d\mu_C \quad ,$$

so that from the property of the Dirac delta function

$$\frac{2}{\alpha E'} \int d\xi P_{\ell'}(\mu_C) P_{\ell}(\mu_L) \delta \left\{ (E - E') - \xi \right\} = \frac{2}{\alpha E'} P_{\ell'}(\mu_C^0) P_{\ell}(\mu_L^0) \quad ,$$

where μ_L^0 and μ_C^0 are now to be functions of energy only:

$$\mu_L^0 = \frac{(A+1)}{2} \left(\frac{E}{E'} \right)^{1/2} - \frac{(A-1)}{2} \left(\frac{E'}{E} \right)^{1/2} \quad ,$$

$$\mu_C^0 = 1 - \frac{2}{\alpha} \left(1 - \frac{E}{E'} \right) \quad .$$

The energy-dependent part of the cross section becomes

$$S_{\ell}(E' \rightarrow E) = (2\ell + 1)P_{\ell}(\mu_L^0) \frac{1}{\alpha E'} \sum_{\ell'} S_{\ell'}(E') P_{\ell'}(\mu_C^0) ,$$

giving finally the macroscopic cross section for the proposed model as

$$\Sigma_s(E' \rightarrow E, \mu_L) = \sum_{\ell} (2\ell + 1)P_{\ell}(\mu_L^0) P_{\ell}(\mu_L) \frac{1}{\alpha E'} \sum_{\ell'} S_{\ell'}(E') P_{\ell'}(\mu_C^0) .$$

In the transport equations, the cross section required is angle independent, so that

$$\Sigma_s(E' \rightarrow E) = 2\pi \int_{-1}^{+1} d\mu_L \Sigma_s(E' \rightarrow E, \mu_L) = 2\pi \sum_{\ell} S_{\ell}(E' \rightarrow E) \int_{-1}^{+1} d\mu_L P_{\ell}(\mu_L)$$

and from

$$\int_{-1}^{+1} d\mu_L P_{\ell}(\mu_L) = \frac{2}{(2\ell + 1)} \delta_{\ell 0} ,$$

then

$$\Sigma_s(E' \rightarrow E) = 4\pi S_0(E' \rightarrow E) = \frac{4\pi}{\alpha E'} \sum_{\ell'} S_{\ell'}(E') P_{\ell'}(\mu_C^0) .$$

If the scattering in the center-of-mass system is isotropic ($\ell' = 0$), then

$$\Sigma_s(E' \rightarrow E) = \frac{\Sigma_s(E')}{\alpha E'} ,$$

where

$$\Sigma_s(E') = 4\pi S_0(E') .$$

This result may also be obtained from direct consideration as follows:

In the center-of-mass system, the probability that a neutron undergoing spherically symmetric scattering will enter the solid angle $d\Omega$ about $\underline{\Omega}$ is equal to

$$\frac{d\Omega}{4\pi} = \frac{2\pi \sin\phi d\phi}{4\pi} = -\frac{1}{2} d\mu_c \quad .$$

The probability that after scattering the neutron will be in any direction is

$$-\frac{1}{2} \int_{-1}^{+1} d\mu_c = 1 \quad .$$

Equal intervals of μ_c have equal probability. For equal intervals of μ_c , the final energy intervals also have equal probability, since dE is directly proportional to $d\mu_c$. This can be seen from the energy angle relation:

$$E - E' = \frac{\alpha E'}{2} (1 - \mu_c) \quad ,$$

and

$$dE = -\frac{\alpha E'}{2} d\mu_c \quad .$$

Since the final energy must lie within the range between $E'(1 - \alpha)$ and E' , the total interval being $\alpha E'$, the probability of scattering from E' into the interval dE about E is then

$$\Sigma_s(E' \rightarrow E) dE = \Sigma_s(E') \frac{dE}{\alpha E'} \quad ,$$

which is the result obtained above.

If the scattering in the center-of-mass is not isotropic, then as the next approximation the $\ell' = 1$ term is retained, so that

$$\Sigma_s(E' \rightarrow E) = \frac{\Sigma_s(E')}{\alpha E'} \left[1 + \frac{S_1(E')}{S_0(E')} \mu_c^0 \right] \quad .$$

The quantity $S_1(E')$ is evaluated from models of neutron-nucleon scattering in the center-of-mass system other than that considered in this section.

The expansion of the macroscopic cross section in Legendre polynomials may be utilized to verify the relation

$$\int_{\Omega} d\Omega \underline{\Omega} \Sigma_s(E' \rightarrow E, \mu_L) = \mu_L^0 \Sigma_s(E' \rightarrow E) \underline{\Omega}' \quad ,$$

used in the first-moment transport equation.

In spherical coordinates the unit directional vector is

$$\underline{\Omega} = \underline{i} \sin \theta \cos \phi + \underline{j} \sin \theta \sin \phi + \underline{k} \cos \theta \quad ,$$

and may be expressed in terms of spherical surface harmonics, $Y_{\ell m}(\theta, \phi)$, as

$$\underline{\Omega} = \left(\frac{4\pi}{3} \right)^{1/2} \left[(-\underline{\epsilon}_1) Y_{1,-1}(\theta, \phi) + (-\underline{\epsilon}_{-1}) Y_{1,1}(\theta, \phi) + \underline{\epsilon}_0 Y_{10}(\theta, \phi) \right]$$

where $\underline{\epsilon}_s (s = 0, \pm 1)$ are spherical basis vectors. With

$$\Sigma_s(\mathbf{E}' \rightarrow \mathbf{E}, \mu_L) = \sum_{\ell} S_{\ell}(\mathbf{E}' \rightarrow \mathbf{E}) P_{\ell}(\cos \theta)$$

and from the orthogonality relation

$$\int d\underline{\Omega} Y_{\ell', m'}(\theta, \phi) P_{\ell}(\cos \theta) = \delta_{\ell \ell'} \frac{4\pi}{2\ell + 1} Y_{\ell m'}(\theta', \phi') \quad ,$$

the integral becomes

$$\int_{\underline{\Omega}} d\underline{\Omega} \underline{\Omega} \Sigma_s(\mathbf{E}' \rightarrow \mathbf{E}, \mu_L) = S_1(\mathbf{E}' \rightarrow \mathbf{E}) \frac{4\pi}{3} \underline{\Omega}' = \Sigma_s(\mathbf{E}' \rightarrow \mathbf{E}) \mu_L^0 \underline{\Omega}' \quad ,$$

where

$$\underline{\Omega}' = \left(\frac{4\pi}{3} \right)^{1/2} \left[(-\underline{\epsilon}_1) Y_{1,-1}(\theta', \phi') + (-\underline{\epsilon}_{-1}) Y_{1,1}(\theta', \phi') + \underline{\epsilon}_0 Y_{10}(\theta', \phi') \right] \quad ,$$

and

$$\frac{4\pi}{3} S_1(\mathbf{E}' \rightarrow \mathbf{E}) = \mu_L \frac{4\pi}{\alpha E'} \sum_{\ell'} S_{\ell'}(\mathbf{E}') P_{\ell'}(\mu_c^0) = \mu_L^0 \Sigma_s(\mathbf{E}' \rightarrow \mathbf{E}) \quad .$$

6. Diffusion-Age Approximation

The transport equations may be cast in terms of a quantity called "lethargy," defined as

$$u = \ln E_0/E$$

where E_0 is some maximum energy. The cross section $\Sigma_s(E' \rightarrow E)$ is transformed in terms of lethargy by writing

$$\begin{aligned} \Sigma_s(E \rightarrow E) &= \frac{4\pi}{\alpha E'} \sum_{\ell'} S_{\ell'}(E') P_{\ell'}(\mu_c^0) = \frac{4\pi S_0(E')}{\alpha E} \frac{E}{E'} \sum_{\ell'} \frac{S_{\ell'}(E')}{S_0(E')} P_{\ell'}(\mu_c^0) \\ &= \frac{\Sigma_s(E')}{E} f(u-u') \end{aligned}$$

where

$$\begin{aligned} f(u-u') &= \frac{e^{-(u-u')}}{\alpha} \sum_{\ell'} \frac{S_{\ell'}(E')}{S_0(E')} P_{\ell'}(\mu_c^0) \quad \text{for} \quad \begin{cases} (u' \leq u < u' + u_m) \\ \text{or} \\ (u - u_m \leq u' \leq u) \end{cases} \\ &= 0 \quad \text{(otherwise),} \end{aligned}$$

and the maximum lethargy is

$$u_m = \ln \frac{1}{(1-\alpha)}$$

By making the above change in variables in the transport equations with

$$-du' = \frac{dE'}{E'}$$

and normalizing the flux so that

$$\int dE \phi(\underline{r}, E) = \phi(\underline{r}) = \int du E \phi(\underline{r}, E) = \int du \phi(\underline{r}, u)$$

and similarly for the current, the transport equations in terms of lethargy become

$$\text{div}_{\underline{r}} \underline{J}(\underline{r}, u) + \Sigma_t(\underline{r}, u) \phi(\underline{r}, u) = \int_{u-u_m}^u du' \phi(\underline{r}, u') \Sigma_s(\underline{r}, u') f(u-u') + S(\underline{r}, u)$$

$$\frac{1}{3} \text{grad}_{\underline{r}} \phi(\underline{r}, u) + \Sigma_t(\underline{r}, u) = \int_{u-u_m}^u du' \underline{J}(\underline{r}, u') \Sigma_s(\underline{r}, u') \mu_L^0 f(u-u') ,$$

$$S(\underline{r}, u) = \chi(u) \frac{\nu_f}{k_{\text{eff}}} \int_{-\infty}^{\infty} du \phi(\underline{r}, u) \Sigma_f(u) ,$$

where the cosine of the scattering angle in the laboratory system and center-of-mass system in lethargy are

$$\mu_L^0 = \frac{(A+1)}{2} e^{-(u-u')/2} - \frac{(A-1)}{2} e^{(u-u')/2}$$

$$\mu_c^0 = 1 - \frac{2}{\alpha} \left[1 - e^{-(u-u')} \right] .$$

A method of solving this set of integro-differential equations is to transform the integral terms into differential forms by expanding the integrands in Taylor series. This is similar to the recasting of the transport equation into a form known as the Fokker-Planck equation, if only the first few terms are retained, and is applicable for systems in which the interactions between particles result in small changes of momentum.

Expanding the reaction rate $\phi(\underline{r}, u') \Sigma_s(\underline{r}, u')$ about the lethargy u in a Taylor series,

$$\begin{aligned} \phi(\underline{r}, u') \Sigma_s(\underline{r}, u') &= \phi(\underline{r}, u) \Sigma_s(\underline{r}, u) + (u'-u) \frac{\partial}{\partial u} \phi(\underline{r}, u) \Sigma_s(\underline{r}, u) \\ &+ \frac{(u'-u)^2}{2} \frac{\partial^2}{\partial u^2} \phi(\underline{r}, u) \Sigma_s(\underline{r}, u) + \dots , \end{aligned}$$

and, substituting in the zeroth moment transport equation, the integrals to evaluate are of the form

$$\int_{u-u_m}^u du' (u'-u)^n f(u-u') \equiv \overline{(u'-u)^n} \equiv \overline{(-\xi)^n} .$$

A similar expansion in the first-moment transport equation of $\underline{J}(\underline{r}, u') \Sigma_s(\underline{r}, u')$ results in integrals of the form

$$\int_{u-u_m}^u du' \mu_L^0 (u'-u)^n f(u-u') \equiv \mu_L^0 \overline{(u'-u)^n} \equiv \mu_L^0 \overline{(-\xi)^n} .$$

These integrals are essentially n^{th} -order moments in energy or lethargy. The property of $f(u-u')$ is

$$\int_{u-u_m}^u du' f(u-u') = 1 \quad ,$$

and the first moment in lethargy ($n = 1$) is the average logarithmic energy loss, which for isotropic scattering in the center-of-mass system is

$$\overline{\xi} = \left\{ 1 - \frac{(1 - \alpha)}{\alpha} u_m \right\} \quad .$$

The zeroth lethargy moment in the second integral leads to the average cosine of the scattering angle in the laboratory system, which for isotropic scattering in the center of mass system is

$$\overline{\mu_L^0} = 2/3A \quad .$$

Substituting the above expansions in the transport equations and keeping terms in second order of smallness, $\overline{\xi^n} = 0$ for $n > 2$ and $\overline{\mu_L^0} (-\overline{\xi^n}) = 0$ for $n > 0$, gives

$$\begin{aligned} \text{div}_{\underline{r}} \underline{J}(\underline{r}, u) + \Sigma_a(\underline{r}, u) \phi(\underline{r}, u) &= -\overline{\xi} \frac{\partial}{\partial u} \phi(\underline{r}, u) \Sigma_s(\underline{r}, u) \\ &+ \frac{\overline{\xi^2}}{2} \frac{\partial^2}{\partial u^2} \phi(\underline{r}, u) \Sigma_s(\underline{r}, u) + S(\underline{r}, u) \quad , \end{aligned}$$

$$\frac{1}{3} \text{grad}_{\underline{r}} \phi(\underline{r}, u) + \Sigma_{tr}(\underline{r}, u) \underline{J}(\underline{r}, u) = 0 \quad ,$$

where the quantity

$$\Sigma_{tr}(\underline{r}, u) = \Sigma_t(\underline{r}, u) - \overline{\mu_L^0} \Sigma_s(\underline{r}, u)$$

is called the transport cross section. The validity of this approximation depends on the mass of the scatterer, since energy exchanges between neutrons and light nuclei may be very large. A scatterer of unit atomic mass may absorb all the energy of the incident neutron.

To this order of approximation, the latter equation, written as,

$$\underline{J}(\underline{r}, u) = -\frac{1}{3\Sigma_{tr}(\underline{r}, u)} \text{grad}_{\underline{r}} \phi(\underline{r}, u) = -D(\underline{r}, u) \text{grad}_{\underline{r}} \phi(\underline{r}, u) \quad ,$$

is known as Fick's law, and $D(\underline{r}, u)$ is called the diffusion coefficient. Substituting this expression for the current into the zeroth-moment transport equation, and since for isotropic scattering in the center-of-mass system $\overline{\xi}$ is independent of energy, the transport equation becomes

$$\begin{aligned} \frac{\partial}{\partial u} \left\{ \overline{\xi} \phi(\underline{r}, u) \Sigma_s(\underline{r}, u) \right\} - \text{div}_{\underline{r}} D(\underline{r}, u) \text{grad}_{\underline{r}} \phi(\underline{r}, u) + \Sigma_a(\underline{r}, u) \phi(\underline{r}, u) \\ = \gamma \frac{\partial^2}{\partial u^2} \left\{ \overline{\xi} \phi(\underline{r}, u) \Sigma_s(\underline{r}, u) \right\} + S(\underline{r}, u) \quad , \end{aligned}$$

where

$$\gamma = \overline{\xi^2} / 2 \overline{\xi} \quad .$$

A method of reducing this equation to first-order derivatives in u is to differentiate with respect to u , substitute this result for the second-order derivative in the original equation, and retain only first powers of γ . The resulting transport equation becomes

$$\frac{\partial}{\partial u} q(\underline{r}, u) - \text{div}_{\underline{r}} D(\underline{r}, u) \text{grad}_{\underline{r}} \phi(\underline{r}, u) + \Sigma_a(\underline{r}, u) \phi(\underline{r}, u) - S(\underline{r}, u) = 0 \quad ,$$

with

$$\begin{aligned} q(\underline{r}, u) = \left\{ \overline{\xi} \phi(\underline{r}, u) \Sigma_s(\underline{r}, u) - \gamma \text{div}_{\underline{r}} D(\underline{r}, u) \text{grad}_{\underline{r}} \phi(\underline{r}, u) \right. \\ \left. + \gamma \Sigma_a(\underline{r}, u) \phi(\underline{r}, u) - \gamma S(\underline{r}, u) \right\} \quad . \end{aligned}$$

The quantity $q(\underline{r}, u)$ is the slowing down density with capture, leakage and source term, and to the order of the second moment of energy this is called the diffusion-age equation.

7. Method of Groups

The method of groups is to divide the energy or lethargy range into intervals u^j, u^{j+1} . The lowest group in energy, ranging from zero to some cut off energy E_T , is called the slow or thermal group. The lethargy range for this group is from $u = u_T (E = E_T)$ to $u = \infty (E = 0)$.

Within this group, the energy distribution of the neutrons is assumed to be Maxwellian, and the parameters associated with the thermal groups are averaged over this distribution. The neutrons above this thermal group will be called fast. This above-thermal group may be neglected (leaving one with a one-group description) or may be lumped into a single fast group (two-group theory), or may be divided into many groups.

Integrating the diffusion-age equation over the thermal group, and with the following definitions of averaged quantities

$$\phi_T(\underline{r}) = \int_{u_T}^{\infty} du \phi(\underline{r}, u) \quad , \quad \Sigma_{aT}(\underline{r}) \phi_T(\underline{r}) = \int_{u_T}^{\infty} du \Sigma_a(\underline{r}, u) \phi(\underline{r}, u) \quad ,$$

$$DT(\underline{r}) \text{grad}_{\underline{r}} \phi_T(\underline{r}) = \int_{u_T}^{\infty} du D(\underline{r}, u) \text{grad}_{\underline{r}} \phi(\underline{r}, u) \quad ,$$

$$S_T(\underline{r}) = \int_{u_T}^{\infty} du S(\underline{r}, u) \quad ,$$

the thermal-group equation is

$$\text{div}_{\underline{r}} D_T(\underline{r}) \text{grad}_{\underline{r}} \phi_T(\underline{r}) - \Sigma_{aT}(\underline{r}) \phi_T(\underline{r}) + q(\underline{r}, u_T) + S_T(\underline{r}) = 0 \quad ,$$

where $q(\underline{r}, \infty) = 0$.

For a one-group theory, the only source of neutrons would be from the fission process, that is, the neutrons are assumed to be born thermal so that $q(\underline{r}, u_T) = 0$, and from the definition of $S(\underline{r}, u)$

$$S_T(\underline{r}) = \frac{\nu_f}{k_{\text{eff}}} \phi_T(\underline{r}) \Sigma_{fT} \quad .$$

For other than one-group theory, the source of neutrons for the thermal group is predominantly from slowing down of neutrons of higher energy, and the usual assumption made is that the fission processes do not

emit neutrons in the slow group [$\chi(u) = 0$ for $u_T \leq u \leq \infty$]. In the thermal-group equation, then, $S_T(\underline{r}) = 0$ and the source term $S(\underline{r}, u_T)$ in the definition of $q(\underline{r}, u_T)$ is also zero. Further, to ease the analysis, it is assumed that fissions occur only in the thermal group, so that the source becomes

$$S(\underline{r}, u) = \chi(u) \frac{\nu_f}{k_{\text{eff}}} \int_{u_T}^{\infty} du \phi(\underline{r}, u) \Sigma_f(\underline{r}, u) = \chi(u) \frac{\nu_f}{k_{\text{eff}}} \Sigma_{fT}(\underline{r}) \phi_T(\underline{r}) .$$

For a homogeneous system or a subregion of the system in which the cross sections are assumed to be constant with respect to r , the basic reactor equations are as follows: for the above-thermal group (fast equation),

$$\frac{\partial}{\partial u} q(\underline{r}, u) - D(u) \nabla^2 \phi(\underline{r}, u) + \Sigma_a(u) \phi(\underline{r}, u) - S(\underline{r}, u) = 0 ,$$

$$q(\underline{r}, u) = \left\{ \left[\frac{\partial}{\partial u} \Sigma_s(u) + \gamma \Sigma_a(u) - \gamma D(u) \nabla^2 \right] \phi(\underline{r}, u) - \gamma S(\underline{r}, u) \right\} ,$$

and for the thermal group,

$$D_T \nabla^2 \phi_T(\underline{r}) - \Sigma_{aT} \phi_T(\underline{r}) + q(\underline{r}, u_T) = 0$$

$$q(\underline{r}, u_T) = \left[\frac{\partial}{\partial u} \Sigma_s(u_T) + \gamma \Sigma_a(u_T) - \gamma D(u_T) \nabla^2 \right] \phi(\underline{r}, u_T) .$$

Before further specializing to a definite number of groups, the above equations may be used to solve for k_{eff} which appears in the source term $S(\underline{r}, u)$. Assume that the spatial dependence equations are of the form

$$\nabla^2 \phi(\underline{r}, u) + \kappa^2(u) \phi(\underline{r}, u) = 0 ,$$

$$\nabla^2 \phi_T(\underline{r}) + \kappa_T^2 \phi(\underline{r}) = 0 ,$$

with the boundary condition that $\phi(\underline{r}, u)$ and $\phi_T(\underline{r})$ are zero on the surface of the system. The quantity $\kappa^2(u)$ (or κ_T^2), called buckling, is the spatial curvature of the flux. It is a measure of the leakage of neutrons out of the system.

Differentiating $q(\underline{r}, u)$ with respect to u and substituting into the fast equation, the result is

$$\begin{aligned} & \frac{\partial}{\partial u} \left[\bar{\xi} \Sigma_s(u) + \gamma \Sigma_a(u) + \gamma D(u) \kappa^2(u) \right] \phi(\underline{r}, u) \\ & + \left[D(u) \kappa^2(u) + \Sigma_a(u) \right] \phi(\underline{r}, u) \\ & - \frac{\nu_f}{k_{\text{eff}}} \Sigma_{fT}(\underline{r}) \phi_T(\underline{r}) \left[\chi(u) + \gamma \frac{\partial}{\partial u} \chi(u) \right] = 0 \end{aligned}$$

This is a first-order differential equation and a solution is [assuming $\chi(u) \gg \gamma \frac{\partial}{\partial u} \chi(u)$, to ease analysis]

$$\left[\bar{\xi} \Sigma_s + \gamma \Sigma_a + \gamma D \kappa^2 \right] \phi(\underline{r}, u) = \frac{\nu_f}{k_{\text{eff}}} \Sigma_{fT} \phi_T(\underline{r}) \times$$

$$\int_{-\infty}^u du' \chi(u') e^{- \int_{u'}^u \frac{[D \kappa^2 + \Sigma_a]}{[\bar{\xi} \Sigma_s + \gamma \Sigma_a + \gamma D \kappa^2]} du''},$$

where it is understood that Σ_s , Σ_a , D , and κ^2 are still dependent upon u . Evaluating the above equation at $u = u_T$, and substituting for $\phi_T(\underline{r})$ from the thermal group equation, there is obtained for the equation for k_{eff}

$$k_{\text{eff}} = \frac{\nu_f \Sigma_{fT}(\underline{r})}{[D_T \kappa_T^2 + \Sigma_{aT}]} \int_{-\infty}^{u_T} du \chi(u) e^{- \int_u^{u_T} \frac{[D \kappa^2 + \Sigma_a]}{[\bar{\xi} \Sigma_s + \gamma \Sigma_a + \gamma D \kappa^2]} du'}$$

Assuming that the source emits neutrons at only one energy, say $u = u_0$, then $\chi(u) = \delta(u - u_0)$, and with the following definitions:

$$L_T^2 = \frac{D_T}{\Sigma_{aT}},$$

$$\tau \kappa^2 = \int_{u_0}^{u_T} du \frac{D \kappa^2}{\left[\frac{\xi}{\xi} \Sigma_s + \gamma \Sigma_a + \gamma D \kappa^2 \right]},$$

and

$$p = e^{- \int_{u_0}^{u_T} du \frac{\Sigma_a}{\left[\frac{\xi}{\xi} \Sigma_s + \gamma \Sigma_a + \gamma D \kappa^2 \right]}},$$

the equation for k_{eff} is

$$k_{\text{eff}} = \frac{\nu_f \Sigma_{fT}(r)}{\Sigma_{aT}} \frac{p e^{-\tau \kappa^2}}{\left[1 + L_T^2 \kappa_T^2 \right]}.$$

The quantity p is the probability that a neutron born with lethargy u_0 will escape being captured in slowing down to lethargy u_T . This is commonly called the resonance escape probability, since this region of energy includes resonance phenomenon. Similarly, the quantity $e^{-\tau \kappa^2}$ is the probability that a neutron will escape diffusing out of the system in slowing down from u_0 to u_T . The factor τ is usually called the age and is defined as (for κ^2 independent of u in this range)

$$\tau(u) = \int_{u_0}^u du' \frac{D(u')}{\left[\frac{\xi}{\xi} \Sigma_s(u') + \gamma \Sigma_a(u') + \gamma D(u') \kappa^2 \right]},$$

that is, the age (in cm^2) of a neutron in slowing down from u_0 to u .

The factor $\left[1 + L_T^2 \kappa_T^2 \right]^{-1}$ is the probability that a thermal neutron will escape diffusing out of the system before being absorbed; L_T is the diffusion length of thermal neutrons.

The effective criticality constant, k_{eff} , may be put in the more familiar form by introducing the macroscopic absorption cross section of the fertile material (fuel), Σ_a^{fuel} . Defining the number of neutrons produced per neutron absorbed in the fuel as

$$\eta = \nu_f \Sigma_{fT} / \Sigma_a^{\text{fuel}},$$

and the thermal utilization factor by

$$f = \Sigma_a^{\text{fuel}} / \Sigma_{aT} ,$$

the effective criticality factor becomes

$$k_{\text{eff}} = \eta f p \frac{e^{-\tau \kappa^2}}{[1 + L_T^2 \kappa^2]} .$$

In a finite system the steady-state neutron balance is maintained when k_{eff} is unity. For an infinitely large system, where the neutron leakage is zero, the flux bucklings κ^2 , and κ_T^2 , or the spatial flux curvatures, are zero, so that

$$\lim_{\kappa_T^2, \kappa^2 \rightarrow 0} k_{\text{eff}} = \eta f p = k_{\infty} ,$$

where k_{∞} is the criticality factor for an infinitely large system.

For a natural uranium system there is a contribution of neutrons from the threshold fissions in U^{238} . A fast effect factor ϵ is then included in the criticality constant, and the resultant definition of k_{∞} is a four-factor formula.

Returning to the multigroup method of solving the basic reactor equation, a two-group formulation is to collapse the neutrons in the energy region above the thermal group into a single group. Integrating the fast equation over the remaining lethargy interval, $u = -\infty$ ($E = \infty$), $u = u_T$, with $q(\underline{r}, -\infty) = 0$, and if definitions of averages analogous to those used in the thermal group are employed, the fast group equation is then

$$\text{div}_{\underline{r}} D_F(\underline{r}) \text{grad}_{\underline{r}} \phi_F(\underline{r}) - \Sigma_{aF}(\underline{r}) \phi_F(\underline{r}) - q(\underline{r}, u_T) + \frac{\nu}{k_{\text{eff}}} \Sigma_{fT} \phi_T(\underline{r}) = 0 .$$

The above equation with the thermal-group equation:

$$\text{div}_{\underline{r}} D_T(\underline{r}) \text{grad}_{\underline{r}} \phi_T(\underline{r}) - \Sigma_{aT}(\underline{r}) \phi_T(\underline{r}) + q(\underline{r}, u_T) = 0 ,$$

and with

$$q(\underline{r}, u_T) = \left[\bar{\xi} \Sigma_s(\underline{r}, u_T) + \gamma \Sigma_a(\underline{r}, u_T) - \gamma \text{div}_{\underline{r}} D(\underline{r}, u_T) \text{grad}_{\underline{r}} \right] \phi(\underline{r}, u_T)$$

are the basic reactor equations for a two-group theory. The slowing down density $q(\underline{r}, u_T)$ is the source term for thermal neutrons and is a removal

(or sink) term for the fast-group neutrons. The extension to a larger number of energy intervals would involve the same slowing down term where the source of neutrons for a group is the slowing down density from the next higher energy group. Usually this term is replaced by a fictitious removal cross section multiplied by the group flux, e.g., in the two-group theory

$$q(\underline{r}, u_T) = \Sigma_{R_F}(\underline{r}) \phi_F(\underline{r}) \quad .$$

8. Adjoint Equations

Consider the general problem of an operator K operating on a function $\phi(\underline{r}, \underline{u}, \underline{\Omega}, t)$ such that

$$K\phi(\underline{r}, \underline{u}, \underline{\Omega}, t) = v\phi(\underline{r}, \underline{u}, \underline{\Omega}, t) .$$

This is similar to a time-dependent reactor equation; that is, let K be an operator on all dynamical variables except time and let $\phi(\underline{r}, \underline{\Omega}, t)$ be separable in time:

$$\phi(\underline{r}, \underline{u}, \underline{\Omega}, t) = \phi(\underline{r}, \underline{u}, \underline{\Omega}) e^{vt} .$$

Then

$$K\phi(\underline{r}, \underline{u}, \underline{\Omega}, t) = \frac{\partial}{\partial t} \phi(\underline{r}, \underline{u}, \underline{\Omega}, t) = v\phi(\underline{r}, \underline{u}, \underline{\Omega}, t) .$$

Now if this equation is likened to the neutron-balance equation in a finite medium, with boundary conditions, the problem becomes an eigenvalue problem. There are usually an infinite set of functions and corresponding values which satisfy this equation. Subscripting the eigenfunctions and eigenvalues as $\{\phi_1, \phi_2, \dots, \phi_\ell, \dots\}$ and $\{v_1, v_2, \dots, v_\ell, \dots\}$, respectively, the equations having particular solutions may be written as

$$K\phi_\ell = v_\ell \phi_\ell ,$$

$$K\phi_k = v_k \phi_k .$$

Multiplying the top equation by ϕ_k and the lower equation by ϕ_ℓ , integrating each over the region in which these equations hold, and subtracting the two, there is obtained

$$\int d\underline{r} d\underline{v} \phi_\ell K\phi_k - \int d\underline{r} d\underline{v} \phi_k K\phi_\ell = (v_k - v_\ell) \int \phi_\ell \phi_k d\underline{r} d\underline{v} .$$

If the eigenfunctions are orthogonal and normalized such that

$$\begin{aligned} \int d\underline{r} d\underline{v} \phi_\ell \phi_k &= 1, \quad \text{for } k = \ell, \\ &= 0, \quad \text{for } k \neq \ell, \end{aligned}$$

then always

$$\int d\underline{r} d\underline{v} \phi_\ell K\phi_k = \int d\underline{r} d\underline{v} \phi_k K\phi_\ell .$$

The operator K is now said to be self-adjoint. To get this relation, the set of eigenfunctions had to form an orthogonal set. In general, the set of

eigenfunctions $\{\phi_\ell\}$ corresponding to the set of eigenvalues $\{v_\ell\}$ of the operator K are not orthogonal. To find such a set, $\{\phi_\ell^+\}$, corresponding to the same set of eigenvalues $\{v_\ell\}$, an equation called an "adjoint equation,"

$$K^+\phi_k^+ = v_k \phi_k^+ ,$$

is formally introduced, such that, proceeding as before,

$$\int d\underline{r} d\underline{v} \phi_\ell K^+\phi_k^+ - \int d\underline{r} d\underline{v} \phi_k^+ K \phi_\ell = (v_k - v_\ell) \int d\underline{r} d\underline{v} \phi_\ell \phi_k^+ .$$

Now since the set $\{\phi_k^+\}$ is to be orthogonal to $\{\phi_\ell\}$, then the adjoint equation, which has solutions $\{\phi_k^+\}$, must be obtained through the prescription

$$\int d\underline{r} d\underline{v} \phi_\ell K^+\phi_k^+ = \int d\underline{r} d\underline{v} \phi_k^+ K \phi_\ell .$$

This relation is also known as Lagrange's identity.

The adjoint equation for the two-group theory (or multigroup theory) is obtained by writing the set of equations in matrix form

$$Kf = \begin{pmatrix} (\text{div}_{\underline{r}} D_F \text{grad}_{\underline{r}} - \Sigma_{a_F} - \Sigma_{R_F}) & \left(\frac{\nu_f}{k_{\text{eff}}} \Sigma_{f_T} \right) \\ (\Sigma_{R_F}) & (\text{div}_{\underline{r}} D_T \text{grad}_{\underline{r}} - \Sigma_{a_T}) \end{pmatrix} \begin{pmatrix} \phi_F \\ \phi_T \end{pmatrix} = 0 .$$

The above quantities are functions of position only and in using the Lagrange identity to find the set of adjoint equations K^+f^+ , the integration over configuration space is performed only over position:

$$\int d\underline{r} f K^+f^+ = \int d\underline{r} f^+ K f .$$

The matrix f^+ is the row matrix of the adjoint fluxes $\phi_F^+(\underline{r})$ and $\phi_T^+(\underline{r})$. If the operation defined by the right-hand side of the Lagrange identity is carried out, the following integrals result:

$$\begin{aligned} \int d\underline{r} f^+ K f &= \int d\underline{r} \left(\phi_F^+(\underline{r}) \phi_T^+(\underline{r}) \right) K f \\ &= \int d\underline{r} \phi_F^+ \left\{ \text{div}_{\underline{r}} D_F \text{grad}_{\underline{r}} \phi_F(\underline{r}) - \Sigma_{a_F} \phi_F(\underline{r}) - \Sigma_{R_F} \phi_F(\underline{r}) + \frac{\nu_f}{k_{\text{eff}}} \Sigma_{f_T} \phi_T(\underline{r}) \right\} \\ &\quad + \int d\underline{r} \phi_T^+ \left\{ \Sigma_{R_F} \phi_F(\underline{r}) + \text{div}_{\underline{r}} D_T \text{grad}_{\underline{r}} \phi_T(\underline{r}) - \Sigma_{a_T} \phi_T(\underline{r}) \right\} . \end{aligned}$$

The integrals involving the spatial operators may be rewritten as

$$\int d\underline{r} \phi^+ \operatorname{div}_{\underline{r}} D \operatorname{grad}_{\underline{r}} \phi = \int d\underline{r} \phi \operatorname{div}_{\underline{r}} D \operatorname{grad}_{\underline{r}} \phi^+$$

with the aid of the divergence theorem (Gauss's theorem) and the condition that the flux and its adjoint vanish on the surface S of the domain. This relation is obtained by starting with the divergence theorem:

$$\int d\underline{r} \operatorname{div}_{\underline{r}} \underline{W}(\underline{r}) = \int dS \underline{n} \cdot \underline{W} \quad .$$

Letting

$$\underline{W}(\underline{r}) = \phi^+(\underline{r}) D(\underline{r}) \operatorname{grad}_{\underline{r}} \phi(\underline{r}) \quad ,$$

and using the relation for the divergence of the product of a scalar and a vector, the theorem may be written in the form

$$\int d\underline{r} D \operatorname{grad}_{\underline{r}} \phi \cdot \operatorname{grad}_{\underline{r}} \phi^+ + \int d\underline{r} \phi^+ \operatorname{div}_{\underline{r}} D \operatorname{grad}_{\underline{r}} \phi = \int dS D \phi^+ \underline{n} \cdot \operatorname{grad}_{\underline{r}} \phi \quad .$$

A similar equation is obtained with roles of ϕ^+ and ϕ reversed, if ϕ and ϕ^+ are interchanged in the definition of $\underline{W}$. Using the condition that ϕ and ϕ^+ vanish on the surface and noting that the scalar product of the gradients in both equations are identical, then it follows that ϕ and ϕ^+ may be interchanged in the original integral.

In the remaining integrals, the interchange of the flux and its adjoint present no difficulties.

Arranging the resultant terms in the form similar to the original integral, then

$$\begin{aligned} \int d\underline{r} f^+ K f &= \int d\underline{r} \phi_F \left\{ \operatorname{div}_{\underline{r}} D_F \operatorname{grad}_{\underline{r}} \phi_F^+(\underline{r}) - \Sigma_{a_F} \phi_F^+(\underline{r}) - \Sigma_{R_F} \phi_F^+(\underline{r}) + \Sigma_{R_F} \phi_T^+(\underline{r}) \right\} \\ &+ \int d\underline{r} \phi_T \left\{ \frac{\nu_f}{k_{\text{eff}}} \Sigma_{f_T} \phi_F^+ + \operatorname{div}_{\underline{r}} D_T \operatorname{grad}_{\underline{r}} \phi_T^+(\underline{r}) - \Sigma_{a_T} \phi_T^+(\underline{r}) \right\} \\ &= \int d\underline{r} f^+ K^+ f \end{aligned}$$

The two-group adjoint equations become, in matrix form,

$$K^+ f^+ = \begin{pmatrix} (\operatorname{div}_{\underline{r}} D_F \operatorname{grad}_{\underline{r}} - \Sigma_{a_F} - \Sigma_{R_F}) & (\Sigma_{R_F}) \\ \left(\frac{\nu_f}{k_{\text{eff}}} \Sigma_{f_T} \right) & (\operatorname{div}_{\underline{r}} D_T \operatorname{grad}_{\underline{r}} - \Sigma_{a_T}) \end{pmatrix} \begin{pmatrix} \phi_F^+ \\ \phi_T^+ \end{pmatrix} = 0 \quad .$$

Note that the adjoint of a matrix results simply from the interchange of rows and columns. This result makes it quite easy to obtain the set of adjoint equations for an n^{th} -group theory. In a one-group theory, the adjoint equation becomes identical to the original equation, and the operator is then called self-adjoint. The adjoint function and the real function are identical in this case.

For equations in which the energy or lethargy dependence is still present, the procedure in obtaining the adjoint equation is the same except that the integration over the energy or lethargy must be included.

9. Perturbation Theory

The steady-state distribution of neutrons in a system will be disturbed if the physical parameters of the system are changed. The eigenvalue (criticality factor) k_{eff} must be altered, commensurate with the perturbation, in order that the perturbed system remain critical. The change in k_{eff} due to variations in the physical parameters is determined by means of perturbation theory.

The set of reactor equations, which now includes the adjoint equations, is

$$\begin{aligned} Kf &= 0 \quad , \\ K^+ f^+ &= 0 \quad . \end{aligned}$$

The perturbed system in a steady-state condition must satisfy the equation

$$K' f' = 0 \quad ,$$

where f' is the solution of the perturbed operator:

$$K' = K + \delta K \quad ,$$

with K and δK being the unperturbed and perturbation operators, respectively.

Multiplying the perturbed equation by the adjoint function f^+ , the adjoint equation by f' , subtracting the two, and integrating over configuration space (volume $d\underline{r}$ for f , f^+ , f' functions of $\underline{r}$ only), there is obtained

$$\int d\underline{r} f^+ K f' - \int d\underline{r} f' K^+ f^+ + \int d\underline{r} f^+ \delta K f' = 0 \quad .$$

The perturbed solution f' is usually expanded in terms of the set of eigenfunctions generated by the unperturbed equation so that f' is also orthogonal to f^+ . From Lagrange's identity, then,

$$\int d\underline{r} f^+ K f' = \int d\underline{r} f' K^+ f^+ \quad .$$

The equation used to determine the change in the eigenvalue k_{eff} when the physical parameters are varied becomes

$$\int d\underline{r} f^+ \delta K f' = 0 \quad .$$

Writing the perturbed parameters as $D' = D + \delta D$, $\Sigma' = \Sigma + \delta \Sigma$, and $\left(\frac{\nu f}{k_{\text{eff}}} \Sigma f_T\right)' = \frac{\nu f \Sigma f_T}{k_{\text{eff}}} + \delta \left(\frac{\nu f \Sigma f_T}{k_{\text{eff}}}\right)$ in the matrix $K' f'$, the perturbation operator δK operating on f' becomes (for two-group theory)

$$\delta K f' = \begin{pmatrix} (\text{div}_{\underline{r}} \delta D_F \text{grad}_{\underline{r}} - \delta \Sigma a_f - \delta \Sigma_{R_F}) & \left(\delta \frac{\nu f}{k_{\text{eff}}} \Sigma f_T\right) \\ (\delta \Sigma_{R_F}) & (\text{div}_{\underline{r}} \delta D_T \text{grad}_{\underline{r}} - \delta \Sigma a_T) \end{pmatrix} \begin{pmatrix} \phi'_F \\ \phi'_T \end{pmatrix} = 0 \quad ,$$

and the perturbation integral becomes

$$\begin{aligned} \int d\underline{r} f^+ \delta K f' &= \int d\underline{r} (\phi_F^+ \phi_T^+) \delta K f' = \int d\underline{r} \phi_F^+ \left\{ \text{div}_{\underline{r}} \delta D_F \text{grad}_{\underline{r}} \phi'_F - \delta \Sigma a_F \phi'_F - \delta \Sigma_{R_F} \phi'_F + \delta \frac{\nu f}{k_{\text{eff}}} \Sigma f_T \phi'_T \right\} \\ &+ \int d\underline{r} \phi_T^+ \left\{ \delta \Sigma_{R_F} \phi'_F + \text{div}_{\underline{r}} \delta D_T \text{grad}_{\underline{r}} \phi'_T - \delta \Sigma a_T \phi'_T \right\} = 0 \quad . \end{aligned}$$

Expanding the quantity

$$\delta \left(\frac{\nu f \Sigma f_T}{k_{\text{eff}}} \right) = \frac{\delta(\nu f \Sigma f_T)}{k_{\text{eff}}} + \nu f \Sigma f_T \delta \left(\frac{1}{k_{\text{eff}}} \right) = \frac{\delta(\nu f \Sigma f_T)}{k_{\text{eff}}} - \nu f \Sigma f_T \frac{\delta k_{\text{eff}}}{k_{\text{eff}}^2}$$

where k_{eff}' is the eigenvalue of the perturbed system, and with the reactor originally critical, $k_{\text{eff}} = 1$, solving for $\delta k_{\text{eff}}/k_{\text{eff}}'$ (reactivity change)

$$\begin{aligned} \left(-\frac{\delta k_{\text{eff}}}{k_{\text{eff}}'} \right) &= \frac{1}{\int d\underline{r} \nu f \Sigma f_T \phi_F^+ \phi_T^+} \int d\underline{r} \left\{ \delta(\nu f \Sigma f_T) \phi_F^+ \phi_T^+ - \delta \Sigma a_F \phi_F^+ \phi_F^+ - \delta \Sigma_{R_F} \phi_F^+ \phi_F^+ \right. \\ &\quad \left. + \delta \Sigma_{R_F} \phi_T^+ \phi_F^+ - \delta \Sigma a_T \phi_T^+ \phi_T^+ - \delta D_F \text{grad}_{\underline{r}} \phi_F^+ \cdot \text{grad}_{\underline{r}} \phi_F^+ - \delta D_T \text{grad}_{\underline{r}} \phi_T^+ \cdot \text{grad}_{\underline{r}} \phi_T^+ \right\} . \end{aligned}$$

The last two terms are from the divergence theorem, namely,

$$\int d\underline{r} \phi^+ \left\{ \text{div}_{\underline{r}} \delta D \text{grad}_{\underline{r}} \phi' \right\} = \int d\underline{r} \delta D \text{grad}_{\underline{r}} \phi^+ \cdot \text{grad}_{\underline{r}} \phi' \quad .$$

The perturbation integral gives the change in the reactivity, which is proportional to the time rate of change of neutron density resulting from certain changes of the physical parameters. Consider, for example, that only the thermal absorption cross section is changed at position $\underline{r}_0$

in the reactor, and assume that at this position the gradient of the flux is zero; then the reactivity change is given by

$$\frac{\delta k_{\text{eff}}}{k_{\text{eff}}'} = \frac{\delta \Sigma_{aT}(\underline{r}_0) \phi_T^+(\underline{r}_0) \phi_T'(\underline{r}_0)}{\int d\underline{r} (\nu_f \Sigma_{fT}) \phi_F^+(\underline{r}) \phi_T'(\underline{r})}.$$

If the fissionable material is uniformly distributed in a region of the reactor (core), then

$$\frac{\delta k_{\text{eff}}}{k_{\text{eff}}'} = \frac{\delta \Sigma_{aT}(\underline{r}_0)}{(\nu \Sigma_{fT})} \frac{\phi_T^+(\underline{r}_0) \phi_T'(\underline{r}_0)}{\int_{\text{core}} d\underline{r} \phi_F^+(\underline{r}) \phi_T'(\underline{r})} = \frac{\delta \Sigma_{aT}}{(\nu \Sigma_{fT})} w(\underline{r}_0).$$

The quantity $w(\underline{r}_0)$ is defined as the statistical weight at the point $\underline{r}_0$ for this particular perturbation. The physical interpretation of this weighting factor (and similarly for the others) is that in a region of high statistical weight the perturbation causes a greater change in reactor period than in a region of low statistical weight. For a change in the diffusion coefficient, the statistical weight is the scalar product of the gradients of the flux and its adjoint.

The adjoint flux is also interpreted as an "importance" function in that for a given change in the reaction rate, $\delta \Sigma_{aT} \phi_T'$, the time rate of change of the neutron density is weighted by the adjoint flux at the position where the change is made.

If the perturbation is small, the statistical weights of the perturbation integral may be evaluated by replacing the perturbed flux ϕ' by the unperturbed quantity ϕ .