Chapter 1

THE NEUTRON TRANSPORT EQUATION

1.1 Introduction

Two methods exist for simulating and modeling neutron transport and interactions in the reactor core, or "neutronics." Deterministic methods solve the Boltzmann transport equation in a numerically approximated manner everywhere throughout a modeled system. Monte Carlo methods model the nuclear system (almost) exactly and then solve the exact model statistically (approximately) anywhere in the modeled system. Although deterministic methods are fast for one-dimensional models, both methods are slow for realistic three-dimensional problems.

1.1.1 Deterministic methods

Deterministic neutronics methods play a fundamental role in reactor core modeling and simulation. A first-principles treatment requires solution of the linearized Boltzmann transport equation. This task demands enormous computational resources because the problem has seven dimensions: three in space, two in direction, and one each in energy and time.

Nowadays reactor core analyses and design are performed using nodal (coarse-mesh) two-group diffusion methods. These methods are based on pre-computed assembly homogenized cross-sections and assembly discontinuity factors obtained by single assembly calculation with reflective boundary conditions (infinite lattice). These methods are very efficient and accurate when applied to the current low-heterogeneous Light Water Reactor (LWR) cores. With the progress in the Nuclear Engineering field new generations of Nuclear Power Plants (NPPs) are considered that will have more complicated rector core designs, such as cores loaded partially with mixed-oxide (MOX) fuel, high burn-up loadings, and cores with advanced fuel assembly and control rode designs. Such heterogeneous cores will have much more pronounced leakage between the unlike assemblies, which will introduce challenges to the current methods for core calculation. First, the use of pre-computed fuel-assembly homogenized cross-section could lead to significant errors in the coarse-mesh solution. On the other hand, the application of the two-group diffusion theory for such heterogeneous cores could also be source for large errors. New core calculation methodologies based on fine-mesh (pin-by-pin), higher-order neutron transport treatment, multi-group methods are needed to be developed to address the difficulties the diffusion approximation meets by improving accuracy, while preserving efficiency of the current reactor core calculations.

The diffusion theory model of neutron transport has played a crucial role in reactor theory since it is simple enough to allow scientific insight, and it is sufficiently realistic to study many important design problems. The mathematical methods used to analyze such a model are the same as those applied in more sophisticated methods such as multi-group neutron transport theory. The neutron flux (ψ) and current (J) in the diffusion theory model are related in a simple way under certain conditions. This relationship between ψ and J is identical in form to a law used in the study of diffusion phenomena in liquids and gases: Fick's law. The use of this law in reactor theory leads to the diffusion approximation, which is a result of a number of simplifying assumptions. On the other hand, higher-order neutron transport codes have always been deployed in nuclear engineering for mostly time-independent problems out-of-core shielding

calculations. With all the limitations of two-group diffusion theory, it is desirable to implement the more accurate, but also more expensive multi-group transport approach.

Replacing two group diffusion nodal (assembly-based) neutronics solvers with multi-group transport (pin-based) solutions can be performed in direct and embedded manner. While studies have been performed utilizing the two deterministic types of methods (depending on techniques to treat angular flux dependence) - the discrete ordinates (S_N) and spherical harmonics (P_N) approximations – for core analysis, the majority of the efforts have been focused on replacing diffusion approximation with Simplified P_3 (SP_3) approach. The SP_3 method has gained popularity in the last 10 years as an advanced method for neutronics calculation. The SP_3 approximation was chosen because of its improved accuracy as compared to the diffusion theory for heterogeneous core problems and efficiency in terms of computing time as compared to higher order transport approximations. The SP_3 approximation is more accurate when applied to transport problems than the diffusion approximation with considerable less computation expense than the discrete ordinates (S_N) or spherical harmonics (P_N) approximations. Another advantage of SP_3 approximation is that it can be solved by straightforward extension of the common nodal diffusion methods with little overhead. It has been shown also that the multi-group SP_3 pin-by-pin calculations can be used for practical core depletion and transient analyses. Recent results obtained elsewhere indicated the importance of consistent cross-section generation and utilization in the SP_3 equations in terms of modeling the P_1 scattering. Since this is an important issue for practical utilization of SP_3 approximation for reactor core analysis.

1.1.2 Stochastic methods

Numerical methods that are known as Monte Carlo methods can be loosely described as statistical simulation methods, where statistical simulation is defined in quite general terms. It can be any method that utilizes sequences of random numbers to perform the simulation. Statistical simulation methods may be contrasted to conventional numerical discretization methods, which typically are applied to ordinary or partial differential equations that describe some underlying physical or mathematical system. In many applications of Monte Carlo, the physical process is simulated directly, and there is no need to even write down the differential equations that describe the behavior of the system. The only requirement is that the physical (or mathematical) system be described by probability density functions (pdf's). Once the pdf's are known, the Monte Carlo simulation can proceed by random sampling from the pdf's. Many simulations are then performed (multiple "trails" or "histories") and the desired result is taken as an average over the number of observations (which may be a single observation or perhaps millions of observations). In many practical applications, one can predict the statistical error (the "variance") in this average result, and hence an estimate of the number of Monte Carlo trials that are needed to achieve a given error.

When it is difficult (impossible, impractical) to describe a physical phenomenon via deterministic equations (balance equations, distribution functions, differential equations, etc.) Monte Carlo method becomes useful (or necessary). In Nuclear Engineering, in the past the method was mainly used for complex "shielding" problems and for benchmarking of deterministic calculations. Today, however, because of the advent of faster computers and parallel computing, the technique is being used more extensively for "normal" calculations. But, as will be discussed later, one should not (cannot) only rely on Monte Carlo calculations because the technique is very expensive/impractical (time and money) for obtaining detail information about a physical system or for performing sensitivity/perturbation studies. In such

situation, deterministic methods are necessary for aiding Monte Carlo and/or for performing the actual simulation.

Using the Monte Carlo method, a model of the medium under study is set up in the computer and individual particles are thrown at the medium or are generated in it, as if coming from a source. The particles are followed, one by one, and the various events in which they participate (collision, absorption, fission, escape, etc.) are recorded. All the events associated with one particle constitute the history of that particle. The present trend in advanced and next generation nuclear reactor core designs is towards increased material heterogeneity and geometry complexity. The continuous energy Monte Carlo method has the capability of modeling such core environments with high accuracy. Because of its statistical nature, Monte Carlo core calculations usually involve a considerable computer time to attain reliable converged results for both integral parameters and local distributions. Number of coupled Monte Carlo depletion code systems have been developed and successfully used in assembly/core depletion reference calculations. Now the tendency is to couple Monte Carlo neutronic calculation with a thermal-hydraulics code to obtain three-dimensional (3D) power and thermal-hydraulic solutions for a reactor core. The investigations performed at PSU showed that performing Monte Carlo based coupled core steady state calculations are feasible. This conclusion indicates that in the future it will be possible to use Monte Carlo method to produce reference results at operating conditions.

1.1.3 Conclusions

For reactor core modeling and simulation, deterministic methods will be used principally in the short term (3–5 years) with Monte Carlo as a benchmarking tool. In the intermediate term (5–10 years) Monte Carlo methods could be used as a hybrid tool with multi-physics coupling to deterministic neutronics and thermal hydraulics codes. In the long term (>10 years) multi-physics codes using non-orthogonal grids will provide complete, high-accuracy design tools, fully integrated into reactor core design and operation.

1.1.4 Basic terms and definitions

Please review Sections 1-1, 1-2, and 1-3 of Chapter 1 of E. E. Lewis and W. F. Miller, *Computational Methods of Neutron Transport*, American Nuclear Society (1993).

1.2 Neutron Boltzmann Equation

Several choices are possible for describing neutron behavior in a medium filled with nuclei. A neutron is a subatomic particle called a baryon having the characteristic strong nuclear force of the standard model. Thus, a quantum mechanical description seems appropriate, leading to an involved system of Schrödinger equations describing neutron motion between and within nuclei. A neutron is also a relativistic particle with variation of its mass over time when travelling near the speed of light. Finally, a neutron possesses wave and classical particle properties simultaneously and therefore a collective description like that of Maxwell's equations also seems appropriate. In reality, a neutron displays all of the above characteristics at one time or another. When a neutron collides with a nucleus, its strong force interacts with all of the individual nucleons. However, between nuclear collisions, neutrons move ballistically. Neutrons with energies above 20 MeV with speeds of more than 20% the speed of light (c), exhibit relativistic motion, but most in a reactor are rarely above $0.17c$. The neutron wavelength is most important for ultra-low-energy neutrons mainly existing in the laboratory. Fortunately, the

classical neutral particle description with quantum mechanics describing collisions emerges as the most appropriate for the investigation of neutron motion within a nuclear reactor.

We now derive the neutron Boltzmann equation, also called the neutron transport equation, to characterize a relatively small number of neutrons colliding in a vast sea of nuclei. Mathematically, a neutron is a neutral point particle, experiencing deflection from or capture by a nucleus at the center of an atom. If conditions are just right, the captured neutron causes a fissile nucleus to fission producing more neutrons. The statistically large number of neutrons interacting in a reactor allows for a continuum-like description through averaging resulting in the linear Boltzmann equation. Also, a statistical mechanical formulation, first attempted by Boltzmann for interacting gases, provides an appropriate description. Boltzmann's equation, based on physical arguments, such as finite particle size, gives a more physically precise picture of particle-particle interaction than is presented here. In his description, all particles, including nuclei, are in motion with like particle collisions allowed. Because of the low density of neutrons in comparison to nuclei in a reactor however, these collisions are infrequent enabling a simplified physical/mathematical theory.

Several forms of the neutron transport equation exist. The integro-differential formulation, arguably the most popular form in neutron transport and reactor physics applications, is presented in Section 1.2. However, other forms of the transport equation exist and are being used such as integral and adjoint forms.

1.2.1 Integro-differential neutron Boltzmann equation

A primary goal of nuclear reactor design is the reliable prediction of neutron production and loss rates. Predictions come from the solution of the neutron conservation equation - hence, the importance of the neutron Boltzmann equation. Of the several possible physical descriptions, we consider the neutron as a classical interacting particle and formulate neutron conservation in a medium.

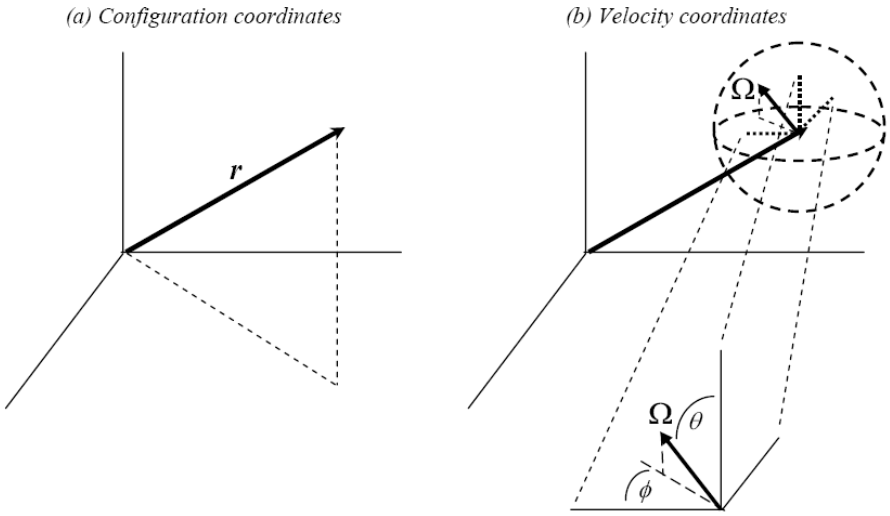
1.2.1.1 Independent variables

Figure 1.1(a) shows a neutron moving at the position denoted by the vector $\boldsymbol{r}$. Figure 1.1(b) shows a second vector Ω in a coordinate system (dotted axes) superimposed on the neutron itself to indicate neutron direction. The Ω-vector specifies a point on the surface of a fictitious sphere of unit radius surrounding the neutron and pointing in its direction of travel. The neutron velocity is therefore, $\boldsymbol{V} \equiv \mathrm{v}\boldsymbol{\Omega}$, where v is the neutron speed giving the classical neutron kinetic energy:

$$E \equiv \frac{1}{2} m \mathrm{v}^2$$

for a neutron of mass m. Along with time, represented by t and measured from a reference time, $\boldsymbol{r}$,Ω,E symbolize the six independent variables of the classical description of neutron motion.

Figure 1.1



1.2.1.2 Dependent variables

For convenience, we combine the position and velocity vectors into a single generalized six-dimensional vector $\boldsymbol{P}\equiv(\boldsymbol{r},\boldsymbol{V})$ defining the neutron phase space. Furthermore, decomposing the velocity vector into speed and direction gives the equivalent representations, $\boldsymbol{P} = (\boldsymbol{r},\Omega,\mathrm{v}) = (\boldsymbol{r},\Omega,E)$. Note that a Jacobian transformation is required between the various phase space transitions. The following derivation uses the latter representation exclusively. The derivation will be a purely heuristic one, i.e. coming from physical intuition rather than from precise mathematical rigor. In this regard, we largely follow the approach of Boltzmann.

The key element of the derivation is to maintain the point particle nature of a neutron while taking advantage of the statistics of large numbers. Thus, point collisions occur in a statistically averaged phase space continuum realized by defining the phase volume element $\Delta\mathbf{P} \equiv \Delta\mathbf{r}\Delta\boldsymbol{\Omega}\Delta E$ about $\boldsymbol{P}$ as shown in Figure 1.2. Note that the unit of solid angle, $\Delta\boldsymbol{\Omega}$**,** is the steradian (*sr*), and that 4π steradians account for all possible directions on a unit sphere.
The volume element of phase space $\Delta\mathbf{P}$ plays a central part in the overall neutron balance. One physically accounts for neutrons entering or leaving through the boundaries of $\Delta\mathbf{r}$ or that are lost or gained within $\Delta\mathbf{r}$. In addition, neutrons enter or leave the phase element through deflection into or out of the direction range $\Delta\boldsymbol{\Omega}$, or by slowing down or speeding up through the energy boundaries of ΔE .

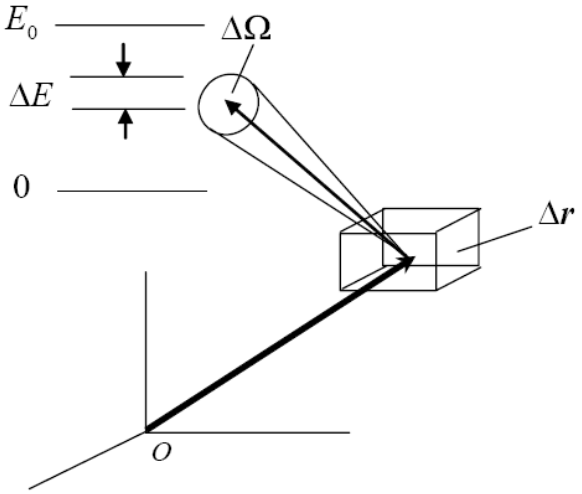
Let $N(\mathbf{r},\boldsymbol{\Omega},E,t)$ be the neutron density distribution:

$$N(\boldsymbol{r},\boldsymbol{\Omega},E,t)\Delta\boldsymbol{P} \equiv \text{Number of neutrons in } \Delta\boldsymbol{P} \text{ at time } t$$

Since $\mathrm{v}\Delta t$ is the distance travelled per neutron of speed v, called the neutron track length, the total track length of all neutrons in $\Delta\mathbf{P}$ is:

$$\mathrm{v}N(\boldsymbol{r},\boldsymbol{\Omega},E,t)\Delta\boldsymbol{P}\Delta t \equiv \text{Total track length in } \Delta\boldsymbol{P} \text{ at time } t \text{ for neutrons of speed v}$$

Figure 1.2. Phase space volume element $\Delta P \equiv \Delta r \Delta\Omega \Delta E$



As shown, the track length serves as the bridge between point-like and continuum particle behavior when characterizing collisions. In the above definition, it is convenient to define the following quantity as the neutron angular flux at time t:

$$\phi(\boldsymbol{r},\boldsymbol{\Omega},E,t) \equiv \mathrm{v}N(\boldsymbol{r},\boldsymbol{\Omega},E,t)$$

representing the total track length per second of all neutrons in $\Delta\mathbf{P}$ per unit of phase space. While the neutron density and flux are associated with a phase space volume element, the neutron angular current vector, $J(\mathbf{r},\boldsymbol{\Omega},E,t)$, is associated with an area. The magnitude of the angular current vector is the rate of neutrons per steradian, energy and area, in the direction $\boldsymbol{\Omega}$ that pass through an area perpendicular to $\boldsymbol{\Omega}$ at time t. Neutrons, passing through the area A oriented with the unit normal $\hat{\mathbf{n}}$, as shown in Figure 1.3, during Δt, enter the volume element $\Delta\mathbf{r} = \hat{\mathbf{n}} \bullet \boldsymbol{\Omega} A \,\mathrm{v}\, \Delta t$. Thus, the total number of neutrons in the phase volume element $\Delta\mathbf{P} = \left[\hat{\mathbf{n}} \bullet \boldsymbol{\Omega} A \,\mathrm{v}\, \Delta t\right]\Delta\boldsymbol{\Omega}\Delta E$ is:

$$N(\boldsymbol{r},\boldsymbol{\Omega},E,t)\left[\hat{\boldsymbol{n}} \bullet \boldsymbol{\Omega} A \mathrm{v} \Delta t\right]\Delta\boldsymbol{\Omega}\Delta E$$

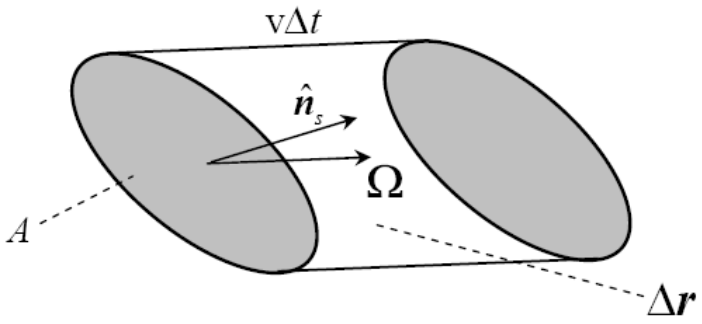
We then conveniently define the angular current vector to be:

$$\boldsymbol{J}(\boldsymbol{r},\boldsymbol{\Omega},E,t) \equiv \mathrm{v}\boldsymbol{\Omega}N(\boldsymbol{r},\boldsymbol{\Omega},E,t)$$

such that $\hat{\mathbf{n}} \bullet J(\mathbf{r},\boldsymbol{\Omega},E,t)\Delta\boldsymbol{\Omega}\Delta E$ is the rate of neutrons per area passing through an area of orientation $\hat{\mathbf{n}}$.

N, ϕ and $\boldsymbol{J}$ are called *dependent* variables since they *depend* on the *independent* variables of phase space and time.

Figure 1.3. Neutrons passing through area A are moving into Δr during Δt



1.2.1.3 Nuclear data

Neutrons primarily experience scattering, capture and fission characterized through probabilities represented by microscopic and macroscopic cross sections. In the following, we assume neutrons interact with inert stationary nuclei. The macroscopic cross section for interaction of type i with the nucleus of nuclide j is:

$$\Sigma_{ij}(\boldsymbol{r},E,t) \equiv \text{Fractional probability of neutron interactions } i \text{ with nuclide } j \text{ per path length travelled}$$

where $i = s_{catter}, c_{apture}, f_{ission}, a_{bsorption} (= c + f)$·$\Sigma_{ij}(\boldsymbol{r},E,t)$ is a product of a microscopic cross section $\sigma_{ij}(E)$ which depends on the nuclide j and reaction type i and the nuclear atomic density, $N_j(\boldsymbol{r},t)$, which can vary spatially. The microscopic cross section nominally represents the area presented to the neutron for an interaction to occur and is a measure of the probability of occurrence. The cross section is fundamental to neutron transport theory and provides the essential element in the continuum characterization of point collisions. Since, as previously shown, the total path length of all neutrons in the element $\Delta\mathbf{P}$ is $\phi(\mathbf{r},\boldsymbol{\Omega},E,t)\Delta\mathbf{P}\Delta t$, the number of interactions of type i per time, or the reaction rate for interaction i in $\Delta\mathbf{P}$ with nuclide j is simply from the definition of cross section:

$$\text{Reaction rate for interaction } i \text{ with nuclide } j \equiv \Sigma_{ij}(\boldsymbol{r},E,t)\phi(\boldsymbol{r},\boldsymbol{\Omega},E,t)\Delta\boldsymbol{P}$$

If we assume individual interactions to be independent events, the total interaction rate of type i is the sum over all J participating nuclear species giving the total macroscopic cross section:

$$\Sigma_i(\boldsymbol{r},E,t) = \sum_{j=1}^{J}\Sigma_{ij}(\boldsymbol{r},E,t) = \sum_{j=1}^{J}N_j(\boldsymbol{r},t)\sigma_{ij}(E)$$

Note that the macroscopic interaction rate is independent of neutron direction and depends only on neutron motion amongst interaction centers (the nuclei). When we next consider neutron deflection or scattering, directional information is essential, however.

The law of deflection, or the differential scattering kernel, is:

$$f_s(\Omega' \bullet \Omega, E' \to E)\Delta\Omega\Delta E \equiv \text{Fractional probability of scattering from direction } \Omega' \text{ and energy } E' \text{ to direction range } \Delta\Omega \text{ and energy range } \Delta E$$

We mostly require, however, the differential scattering cross section for the j^{th} nuclide:

$$\Sigma_{sj}(r, \Omega' \bullet \Omega, E' \to E, t) \equiv \Sigma_{sj}(r, E', t) f_{sj}(\Omega' \bullet \Omega, E' \to E)$$

Scattering, assumed rotationally invariant, depends only on the cosine of the angle between the incoming $\mathbf{\Omega}'$ and scattered $\mathbf{\Omega}$ neutron directions, $\mathbf{\Omega}' \bullet \mathbf{\Omega}$. We normalize the scattering kernel such that neutrons must appear in some direction and energy range:

$$\int_0^\infty dE \int_{4\pi} d\Omega f_s(\Omega' \bullet \Omega, E' \to E) \equiv 1$$

Assuming that the speed of light is an upper limit, the integration is actually over a finite range $[0, E_0]$.

The scattering law f_{sj} is generally independent of time and position. The scattering cross section for an individual nuclide, however, includes the atomic density, which can provide a time variation of the differential scattering cross section.

Neutrons from fission are either prompt or delayed through subsequent nuclear decay and emission. Here, we consider only prompt neutrons. The neutrons, produced isotropically, appear in an energy and direction range according to the distribution $\chi(E)$:

$$\frac{\chi(E)}{4\pi}\Delta\Omega\Delta E \equiv \text{Fractional probability of a fission neutron appearing in the direction range } \Delta\Omega \text{ and energy range } \Delta E$$

with normalization:

$$\int_0^\infty dE \chi(E) \equiv 1$$

In addition, we shall require the average number of neutrons produced per fission, $\nu(E)$.

With the notation now in place, an accounting of the total number of neutrons in the phase space volume element $\Delta\mathbf{P}$ becomes our focus.

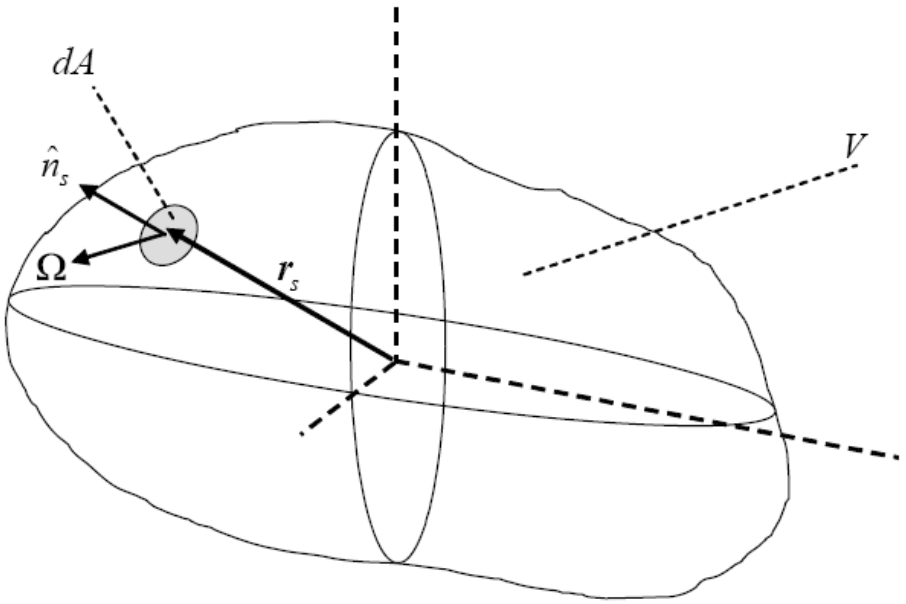
1.2.1.4 Contributions to the total neutron balance

We now account for the net number of neutrons within an arbitrary volume V (shown in Figure 1.4) and in the partial phase space element $\Delta\mathbf{\Omega}\Delta E$ during a time Δt. In words, the neutron balance in the entire volume V and partial element $\Delta\mathbf{\Omega}\Delta E$ is:

Number at time $t+\Delta t$	=	Number at time t	+			
			+	Number gained during Δt	−	Number lost during Δt

All contributions to the neutron balance, which we now consider separately, are in terms of the dependent variables.

Figure 1.4. General transport medium



1.1.4.1.1 Total number of neutrons

The total number of neutrons in $V\Delta\mathbf{\Omega}\Delta E$ at times t and $t+\Delta t$ is:

$$\Delta\Omega\Delta E\int_V drN(\mathbf{r},\Omega,E,t)$$

$$\Delta\Omega\Delta E\int_V drN(\mathbf{r},\Omega,E,t+\Delta t)$$

1.1.4.1.2 Scattering gain

Neutrons from all points within V are scattered into the element $\Delta\mathbf{\Omega}\Delta E$. The total number scattered during Δt from any element $dE'd\mathbf{\Omega}'$ (at time t) is therefore the total scattering rate in V multiplied by Δt:

$$\Delta t\int_V dr\Sigma_s(\mathbf{r},E',t)\phi(\mathbf{r},\Omega',E',t)dE'd\Omega'$$

and of these:

$$f_s(\Omega'\bullet\Omega,E'\to E)\Delta\Omega\Delta E$$

reach $\Delta\mathbf{\Omega}\Delta E$. Thus, the total number scattering into $\Delta\mathbf{\Omega}\Delta E$ during Δt within V is the integration over all possible contributions from all differential phase space elements $dE'd\mathbf{\Omega}'$:

$$\Delta\Omega\Delta E\Delta t\int_V dr\int_0^\infty dE'\int_{4\pi}d\Omega' f_s(\Omega'\bullet\Omega,E'\to E)\Sigma_s(\mathbf{r},E',t)\phi(\mathbf{r},\Omega',E',t)$$

1.1.4.1.3 Fission production

The number of fissions occurring within V during Δt in any differential element $dE'd\mathbf{\Omega}'$ is:

$$\Delta t\int_V dr\Sigma_f(\mathbf{r},E',t)\phi(\mathbf{r},\Omega',E',t)dE'd\Omega'$$

For each fission, $\frac{\chi(E)}{4\pi}\nu(E')\Delta\mathbf{\Omega}\Delta E$ neutrons appear in $\Delta\mathbf{\Omega}\Delta E$ giving a total gain from fission in $V\Delta\mathbf{\Omega}\Delta E$ of:

$$\Delta\Omega\Delta E\Delta t\int_V dr\frac{\chi(E)}{4\pi}\int_0^\infty dE'\int_{4\pi}d\Omega'\nu(E')\Sigma_f(\mathbf{r},E',t)\phi(\mathbf{r},\Omega',E',t)$$

1.1.4.1.4 Losses from absorption and scattering

The number of neutrons lost due to absorption in $V\Delta\mathbf{\Omega}\Delta E$ is:

$$\Delta\boldsymbol{\Omega}\Delta E\Delta t\int_V dr\Sigma_a\left(\boldsymbol{r},E,t\right)\phi\left(\boldsymbol{r},\boldsymbol{\Omega},E,t\right)$$

Here, absorption refers to loss independently of whether a neutron causes a fission or not.

In addition, a neutron is lost when it scatters out of the direction range $\Delta\boldsymbol{\Omega}$ or energy range ΔE . The number lost from scattering out of $V\Delta\boldsymbol{\Omega}\Delta E$ is therefore:

$$\Delta\boldsymbol{\Omega}\Delta E\Delta t\int_V dr\left[\int_0^\infty dE'\int_{4\pi} d\boldsymbol{\Omega}' f_s\left(\boldsymbol{\Omega}'\bullet\boldsymbol{\Omega},E\to E'\right)\right]\Sigma_s\left(\boldsymbol{r},E,t\right)\phi\left(\boldsymbol{r},\boldsymbol{\Omega},E,t\right)$$

or, from the scattering kernel normalization:

$$\Delta\boldsymbol{\Omega}\Delta E\Delta t\int_V dr\Sigma_s\left(\boldsymbol{r},E,t\right)\phi\left(\boldsymbol{r},\boldsymbol{\Omega},E,t\right)$$

1.1.4.1.5 Losses from streaming out of V

Consider the elemental area dA on the surface of V with outward normal $\hat{\mathbf{n}}_s$ (see Figure 1.4). By definition of the current vector, the number of neutrons "leaking out" of dA from the element $\Delta\boldsymbol{\Omega}\Delta E$ during Δt is:

$$\Delta\boldsymbol{\Omega}\Delta E\Delta t\ \hat{\boldsymbol{n}}_s\bullet\boldsymbol{J}\left(\boldsymbol{r},\boldsymbol{\Omega},E,t\right)dA$$

Thus, over the entire surface of V, the total leakage is:

$$\Delta\boldsymbol{\Omega}\Delta E\Delta t\int_A dA\hat{\boldsymbol{n}}_s\bullet\boldsymbol{J}\left(\boldsymbol{r}_s,\boldsymbol{\Omega},E,t\right)=\Delta\boldsymbol{\Omega}\Delta E\Delta t\int_V dr\nabla\bullet\boldsymbol{J}\left(\boldsymbol{r},\boldsymbol{\Omega},E,t\right)$$

where the divergence theorem [2] has transformed the surface integration into a volume integration.

1.2.1.4 Total balance: the neutron Boltzmann equation

Putting all contributions together, dividing by $\Delta t\Delta\boldsymbol{\Omega}\Delta E$ and taking the limit as Δt , $\Delta\boldsymbol{\Omega}$, ΔE approach 0 gives the overall balance in any partial element $d\boldsymbol{\Omega}dE$ over the entire volume at time t:

$$\int_V dr \left\{ \begin{array}{l} \left[\frac{1}{\mathrm{v}} \frac{\partial}{\partial t} + \boldsymbol{\Omega} \bullet \nabla + \Sigma(\boldsymbol{r}, E, t) \right] \phi(\boldsymbol{r}, \boldsymbol{\Omega}, E, t) - \\ - \int_0^\infty dE' \int_{4\pi} d\boldsymbol{\Omega}' \Sigma_s(\boldsymbol{r}, \boldsymbol{\Omega}' \bullet \boldsymbol{\Omega}, E' \to E) \phi(\boldsymbol{r}, \boldsymbol{\Omega}', E', t) - \\ - \frac{\chi(E)}{4\pi} \int_0^\infty dE' \int_{4\pi} d\boldsymbol{\Omega}' \nu(E') \Sigma_f(\boldsymbol{r}, E', t) \phi(\boldsymbol{r}, \boldsymbol{\Omega}', E', t) \end{array} \right\} = 0$$

where the total macroscopic and the differential scattering cross sections are:

$$\Sigma(\boldsymbol{r}, E, t) \equiv \Sigma_a(\boldsymbol{r}, E, t) + \Sigma_s(\boldsymbol{r}, E, t)$$

$$\Sigma_s(\boldsymbol{r}, \boldsymbol{\Omega}' \bullet \boldsymbol{\Omega}, E' \to E, t) \equiv \Sigma_s(\boldsymbol{r}, E', t) f_s(\boldsymbol{\Omega}' \bullet \boldsymbol{\Omega}, E' \to E)$$

Finally, because the volume is arbitrary and assuming a continuous integrand, the above integral is zero only if the integrand is zero yielding the following neutron Boltzmann equation:

$$\begin{aligned} &\left[\frac{1}{\mathrm{v}} \frac{\partial}{\partial t} + \boldsymbol{\Omega} \bullet \nabla + \Sigma(\boldsymbol{r}, E, t) \right] \phi(\boldsymbol{r}, \boldsymbol{\Omega}, E, t) = \\ &= \int_0^\infty dE' \int_{4\pi} d\boldsymbol{\Omega}' \Sigma_s(\boldsymbol{r}, \boldsymbol{\Omega}' \bullet \boldsymbol{\Omega}, E' \to E) \phi(\boldsymbol{r}, \boldsymbol{\Omega}', E', t) + \\ &+ \frac{\chi(E)}{4\pi} \int_0^\infty dE' \int_{4\pi} d\boldsymbol{\Omega}' \nu(E') \Sigma_f(\boldsymbol{r}, E', t) \phi(\boldsymbol{r}, \boldsymbol{\Omega}', E', t) + Q(\boldsymbol{r}, \boldsymbol{\Omega}, E, t) \end{aligned} \qquad \text{Eq.(1-1)}$$

We include an external volume source rate of emission from non-flux related events, $Q(\mathbf{r}, \boldsymbol{\Omega}, E, t)$, for completeness.

Equation (1-1) is a linear integro-differential equation and as such requires boundary and initial conditions. We will fashion these conditions after the particular benchmark considered.

For steady state problems we assume that all nuclear data to be time independent and:

$$\lim_{t \to \infty} \phi(\boldsymbol{r}, \boldsymbol{\Omega}, E, t) = 0$$

Then through integration over all time, the steady state form of Eq. (1-1) becomes:

$$\left[\Omega \bullet \nabla + \Sigma(r,E)\right]\phi(r,\Omega,E) =$$
$$= \int_0^\infty dE' \int_{4\pi} d\Omega' \Sigma_s(r,\Omega' \bullet \Omega, E' \to E)\phi(r,\Omega',E') +$$
$$+ \frac{\chi(E)}{4\pi} \int_0^\infty dE' \int_{4\pi} d\Omega' \nu(E')\Sigma_f(r,E')\phi(r,\Omega',E') + Q(r,\Omega,E) \qquad \text{Eq.(1-2)}$$

where

$$\phi(r,\Omega,E) \equiv \int_0^\infty dt \phi(r,\Omega,E,t)$$

The steady state source distribution $Q(\mathbf{r},\mathbf{\Omega},E)$ now incorporates the initial condition.

The neutron transport equation given by Eq. (1-2) is the source of all the other transport equations in this compendium. Obviously, Eq. (1-2), being an integro-differential equation in six independent variables, does not lend itself to simple analytical or numerical solutions. Therefore, we require further simplification to enable analytical solution representations for eventual numerical evaluation.

Monte Carlo and other sophisticated deterministic methods solve Eq. (1-2) numerically; but these methods contain numerical and sampling errors. It is also possible to solve Eq. (1-2) in the most analytically pure way possible. Most of the solutions come from other forms of Eq. (1-2) that provide the necessary simplicity for further analytical and numerical investigation. We now consider these forms.

1.2.2 Additional forms of the neutron transport equation

It is of interest to reformulate Eq. (1-2) in the various versions used for further analytical and numerical investigation. There are at least eight (and probably more) equivalent forms of Eq. (1-2) not counting Monte Carlo including:

- integral;
- even/odd parity;
- slowing down kernel;
- multiple collision;
- invariant embedding;
- singular integral;
- Green's function;
- pseudo flux.

Each form has a particular mathematical property facilitating a class of solutions. For example, the multiple collision form is appropriate for highly absorbing media. Invariant embedding is useful for half-space problems, whereas the pseudo flux form is appropriate for isotropic

scattering in multi-dimensions. The Green's function representation is best suited for highly heterogeneous 1-D plane media in the multi-group approximation.

In the following sections, we consider the integral transport equation, and derivative forms of neutron transport equation such as monoenergetic and multi-group approximations in 3-D and specifically in 1-D geometries, as they enable analytical and simple numerical solutions and are ubiquitous in the literature.

1.2.2.1 The integral equation

The integral transport equation is essentially integration along the characteristic defining the neutron path. If a neutron travels in direction $\mathbf{\Omega}$, shown in Figure 1.5, between the points specified by vectors $\mathbf{r}'$ and $\mathbf{r}$, the following relationship holds:

$$\boldsymbol{r} = \boldsymbol{r}' + s\mathbf{\Omega}$$

where s is the magnitude of the vector $\mathbf{r} - \mathbf{r}'$. Since the derivative along the neutron path is:

$$\frac{d}{ds} = \frac{\partial \boldsymbol{r}'}{\partial s} \bullet \nabla_{r'}$$

where the gradient is with respect to $\mathbf{r}'$, evaluation of Eq. (1-2) at $\mathbf{r}'$ gives:

$$\left[\frac{d}{ds} - \Sigma\left(\boldsymbol{r}', E\right)\right]\phi\left(\boldsymbol{r}', \mathbf{\Omega}, E\right) = -q\left(\boldsymbol{r}', \mathbf{\Omega}, E\right) \qquad \text{Eq.(1-3)}$$

where the collision source is

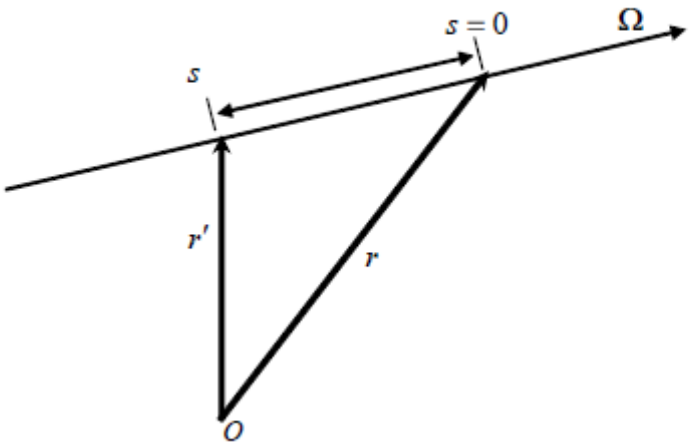
$$q\left(\boldsymbol{r}, \mathbf{\Omega}, E\right) = \int_0^\infty dE' \int_{4\pi} d\mathbf{\Omega}' \Sigma_s\left(\boldsymbol{r}, \mathbf{\Omega}' \bullet \mathbf{\Omega}, E' \to E\right)\phi\left(\boldsymbol{r}, \mathbf{\Omega}', E'\right) + \\ + \frac{\chi(E)}{4\pi} \int_0^\infty dE' \int_{4\pi} d\mathbf{\Omega}' \nu\left(E'\right)\Sigma_f\left(\boldsymbol{r}, E'\right)\phi\left(\boldsymbol{r}, \mathbf{\Omega}', E'\right) + Q\left(\boldsymbol{r}, \mathbf{\Omega}, E\right) \qquad \text{Eq.(1-4)}$$

Further, if we define the optical depth, or mean free path, as:

$$\tau\left(\boldsymbol{r}, \boldsymbol{r}', E\right) \equiv \int_0^{|r-r'|} ds' \Sigma\left(\boldsymbol{r}'\left(s'\right), E\right)$$

and assume we know $q(\mathbf{r}, \mathbf{\Omega}, E)$, the solution to Eq. (1-3), viewed as a first order ordinary differential equations, is:

Figure 1.5. Neutron motion along direction Ω



$$\phi(\mathbf{r},\Omega,E)=\phi(\mathbf{r}',\Omega,E)e^{-\tau(r,r',E)}+\int_0^s ds' e^{-\tau(r,r'(s'),E)}q(\mathbf{r}'(s'),\Omega,E) \qquad \text{Eq.(1-5)}$$

and becomes:

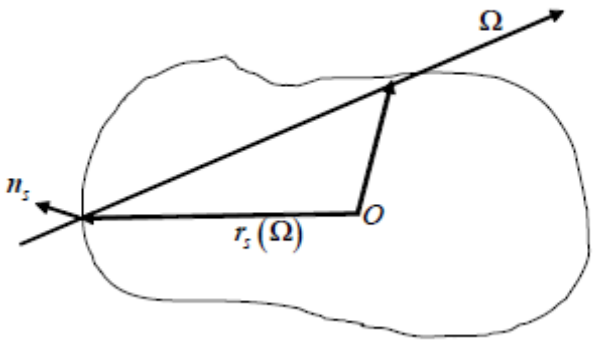
$$\phi(\mathbf{r},\Omega,E)=\phi(\mathbf{r}_s(\Omega),\Omega,E)e^{-\tau(r,r_s(\Omega),E)}\Theta(-\hat{n}_s\bullet\Omega)+ \\ +\int_0^{|r-r_s|} ds' e^{-\tau(r,r-s'\Omega,E)}q(\mathbf{r}-s'\Omega,\Omega,E) \qquad \text{Eq.(1-6)}$$

for $\mathbf{r}'=\mathbf{r}_s$ on the boundary of the medium with outward normal surface $\hat{\mathbf{n}}_s$ shown in Figure 1.6. Note that the distance to the point on the surface from the origin, $\mathbf{r}_s(\mathbf{\Omega})$, depends on the neutron direction. $\mathbf{\Theta}(-\hat{\mathbf{n}}_s\bullet\mathbf{\Omega})$ is the Heaviside step function representing only incoming neutrons where $\phi(\mathbf{r}_s,\mathbf{\Omega},E)$ is known for all incoming directions. We do not consider re-entrant boundaries. Therefore, Eqs. (1-6) and (1-4) constitute a Fredholm integral equation of the second kind for the angular flux. We obtain the scalar, or angularly integrated, flux:

$$\phi(\mathbf{r},E)=\int_{4\pi} d\mathbf{\Omega}\phi(\mathbf{r},\mathbf{\Omega},E) \qquad \text{Eq.(1-7)}$$

through integration of Eq. (1-5):

Figure 1.6. Transport along a neutron direction



$$\phi(\boldsymbol{r},E) = \int_{\hat{n}_s \bullet \Omega < 0} d\Omega \phi\left(r_s(\Omega),\Omega,E\right) e^{-\tau\left(r,r_s(\Omega),E\right)} + \int_{4\pi} d\Omega \int_0^{|r-r_s|} ds' e^{-\tau(r,r',E)} q\left(\boldsymbol{r}'(s'),\Omega,E\right) \quad \text{Eq.(1-8)}$$

By substitution of the differential volume element, $d\mathbf{r}' = s'^2\, d\boldsymbol{\Omega} ds'$, Eq. (1-8) becomes:

$$\phi(\boldsymbol{r},E) = \int_{\hat{n}_s \bullet \Omega < 0} d\Omega \phi\left(r_s(\Omega),\Omega,E\right) e^{-\tau\left(r,r_s(\Omega),E\right)} + \int_V d\boldsymbol{r}' \frac{e^{-\tau(r,r',E)}}{|\boldsymbol{r}-\boldsymbol{r}'|^2} q\left(\boldsymbol{r}', \frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|}, E\right) \quad \text{Eq.(1-9)}$$

Note that Eq. (1-9) is not an integral equation for the scalar flux since the scalar flux does not generally appear under the integral. However, we can find an integral equation for the scalar flux under certain circumstances. If scattering is isotropic and the source is isotropically emitting, then:

$$f_s\left(\Omega' \bullet \Omega, E' \to E\right) = \frac{1}{4\pi} f_s\left(E' \to E\right)$$

$$Q(\boldsymbol{r},\Omega,E) = \frac{1}{4\pi} Q(\boldsymbol{r},E)$$

and Eq. (1-9) reduces to:

$$\phi(\boldsymbol{r},E)=\int\limits_{\hat{n}_s\bullet\boldsymbol{\Omega}<0} d\boldsymbol{\Omega}\phi\left(\boldsymbol{r}_s(\boldsymbol{\Omega}),\boldsymbol{\Omega},E\right)e^{-\tau\left(r,r_s(\Omega),E\right)}+$$
$$+\int\limits_V d\boldsymbol{r}'\frac{e^{-\tau(r,r',E)}}{4\pi\left|\boldsymbol{r}-\boldsymbol{r}'\right|^2}\left[\int\limits_0^\infty dE'\Sigma\left(\boldsymbol{r}',E'\rightarrow E\right)\phi\left(\boldsymbol{r}',E'\right)+Q\left(\boldsymbol{r}',E\right)\right] \qquad \text{Eq.(1-10)}$$

with

$$\Sigma\left(\boldsymbol{r},E'\rightarrow E\right)\equiv\Sigma\left(\boldsymbol{r},E'\right)f_s\left(E'\rightarrow E\right)+\nu\left(E'\right)\Sigma_f\left(\boldsymbol{r},E'\right)\chi\left(E\right)$$

and

$$Q\left(\boldsymbol{r},E\right)=\int\limits_{4\pi} d\boldsymbol{\Omega}Q\left(\boldsymbol{r},\boldsymbol{\Omega},E\right)$$

Equation (4) then gives the angular flux for the collision source:

$$q\left(\boldsymbol{r},\boldsymbol{\Omega},E\right)=\frac{1}{4\pi}\left\{\int\limits_0^\infty dE'\Sigma\left(\boldsymbol{r}',E'\rightarrow E\right)\phi\left(\boldsymbol{r},E'\right)+Q\left(\boldsymbol{r},E\right)\right\} \qquad \text{Eq.(1-11)}$$

If there is no flux passing through the boundary from the vacuum into the medium, $\phi(\mathbf{r}_s,\boldsymbol{\Omega},E)\equiv 0$, for $\hat{\mathbf{n}}_s\bullet\boldsymbol{\Omega}<0$ and if the nuclear properties are uniform, Eq. (1-10) further simplifies to:

$$\phi\left(\boldsymbol{r},E\right)=\int\limits_V d\boldsymbol{r}'\frac{e^{-\Sigma(E)\left|r-r'\right|}}{4\pi\left|\boldsymbol{r}-\boldsymbol{r}'\right|^2}\left[\int\limits_0^\infty dE'\Sigma\left(E'\rightarrow E\right)\phi\left(\boldsymbol{r}',E'\right)+Q\left(\boldsymbol{r}',E\right)\right] \qquad \text{Eq.(1-12)}$$

This equation represents the fundamental neutron transport equation for a 3-D medium with energy dependence and is especially appealing in the multiple collision approximation when absorption dominates. One can also numerically solve Eq. (1-12) through collision probability methods to find fluxes for cross section homogenization.

1.2.3 Derivative forms of the neutron transport equation

Mathematical tractability is the key to generating analytical benchmarks. In its six-dimensional space, the steady state transport equation is anything but mathematically tractable. To make it so, we must reduce the number of independent variables leading to the two approximations in the energy variable to follow. The monoenergetic, or one-group, approximation is a special case of the multi-group approximation but is so ubiquitous in the literature and particularly physically instructive, we consider it separately.

1.2.3.1 Monoenergetic approximation

Because of its simplicity, the monoenergetic approximation, also called one-group approximation, is the most widely considered neutron transport model both analytically and numerically. The model serves as a relatively simple test case to observe the efficiency of new mathematical and numerical methods. The one-group approximation retains the fundamental features of the neutron transport process yet lends itself to theoretical consideration.
As with all approximations, we begin with Eq. (1-2) rewritten here:

$$\begin{aligned}&\left[\Omega\bullet\nabla+\Sigma\left(r,E\right)\right]\phi\left(r,\Omega,E\right)=\\&=\int_0^\infty dE'\int_{4\pi}d\Omega'\Sigma_s\left(r,\Omega'\bullet\Omega,E'\to E\right)\phi\left(r,\Omega',E'\right)+\\&+\frac{\chi\left(E\right)}{4\pi}\int_0^\infty dE'\int_{4\pi}d\Omega'\,\nu\left(E'\right)\Sigma_f\left(r,E'\right)\phi\left(r,\Omega',E'\right)+Q\left(r,\Omega,E\right)\end{aligned}\qquad\text{Eq.(1-2)}$$

A physically based derivation gives the one-group form directly, while the multigroup form of the next section straightforwardly produces the same result as a degenerate multigroup approximation.

To obtain the one-group form, we assume neutrons scatter elastically from a nucleus of infinite mass, and therefore do not lose energy. The details of elastic scattering are found in nearly every reactor physics text; however, the derivation provided here is more mathematically and physically intuitive than most.

An elastic collision between a neutron and nucleus of masses m and M respectively is one that leaves the internal (binding) energy of the nucleus unchanged. The collision occurs instantaneously between two mathematical point particles as shown in Figure 1.7(a) in the physical laboratory (**L**) reference frame. In what follows, a primed quantity refers to before collision and unprimed after collision. The vectors $\boldsymbol{r'}(t)$ and $\boldsymbol{R'}(t)$ define the neutron and nucleus positions at time t and the vector $\boldsymbol{R}_{cm}(t)$:

$$\boldsymbol{R}_{cm}\left(t\right)\equiv\frac{1}{m+M}\left[m\boldsymbol{r}'\left(t\right)+M\boldsymbol{R}'\left(t\right)\right]=\frac{1}{1+A}\left[\boldsymbol{r}'\left(t\right)+A\boldsymbol{R}'\left(t\right)\right]\qquad\text{Eq.(1-13)}$$

defines the position of the center of mass in **L** where A is the mass ratio M/m. To the colliding particles of constant velocity, the center of mass remains stationary before and after collision. For a nucleus initially at rest ($\mathbf{V'\equiv 0}$) and a neutron moving with velocity $\mathbf{v'}$ toward the nucleus, the velocity of the center of mass in the laboratory reference frame is the time derivative of $\boldsymbol{R}_{cm}(t)$:

$$\boldsymbol{V}_{cm}=\frac{1}{1+A}\boldsymbol{v}'\qquad\text{Eq.(1-14)}$$

The most convenient view of elastic scattering is from the center of mass reference frame (**C**) created by imposing a velocity of $-\mathbf{V}_{cm}$ on the laboratory reference frame shown in Figure 1.7(b). The particle velocities in **C** before collision are therefore:

$$\boldsymbol{v}_c' = \boldsymbol{v}' - \boldsymbol{V}_{cm} = \frac{A}{1+A}\boldsymbol{v}',\ \boldsymbol{V}_c' = -\boldsymbol{V}_{cm} \qquad \text{Eq.(1-15)}$$

respectively, and the total linear momentum in **C** is zero, since:

$$\boldsymbol{M}_c' = \boldsymbol{v}' - \boldsymbol{V}_{cm} - A\boldsymbol{V}_{cm} = 0$$

Figure 1.7(c) shows the particle velocity vectors **v**, and **V** in **L** after collision. Again, if we impose -$\boldsymbol{V}_{cm}$, also shown, the corresponding velocities in **C** after collision result. Since the total momentum after collision in **C** is also zero from conservation:

$$\boldsymbol{M}_c = \boldsymbol{v}_c + A\boldsymbol{V}_c = 0$$

the velocity of the nucleus in **C** after collision therefore is:

$$\boldsymbol{V}_c = -\frac{1}{A}\boldsymbol{v}_c \qquad \text{Eq.(1-16)}$$

which is in the exact opposite direction of the neutron. Conservation of kinetic energy in **C** requires:

$$\frac{1}{2}v_c'^2 + \frac{A}{2}V_c'^2 = \frac{1}{2}v_c^2 + \frac{A}{2}V_c^2$$

and since $\boldsymbol{M}_c' = \boldsymbol{v}_c' + A\boldsymbol{V}_c' = \boldsymbol{0}$, $\boldsymbol{V}_c' = -\boldsymbol{v}_c'/A$, we have:

$$v_c = v_c',\ V_c = V_c' \qquad \text{Eq.(1-17)}$$

Thus, the particles' speed before and after collision remains unchanged in **C**.

The scattering angles made by the velocity vectors with respect to the incident neutron direction in **L** and **C**, $\boldsymbol{\theta_0}$ and $\boldsymbol{\theta_c}$, and their corresponding cosines, $\boldsymbol{\mu_0}$, $\boldsymbol{\mu_c}$ are also shown in Figure 1.7(c). For future reference, in terms of the neutron direction before **Ω'** and after collision **Ω**, we define:

$$\mu_0 \equiv \Omega' \bullet \Omega \qquad \text{Eq.(1-18)}$$

Because of the rotational invariance experienced by scattering of perfectly spherical point particles, the collision dynamics will depend only on $\boldsymbol{\mu_0}$.

To obtain a fundamental relationship between the energy before and after collision and the scattering angle in **C**, we form the following expression:

$$v^2 \equiv \boldsymbol{v} \bullet \boldsymbol{v} = \left(\boldsymbol{v}_c + \boldsymbol{V}_{cm}\right) \bullet \left(\boldsymbol{v}_c + \boldsymbol{V}_{cm}\right) = v_c^2 + 2V_{cm}v_c\mu_c + V_{cm}^2$$

to give using Eq. (1-14)

Figure 1.7(a). Laboratory (L) reference frame before collision

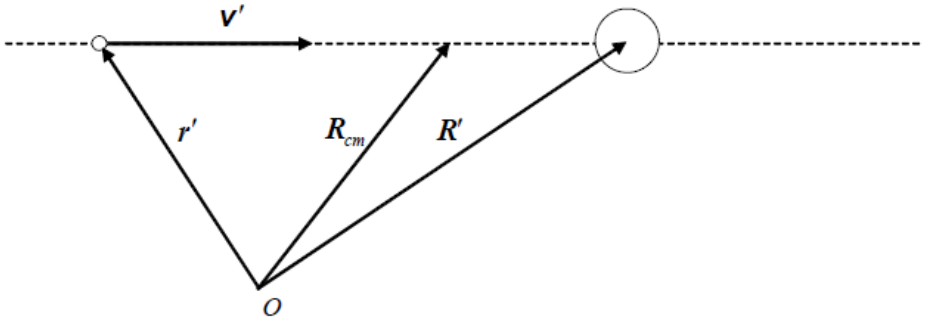


Figure 1.7(b). Center of mass (C) reference frame before collision

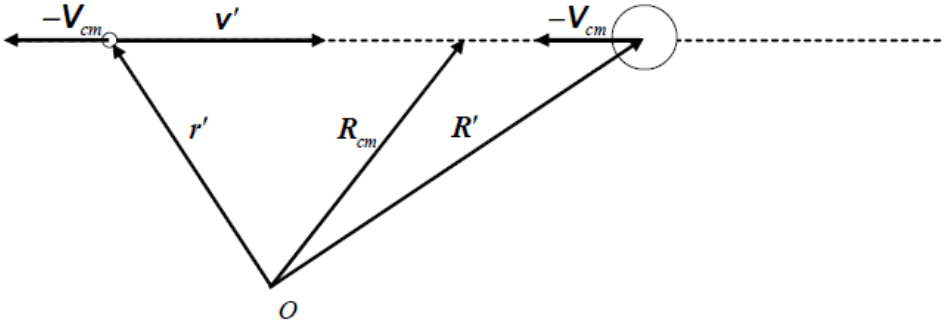
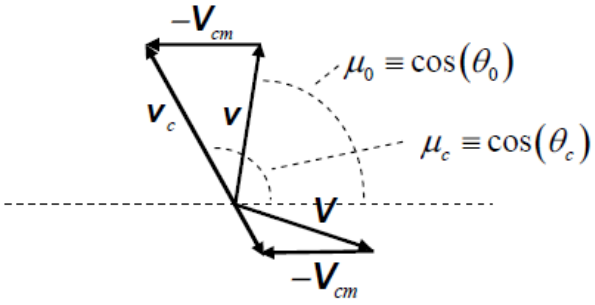


Figure 1.7(c). L and C after collision



$$E = \frac{1}{2}\left[\left(1+\alpha\right)+\left(1-\alpha\right)\mu_c\right]E' \qquad \text{Eq.(1-19)}$$

where the collision parameter is:

$$\alpha \equiv \left[\frac{A-1}{A+1}\right]^2 \qquad \text{Eq.(1-20)}$$

Since from Figure 1.7(c), we deduce that:

$$V_{cm} = -v_c \mu_c + v \mu_0$$

and using Eqs. (1-14) and (1-17), we can relate the scattering angle in the laboratory and center of mass frames:

$$\mu_0 = \frac{A\mu_c + 1}{\left(A^2 + 2A\mu_c + 1\right)^{1/2}} \qquad \text{Eq.(1-21)}$$

or rearranging:

$$\mu_c(\mu_0) = \frac{1}{A}\left[\sqrt{\left(A^2+1\right)\mu_0^2 + \left(1-\mu_0^2\right)^2 - 1} - \left(1-\mu_0^2\right)\right] \qquad \text{Eq.(1-22)}$$

Now recall the differential scattering kernel [defined just prior to Eq. (1-1)]:

$$\Sigma_s\left(r, \boldsymbol{\Omega}' \bullet \boldsymbol{\Omega}, E' \to E\right) = \Sigma_s\left(r, E'\right) f_s\left(\boldsymbol{\Omega}' \bullet \boldsymbol{\Omega}, E' \to E\right) \qquad \text{Eq.(1-23)}$$

with normalization:

$$\int_0^\infty dE \int_{4\pi} d\boldsymbol{\Omega} f_s\left(\boldsymbol{\Omega}' \bullet \boldsymbol{\Omega}, E' \to E\right) \equiv 1 \qquad \text{Eq.(1-24)}$$

Based on energy and momentum conservation, we express the law for scattering through an angle $\boldsymbol{\theta_0}$ in the laboratory frame, and correspondingly through angle $\boldsymbol{\theta_c}$ in the center of mass frame as:

$$f_s\left(\boldsymbol{\Omega}' \bullet \boldsymbol{\Omega}, E' \to E\right) \equiv p_s\left(\mu_0, E'\right) \delta\left(E - \frac{1}{2}\left[\left(1+\alpha\right) + \left(1-\alpha\right)\mu_c\right] E'\right) \qquad \text{Eq.(1-25)}$$

where the delta function enforces the correct kinematics for a given scattering angle. The first factor maintains the normalization with:

$$\int_{4\pi} d\mathbf{\Omega} p_s\left(\mu_0, E'\right) \equiv 1 \qquad \text{Eq.(1-26)}$$

From conservation of probability between the two reference frames:

$$p_s\left(\mu_0, E'\right) = p_s^c\left(\mu_c, E'\right)\left|\frac{d\mu_c}{d\mu_0}\right| \qquad \text{Eq.(1-27)}$$

the scattering kernel then becomes:

$$\begin{aligned}&\Sigma_s\left(r, \mathbf{\Omega}' \bullet \mathbf{\Omega}, E' \to E\right) = \\ &= \Sigma_s\left(r, E'\right) p_s^c\left(\mu_c, E'\right)\left|\frac{d\mu_c}{d\mu_0}\right| \delta\left(E - \frac{1}{2}\left[\left(1+\alpha\right) + \left(1-\alpha\right)\mu_c\right]E'\right)\end{aligned} \qquad \text{Eq.(1-28)}$$

where, from Eq. (22):

$$\frac{d\mu_c}{d\mu_0} = \frac{\mu_0}{A}\left[\frac{A^2 + 1 - 2\left(1-\mu_0^2\right)}{\sqrt{\left(A^2+1\right)\mu_0^2 + \left(1-\mu_0^2\right)^2 - 1}} + 2\right]$$

Note that we introduce angular dependence in the laboratory representation through the transformation between **C** and **L** coordinates.

Finally, when $\boldsymbol{A \to \infty}$, $\boldsymbol{\alpha \to 1}$ Eq. (28) gives:

$$\Sigma_s\left(r, \mathbf{\Omega}' \bullet \mathbf{\Omega}, E' \to E\right) \to \Sigma_s\left(r, \mathbf{\Omega}' \bullet \mathbf{\Omega}, E\right)\delta\left(E - E'\right) \qquad \text{Eq.(1-29)}$$

whith

$$\Sigma_s\left(r, \mathbf{\Omega}' \bullet \mathbf{\Omega}, E\right) \equiv \Sigma_s\left(r, E\right) p_s^c\left(\mu_c\left(\mu_0\right), E\right) \qquad \text{Eq.(1-30)}$$

Equation (1-29) confirms the intuitive notion that a neutron scatters elastically without energy loss on collision with an infinite mass.

If, in addition, neutrons from fission and the external source appear only at energy $\boldsymbol{E_0}$, then:

$$\begin{aligned}Q\left(r, \mathbf{\Omega}, E\right) &\equiv Q\left(r, \mathbf{\Omega}\right)\delta\left(E - E_0\right) \\ \chi\left(E\right) &\equiv \delta\left(E - E_0\right)\end{aligned} \qquad \text{Eq.(1-31)}$$

When we introduce Eqs. (1-29) and (1-31) into Eq. (1-2) after integrating over the delta function in the collision term, there results:

$$\begin{aligned}&\left[\Omega\bullet\nabla+\Sigma\left(r,E\right)\right]\phi\left(r,\Omega,E\right)=\\&=\int_{4\pi}d\Omega'\Sigma_s\left(r,\Omega'\bullet\Omega,E'\right)\phi\left(r,\Omega',E\right)+\\&+\left[\frac{1}{4\pi}\int_0^\infty dE'\int_{4\pi}d\Omega'\nu\left(E'\right)\Sigma_f\left(r,E'\right)\phi\left(r,\Omega',E'\right)+Q\left(r,\Omega\right)\right]\delta\left(E-E_0\right)\end{aligned}\qquad \text{Eq.(1-32)}$$

Since all scattered and fission source neutrons appear at a single energy E_0, physical consistency requires neutrons to be at that energy or expressed formally:

$$\phi\left(r,\Omega,E\right)=\phi\left(r,\Omega\right)\delta\left(E-E_0\right)\qquad \text{Eq.(1-33)}$$

where mathematical consistency requires:

$$\phi\left(r,\Omega\right)\equiv\int_0^\infty dE\phi\left(r,\Omega,E\right)$$

When we introduced Eq. (1-33) into Eq. (1-32), the one-group approximation emerges:

$$\begin{aligned}&\left[\Omega\bullet\nabla+\Sigma\left(r,E_0\right)\right]\phi\left(r,\Omega\right)=\\&=\int_{4\pi}d\Omega'\Sigma_s\left(r,\Omega'\bullet\Omega,E_0\right)\phi\left(r,\Omega'\right)+\\&+\frac{1}{4\pi}\nu\left(E_0\right)\Sigma_f\left(r,E_0\right)\int_{4\pi}d\Omega'\phi\left(r,\Omega'\right)+Q\left(r,\Omega\right)\end{aligned}\qquad \text{Eq.(1-34)}$$

Energy is now just a passive parameter, which we can ignore.

In three dimensions, Eq. (1-34) is still mathematically intractable so we need to make additional simplifications to realize analytical solutions.

1.2.3.2 Multigroup approximation

We initiate the multigroup approximation to Eq. (1-2) by partitioning the total energy interval of interest into *G* energy groups:

$$\Delta E_g=\left[E_g,E_{g-1}\right],\ \ g=1,2,\ldots,G$$

where $g = 1$ is the highest group. By expressing the energy integrals of the scattering and fission sources as sums over all groups, without loss of generality, the integrals in Eq. (1-2) become:

$$\int_0^\infty dE' \int_{4\pi} d\Omega' \Sigma_s(r, \Omega' \bullet \Omega, E' \to E) \phi(r, \Omega', E') =$$

$$= \sum_{g'=1}^{G} \int_{\Delta E_{g'}} dE' \int_{4\pi} d\Omega' \Sigma_s(r, E') f_s(\Omega' \bullet \Omega, E' \to E) \phi(r, \Omega', E')$$

and:

$$\int_0^\infty dE' \nu(E') \Sigma_f(r, E') \phi(r, E') = \sum_{g'=1}^{G} \int_{\Delta E_{g'}} dE' \nu(E') \Sigma_f(r, E') \phi(r, E')$$

By integrating Eq. (2) over ΔE_g, we therefore have:

$$\left[\Omega \bullet \nabla \int_{\Delta E_g} dE \phi(r, \Omega, E) + \int_{\Delta E_g} dE \Sigma(r, E) \phi(r, \Omega, E) \right] =$$

$$= \sum_{g'=1}^{G} \int_{\Delta E_g} dE \int_{\Delta E_{g'}} dE' \int_{4\pi} d\Omega' \Sigma_s(r, \Omega' \bullet \Omega, E' \to E) \phi(r, \Omega', E') +$$

$$+ \frac{1}{4\pi} \int_{\Delta E_g} dE \chi(E) \sum_{g'=1}^{G} \int_{\Delta E_{g'}} dE' \nu(E') \Sigma_f(r, E') \phi(r, E') + \int_{\Delta E_g} dE Q(r, \Omega, E) \qquad \text{Eq.(1-35)}$$

At this point, we introduce the multigroup approximation:

$$\phi(r, \Omega, E) = f(E) \phi_g(r, \Omega)$$
$$Q(r, \Omega, E) = g(E) Q_g(r, \Omega) \qquad \text{Eq.(1-36)}$$

stating the flux and source within each group, $E \in E_g$ are separable functions of energy and r, Ω. The following normalizations:

$$\int_{\Delta E_g} dE f(E) \equiv 1, \quad \int_{\Delta E_g} dE g(E) \equiv 1 \qquad \text{Eq.(1-37)}$$

are also required with $f(E)$ and $g(E)$ assumed to be piecewise smooth functions of E. Then, with the multigroup approximation, Eq. (1-35) becomes:

$$\left[\Omega \bullet \nabla \phi_g(r, \Omega) + \Sigma_g(r) \phi_g(r, \Omega) \right] =$$

$$= \sum_{g'=1}^{G} \int_{4\pi} d\Omega' \Sigma_{sgg'}(r, \Omega' \bullet \Omega) \phi_{g'}(r, \Omega') +$$

$$+ \frac{1}{4\pi} \chi_g \sum_{g'=1}^{G} \nu_{g'} \Sigma_{fg'}(r) \phi_{g'}(r) + Q_g(r, \Omega) \qquad \text{Eq.(1-38)}$$

with the following definitions of the group parameters:

$$\Sigma_g(\boldsymbol{r}) \equiv \int_{\Delta E_g} dE f(E)\Sigma(\boldsymbol{r},E)$$

$$\Sigma_{sgg'}(\boldsymbol{r},\boldsymbol{\Omega}'\bullet\boldsymbol{\Omega}) \equiv \int_{\Delta E_g} dE \int_{\Delta E_{g'}} dE'\Sigma_s(\boldsymbol{r},\boldsymbol{\Omega}'\bullet\boldsymbol{\Omega},E'\to E) f(E') \qquad \text{Eq.(1-39)}$$

$$\nu_g\Sigma_{fg}(\boldsymbol{r}) \equiv \int_{\Delta E_g} dE f(E)\nu(E)\Sigma_f(\boldsymbol{r},E)$$

$$\chi_g \equiv \int_{\Delta E_g} dE\chi(E)$$

In more convenient vector notation, Eq. (1-38) is:

$$\begin{aligned}\left[\boldsymbol{\Omega}\bullet\nabla+\Sigma(\boldsymbol{r})\right]\boldsymbol{\phi}(\boldsymbol{r},\boldsymbol{\Omega}) &= \\ = \int_{4\pi} d\boldsymbol{\Omega}'\Sigma_s(\boldsymbol{r},\boldsymbol{\Omega}'\bullet\boldsymbol{\Omega})\boldsymbol{\phi}(\boldsymbol{r},\boldsymbol{\Omega}') &+ \\ + \frac{1}{4\pi}\chi\left[\nu\Sigma_f(\boldsymbol{r})\right]^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{r}) &+ \boldsymbol{Q}(\boldsymbol{r},\boldsymbol{\Omega})\end{aligned} \qquad \text{Eq.(1-40)}$$

with the group flux and source vectors:

$$\boldsymbol{\phi}(\boldsymbol{r},\boldsymbol{\Omega}) = \left\{\phi_g(\boldsymbol{r},\boldsymbol{\Omega}),\ g=1,\ldots,G\right\}$$
$$\boldsymbol{Q}(\boldsymbol{r},\boldsymbol{\Omega}) = \left\{Q_g(\boldsymbol{r},\boldsymbol{\Omega}),\ g=1,\ldots,G\right\}$$

and the group "constants":

$$\begin{aligned}&\Sigma(\boldsymbol{r}) \equiv diag\left\{\Sigma_g(\boldsymbol{r}),\ g=1,\ldots,G\right\} \\ &\nu\Sigma_f(\boldsymbol{r}) \equiv \left\{\nu_g\Sigma_{fg}(\boldsymbol{r}),\ g=1,\ldots,G\right\} \\ &\Sigma_s(\boldsymbol{r},\boldsymbol{\Omega}'\bullet\boldsymbol{\Omega}) \equiv \left\{\Sigma_{sgg'}(\boldsymbol{r},\boldsymbol{\Omega}'\bullet\boldsymbol{\Omega}),\ g,g'=1,\ldots,G\right\} \\ &\chi \equiv \left\{\chi_g,\ g=1,\ldots,G\right\}\end{aligned} \qquad \text{Eq.(1-41)}$$

The multigroup approximation is the basis of nearly all reactor physics codes, making it one of most widely used approximations of neutron transport and diffusion theory. For inner/outer iterative numerical algorithms, one can reformulate the multigroup approximation as a series of one-group equations.

1.2.3.3One-dimensional plane symmetry

We obtain the 1-D transport equation for plane symmetry when the medium is transversely infinite (in the *yz* plane) with cross section and source variation only in the *x* direction. For this case, Eq. (1-2) becomes:

$$\begin{aligned}&\left[\boldsymbol{\Omega}\bullet\nabla+\Sigma\left(x,E\right)\right]\phi\left(\boldsymbol{r},\boldsymbol{\Omega},E\right)=\\&=\int_0^\infty dE'\int_{4\pi}d\boldsymbol{\Omega}'\Sigma_s\left(x,\boldsymbol{\Omega}'\bullet\boldsymbol{\Omega},E'\rightarrow E\right)\phi\left(\boldsymbol{r},\boldsymbol{\Omega}',E'\right)+\\&+\frac{\chi\left(E\right)}{4\pi}\int_0^\infty dE'\nu\left(E'\right)\Sigma_f\left(x,E'\right)\phi\left(\boldsymbol{r},E'\right)+Q\left(x,\boldsymbol{\Omega},E\right)\end{aligned}\qquad \text{Eq.(1-42)}$$

When we integrate Eq. (1-42) over the transverse ***yz*** plane, there results:

$$\begin{aligned}&\left[\mu\frac{\partial}{\partial x}+\Sigma\left(x,E\right)\right]\phi\left(x,\boldsymbol{\Omega},E\right)=\\&=\int_0^\infty dE'\int_{4\pi}d\boldsymbol{\Omega}'\Sigma_s\left(x,\boldsymbol{\Omega}'\bullet\boldsymbol{\Omega},E'\rightarrow E\right)\phi\left(x,\boldsymbol{\Omega}',E'\right)+\\&+\frac{\chi\left(E\right)}{4\pi}\int_0^\infty dE'\nu\left(E'\right)\Sigma_f\left(x,E'\right)\phi\left(x,E'\right)+Q\left(x,\boldsymbol{\Omega},E\right)\end{aligned}\qquad \text{Eq.(1-43)}$$

Now:

$$\phi\left(x,\boldsymbol{\Omega},E\right)\equiv\int_{-\infty}^{\infty}dz\int_{-\infty}^{\infty}dy\phi\left(x,y,z,\boldsymbol{\Omega},E\right)$$

$$Q\left(x,\boldsymbol{\Omega},E\right)\equiv\int_{-\infty}^{\infty}dz\int_{-\infty}^{\infty}dyQ\left(x,y,z,\boldsymbol{\Omega},E\right)$$

and the ***x***-direction (cosine) $\boldsymbol{\mu}$ is:

$$\mu\equiv\boldsymbol{\Omega}\bullet\hat{\boldsymbol{x}}$$

Since the differential scattering cross section is rotationally invariant with respect to the angle of scattering:

$$\Sigma_s\left(x,\boldsymbol{\Omega}'\left(\mu',\vartheta'\right)\bullet\boldsymbol{\Omega}\left(\mu,\vartheta\right),E'\rightarrow E\right)=\Sigma_s\left(x,\mu',\mu,\vartheta-\vartheta',E'\rightarrow E\right)\qquad \text{Eq.(1-44)}$$

where we explicitly show the dependence on the polar and azimuthal angles of the particle directions (see Figure 1.1). Upon integration over the azimuth θ of the scattered direction:

$$\Sigma_s\left(x,\mu',\mu,E'\to E\right)\equiv\int_0^{2\pi}d\vartheta\Sigma_s\left(x,\boldsymbol{\Omega}'\bullet\boldsymbol{\Omega},E'\to E\right) \qquad \text{Eq.(1-45)}$$

Eq. (1-43) becomes:

$$\left[\mu\frac{\partial}{\partial x}+\Sigma\left(x,E\right)\right]\phi\left(x,\mu,E\right)=$$
$$=\int_0^{\infty}dE'\int_{-1}^{1}d\mu'\Sigma_s\left(x,\mu',\mu,E'\to E\right)\phi\left(x,\mu',E'\right)+ \qquad \text{Eq.(1-46)}$$
$$+\frac{1}{2}\chi\left(E\right)\int_0^{\infty}dE'\nu\left(E'\right)\Sigma_f\left(x,E'\right)\phi\left(x,E'\right)+Q\left(x,\mu,E\right)$$

with:

$$\phi\left(x,\mu,E\right)\equiv\frac{1}{2\pi}\int_0^{2\pi}d\vartheta\phi\left(x,\boldsymbol{\Omega}\left(\mu,\vartheta\right),E\right)$$

$$Q\left(x,\mu,E\right)\equiv\frac{1}{2\pi}\int_0^{2\pi}d\vartheta Q\left(x,\boldsymbol{\Omega}\left(\mu,\vartheta\right),E\right)$$

Commonly, we express the scattering kernel as in a Legendre expansion representation:

$$\Sigma_s\left(x,\boldsymbol{\Omega}'\bullet\boldsymbol{\Omega},E'\to E\right)=\sum_{l=0}^{\infty}\frac{\left(2l+1\right)}{4\pi}\Sigma_{sl}\left(x,E'\to E\right)P_l\left(\boldsymbol{\Omega}'\bullet\boldsymbol{\Omega}\right) \qquad \text{Eq.(1-47)}$$

where the scattering coefficients are (from orthogonality):

$$\Sigma_{sl}\left(x,E'\to E\right)\equiv 2\pi\int_{-1}^{1}d\mu_0P_l\left(\mu_0\right)\Sigma_s\left(x,\mu_0,E'\to E\right) \qquad \text{Eq.(1-48)}$$

Equation (1-45) then becomes:

$$\Sigma_s\left(x,\mu',\mu,E'\to E\right)=\sum_{l=0}^{\infty}\frac{\left(2l+1\right)}{2}\Sigma_{sl}\left(x,E'\to E\right)P_l\left(\mu'\right)P_l\left(\mu\right) \qquad \text{Eq.(1-49)}$$

We have applied the addition theorem for Legendre polynomials, in the form:

$$P_l(\mu')P_l(\mu)=\frac{1}{2\pi}\int_0^{2\pi}d\vartheta P_l(\Omega'\bullet\Omega) \qquad \text{Eq.(1-50)}$$

to obtain Eq. (1-49). With Eq. (1-49), Eq. (1-46) becomes:

$$\left[\mu\frac{\partial}{\partial x}+\Sigma(x,E)\right]\phi(x,\mu,E)=$$
$$=\frac{1}{2}\sum_{l=0}^{\infty}(2l+1)\int_0^{\infty}dE'\Sigma_{sl}(x,E'\to E)P_l(\mu)\phi_l(x,E')+ \qquad \text{Eq.(1-51)}$$
$$+\frac{1}{2}\chi(E)\int_0^{\infty}dE'\nu(E')\Sigma_f(x,E')\phi_0(x,E')+Q(x,\mu,E)$$

where the l^{th} Legendre moment of the angular flux is:

$$\phi_l(x,E)\equiv\int_{-1}^{1}d\mu P_l(\mu)\phi(x,\mu,E)$$

Similarly, the multigroup approximation [Eq. (1-51)] for plane geometry is:

$$\left[\mu\frac{\partial}{\partial x}+\Sigma_g(x)\right]\phi_g(x,\mu)=$$
$$=\frac{1}{2}\sum_{l=0}^{\infty}(2l+1)\sum_{g'=1}^{G}\Sigma_{slgg'}(x)P_l(\mu)\phi_{lg'}(x)+ \qquad \text{Eq.(1-52)}$$
$$+\frac{1}{2}\chi_g\sum_{g'=1}^{G}\nu_{g'}\Sigma_{fg'}(x)\phi_{0g'}(x)+Q_g(x,\mu)$$

with:

$$\phi_{lg}(x)\equiv\int_{-1}^{1}d\mu P_l(\mu)\phi_g(x,\mu)$$

and

$$\Sigma_{slgg'}(x)\equiv\int_{\Delta E_g}dE\int_{\Delta E_{g'}}dE'\Sigma_{sl}(x,E'\to E)f(E')$$

1.3 The Neutron Kinetics Equations

The neutron transport equation without delayed neutrons,

$$\left[\frac{1}{\upsilon}\frac{\partial}{\partial t}+\hat{\Omega}\cdot\vec{\nabla}+\sigma(\vec{r},E)\right]\psi(\vec{r},\hat{\Omega},E,t)$$
$$=q_{ex}(\vec{r},\hat{\Omega},E,t)+\int dE'\int d\Omega'\sigma_s(\vec{r},E'\rightarrow E,\hat{\Omega}'\cdot\hat{\Omega})\psi(\vec{r},\hat{\Omega},E,t) \qquad \text{Eq.(1-53)}$$
$$+\chi(E)\int dE'\nu\sigma(\vec{r},E')\int d\Omega'\psi(\vec{r},\hat{\Omega}',E',t)$$

assumes that all neurons are emitted instantaneously at the time of fission. In fact, small fraction of neutrons is emitted later due to certain fission products. To ascertain the time-dependent behavior of a nuclear reactor, one must account for the emission of these so-called delayed neutrons, for the small fraction of neutrons that are delayed make the chain reaction far more sluggish under most conditions than would first appear.

To derive the neutron kinetics equations, we return to the time-dependent equation

$$\frac{1}{\upsilon}\frac{\partial}{\partial t}\psi(\vec{r},\hat{\Omega},E,t)+\hat{\Omega}\cdot\vec{\nabla}\psi(\vec{r},\hat{\Omega},E,t)+\sigma(\vec{r},E)\psi(\vec{r},\hat{\Omega},E,t) \qquad \text{Eq.(1-54)}$$
$$=q_s(\vec{r},\hat{\Omega},E,t)+q_{ex}(\vec{r},\hat{\Omega},E,t)+q_f(\vec{r},E,t)$$

When delayed neutrons are considered, we express the fission contribution to the emission density as

$$q_f=\underbrace{q_p}_{\substack{\text{emission density}\\ \text{for prompt neutrons}}}+\underbrace{q_d}_{\substack{\text{emission density}\\ \text{for delayed neutrons}}} \qquad \text{Eq.(1-55)}$$

To represent q_p, we assume that for the i^{th} fissionable isotope, a fraction β^i of the fission neutrons is delayed. This delayed fraction is small, ranging from 0.0065 for ^{235}U to about 0.0022 for ^{239}Pu. The fraction of prompt neutrons must then be (1- β^i).

The rate of prompt fission neutrons produced per unit volume from isotope *i* is just

$$(1-\beta^i)\int dE'\nu\sigma_f^i(\vec{r},E')\phi(\vec{r},E') \qquad \text{Eq.(1-56)}$$

To obtain the rate at which prompt neutrons are produced we sum over the isotope index *i* yielding

$$q_p(\vec{r},E,t)=\chi_p(E)\sum_i(1-\beta^i)\int dE'\nu\sigma_f^i(\vec{r},E')\phi(\vec{r},E') \qquad \text{Eq.(1-57)}$$

The delayed neutrons arise from the decay of variety of fission products. For neutron kinetics considerations these are usually divided into six groups, each with a characteristic decay constant λ_l, for each fissionable isotope i, with a characteristic yield β^i_l, where

$$\beta^i = \sum_l \beta^i_l \qquad \text{Eq.(1-58)}$$

If the concentration of the fission product precursors of type l is $C_l(\vec{r},E)$ per unit volume, then the number of delayed neutrons produced by precursor type l per unit time per unit volume will just be $\lambda_l C_l(\vec{r},t)$. Now suppose that the probability that the delayed neutrons from precursor type l will have an energy between E and $E+dE$ is $\chi_l(E)dE$. We find the contribution of the delayed neutrons to the emission density to be

$$q_d(\vec{r},E,t) = \sum_l \chi_l(E)\lambda_l C_l(\vec{r},E') \qquad \text{Eq.(1-59)}$$

Hence,

$$\left[\frac{1}{\upsilon}\frac{\partial}{\partial t} + \hat{\Omega}\cdot\vec{\nabla} + \sigma(\vec{r},E)\right]\psi(\vec{r},\hat{\Omega},E,t)$$

$$\begin{aligned} &= q_{ex}(\vec{r},\hat{\Omega},E,t) + \int dE' \int d\Omega'' \sigma_s(\vec{r},E'\to E,\hat{\Omega}'\cdot\hat{\Omega})\psi(\vec{r},\hat{\Omega},E',t) \\ &+ \chi_p(E)\sum_i (1-\beta^i)\int dE' \nu\sigma^i_f(\vec{r},E')\phi(\vec{r},E') \\ &+ \sum_l \chi_l(E)\lambda_l C_l(\vec{r},E') \end{aligned} \qquad \text{Eq.(1-60)}$$

Before this equation may be solved, an additional equation must be available for each precursor concentration. Since each precursor emits one delayed neutron, the rate of production of precursor type l is

$$\sum_i \beta^i_l \int dE' \nu\sigma^i_f(\vec{r},E')\phi(\vec{r},E',t) \qquad \text{Eq.(1-61)}$$

while the decay rate is $\lambda_l C_l(\vec{r},t)$. Hence the net rate of change in the precursor concentration is

$$\frac{\partial}{\partial t} C_l(\vec{r},t) = \sum_i \beta^i_l \int dE' \nu\sigma^i_f(\vec{r},E')\phi(\vec{r},E',t) - \lambda_l C_l(\vec{r},t) \qquad \text{Eq.(1-62)}$$

The Equations 60 and 61 are referred to as the neutron kinetics equations.

The foregoing equations may be generalized along two lines that are worthy to mention. First, we have made the assumption that the prompt and delayed spectra χ^i_p and χ^i_l are independent

of the isotope producing the fission. This ansatz is invariably employed in problems where delayed neutrons are ignored, since the neglected deviations are insignificant. In kinetics problems neglect of the isotope dependence of the delayed neutron spectra may sometimes lead to significant errors. It is then necessary to derive somewhat more general forms of the kinetics equations in which isotope dependent prompt and delayed spectra are used. Since this generalization causes no generic changes in computational methods, the derivation of the equations is left as an exercise.

Kinetics equations also frequently involve time-dependent cross-sections; a re-derivation of the foregoing equations would then simply introduce the time parameter *t* in each of the cross-sections appearing in the neutron kinetics equations. In kinetics calculations the time-dependence would be predetermined as a function of time. This would be the case, for example, if a control rod were to be inserted into a reactor core at a specified rate.

More generally, changes in cross-sections resulting from thermal-hydraulic or other feedback mechanisms are induced by the fact that the heat of fission causes the temperature in the reactor to change; this in turn results in changes in the number densities and therefore the macroscopic cross-sections appearing in the kinetics equations. The inclusion of these feedback effects for so-called reactor dynamics calculations is outside the scope of this text. However, we note that in most dynamics calculations the kinetics equations are treated as a separate module into which the time-dependent cross-sections are input.

1.4 The Time-Independent Transport Equation

The vast majority of numerical transport equations are carried out using a form of the equations in which time dependence is not treated explicitly. For non-multiplying systems in which the external sources are time-independent and nonnegative there will always be nonnegative solutions to the time-independent form of the transport equation

$$[\hat{\Omega}\cdot\vec{\nabla}+\sigma(\vec{r},E)]\psi(\vec{r},\hat{\Omega},E)=q_{ex}(\vec{r},\hat{\Omega},E)+\int dE'\int d\Omega'\sigma_s(\vec{r},E'\to E,\hat{\Omega}'\cdot\hat{\Omega})\psi(\vec{r},\hat{\Omega},E') \quad \text{Eq.(1-63)}$$

if the boundary conditions are also time-independent. For multiplying systems, the situation is less straightforward, for the critical state of system must be considered.

1.4.1 Fixed Source and Eigenvalue Problems

Physically, a system containing fissionable material is said to be critical if there is a self-sustaining time-independent chain reaction in the absence of external source of neutrons. That is to say, if neutrons are inserted into a critical system, then after sufficient time has elapsed for the decay of transient effects, a time-independent asymptotic distribution of neutrons will exists in which the rate of fission neutron production is just equal to the losses due absorption and leakage from the system. If such an equilibrium cannot be established, the asymptotic distribution of neutrons – called fundamental mode – will not be steady state and will either increase or decrease with time exponentially as indicated in Figure 1.8. The system then is said to be supercritical or subcritical, respectively. If neutrons from a time-independent external source are supplied, a subcritical system will eventually come to an equilibrium state characterized by a time-independent neutron flux distribution in which the production rate of external and fission neutrons is in equilibrium with the absorption and leakage from the system. However, if the system is critical or supercritical, no such equilibrium can exist in the presence of an external source, and the neutron flux distribution will be an increasing function of time. This flux behavior is qualitatively depicted in Figure 1.9.

Figure 1.8. Time dependence of the flux for a source-free multiplying medium

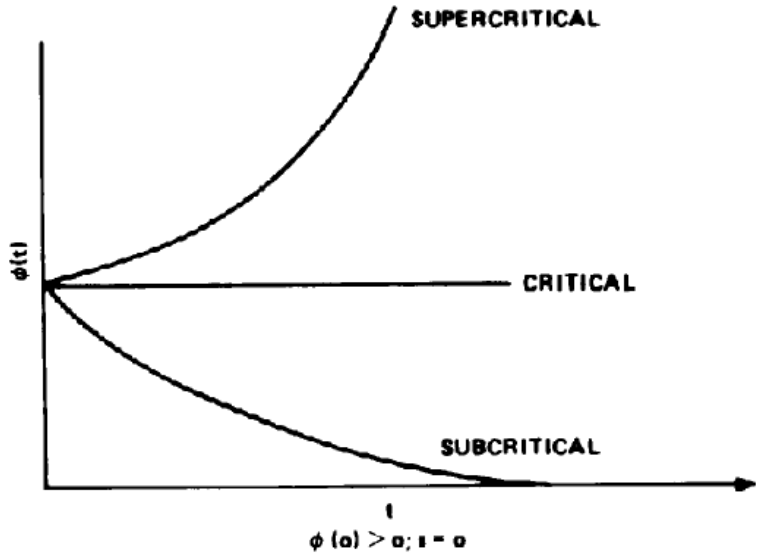
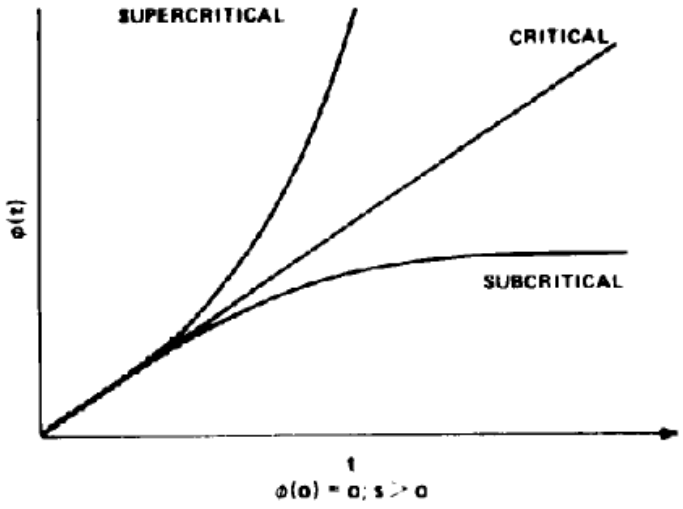


Figure 1.9 Time dependence of the flux a multiplying medium with a known source



Mathematically, a system is critical if a time-independent nonnegative solution to the source-free transport equation can be found. Hence, from the transport equation without delayed neutrons, Eq. 53, one must have a solution to

$$[\hat{\Omega}\cdot\vec{\nabla}+\sigma(\vec{r},E)]\psi(\vec{r},\hat{\Omega},E)$$
$$=\int dE'\int d\Omega'\sigma_s(\vec{r},E'\to E,\hat{\Omega}'\cdot\hat{\Omega})\psi(\vec{r},\hat{\Omega},E') \qquad \text{Eq.(1-64)}$$
$$+\chi(E)\int dE'\nu\sigma_f(\vec{r},E')\int d\hat{\Omega}'\psi(\vec{r},\hat{\Omega}',E'),\qquad \vec{r}\in V$$

with appropriate boundary conditions, for example,

$$\psi(\vec{r},\hat{\Omega},E)=0,\qquad \hat{n}\cdot\hat{\Omega}<0,\ \vec{r}\in\Gamma \qquad \text{Eq.(1-65)}$$

where V is the volume of the system and Γ is its surface. For a subcritical system there must exist a solution to the time-independent form of Eq. 53 in the presence of external sources

$$[\hat{\Omega}\cdot\vec{\nabla}+\sigma(\vec{r},E)]\psi(\vec{r},\hat{\Omega},E)$$
$$=q_{ext}(\vec{r},\hat{\Omega},E)+\int dE'\int d\Omega'\sigma_s(\vec{r},E'\to E,\hat{\Omega}'\cdot\hat{\Omega})\psi(\vec{r},\hat{\Omega},E') \qquad \text{Eq.(1-66)}$$
$$+\chi(E)\int dE'\nu\sigma_f(\vec{r},E')\int d\hat{\Omega}'\psi(\vec{r},\hat{\Omega}',E'),\qquad \vec{r}\in V$$

where we may also have a known distribution of neutrons entering the system across its surface:

$$\psi(\vec{r},\hat{\Omega},E)=\hat{\Psi}(\vec{r},\hat{\Omega}),\qquad \hat{n}\cdot\hat{\Omega}<0,\ \vec{r}\in\Gamma \qquad \text{Eq.(1-67)}$$

There is a difficulty in using Eq. 1-64 as it stands. In most situations the configuration under consideration will not be exactly critical until fine adjustments have been made in composition and/or geometry. But if we try to find a solution to Eq. 1-64 and find that none exists, it tells us nothing about whether the system is subcritical or supercritical or by how much, and therefore no useful information is gained as to how the system parameters might be adjusted to obtain criticality. For this reason criticality calculations are normally cast into the form of Eigenvalue problems, where the Eigenvalue provides a measure of whether the system is critical or subcritical and by how much. The two most common formulations are the time-absorption and multiplication eigenvalues, reefed to as α and k, respectively.

1.4.1.1 The α Eigenvalue

Suppose that we look for asymptotic solutions of Eq. 1-64 in the form

$$\psi(\vec{r},\hat{\Omega},E,t)=\psi_\alpha(\vec{r},\hat{\Omega},E)\exp[\alpha t] \qquad \text{Eq.(1-68)}$$

where the solution satisfies the boundary conditions. By insertion in Eq. 1-53 and setting q_{ex} to zero, we obtain the eigenvalue equation:

$$\left[\hat{\Omega}\cdot\vec{\nabla}+\sigma(\vec{r},E)+\frac{\alpha}{\upsilon}\right]\psi_\alpha(\vec{r},\hat{\Omega},E)$$
$$=\int dE'\int d\Omega'\sigma_s(\vec{r},E'\to E,\hat{\Omega}'\cdot\hat{\Omega})\psi_\alpha(\vec{r},\hat{\Omega},E') \qquad \text{Eq.(69)}$$
$$+\chi(E)\int dE'\,\nu\sigma_f(\vec{r},E')\int d\hat{\Omega}'\psi(\vec{r},\hat{\Omega}',E')$$

In general there will be a spectrum of eigenvalues for which the equation has a solution. However, at long times, only nonnegative solutions corresponding to the largest real component of α will predominate. From our physical definition of criticality we have, for α_0, the eigenvalue with the largest real part,

$$\mathrm{Re}\,\alpha_0\begin{cases}>0 & \text{supercritical,}\\ =0 & \text{critical,}\\ <0 & \text{subritical.}\end{cases}$$

Moreover, the magnitude of Re[α_0] provides a measure of how far from criticality the system is.

1.4.1.2 The k Eigenvalue

The *k* eigenvalue form of the criticality problem is formulated by assuming that *v*, the average number of neutrons per fission, can be adjusted to obtain a time-independent solution to Eq. 1-64. Hence we replace *v* by *v/k* and write

$$\left[\hat{\Omega}\cdot\vec{\nabla}+\sigma(\vec{r},E)+\frac{\alpha}{\upsilon}\right]\psi(\vec{r},\hat{\Omega},E)$$
$$=\int dE'\int d\Omega'\sigma_s(\vec{r},E'\to E,\hat{\Omega}'\cdot\hat{\Omega})\psi_\alpha(\vec{r},\hat{\Omega},E') \qquad \text{Eq.(1-70)}$$
$$+\frac{\chi(E)}{k}\int dE'\,\nu\sigma_f(\vec{r},E')\int d\hat{\Omega}'\psi(\vec{r},\hat{\Omega}',E')$$

Once again we have an eigenvalue problem. From our physical definition of criticality it is apparent that any chain reaction can be made critical if the number of neutrons per fission can be adjusted between zero and infinity. Thus there will be a largest value of *k*, for which a nonnegative fundamental mode solution can be found. Clearly the system is critical if this largest value of is *k = 1*. A value of *k < 1* implies that the hypothetical number of neutrons per fission, *v/k*, required to make the system just critical is larger than *v*, the number available in reality. Hence the system is subcritical. Conversely, for *k > 1*, fewer neutrons per fission are required to make the system critical than are produced in reality, and thus the system is supercritical. To summarize,

$$k\begin{cases}>1 & \text{supercritical,}\\ =1 & \text{critical,}\\ <1 & \text{subritical.}\end{cases}$$

For most reactor criticality calculations the k rather than α eigenvalue is used for several reasons. First, as indicated by Eq. 69, the α eigenvalue equation has the same form as the time-independent transport equation but with α/υ added to the absorption cross-section. For this

reason this formulation is normally referred to as the time-absorption eigenvalue. If the system is subcritical, however, α will be negative, and situation is likely to arise, such as in voided regions where the pseudo total cross-section that include α/υ term will be negative. Such negative cross-sections are problematic for many of the numerical algorithms used to solve the transport equation.

A second drawback arises from the fact that the α eigenvalue causes the removal of neutrons from the system to be inversely proportional to their speed. Hence for supercritical systems α/υ absorption will cause more neutrons to be removed from low energies and result in a neutron energy spectrum that is shifted upward in energy compared to that of a just critical system with $\alpha = 0$. Conversely, in a subcritical system the negative value of α causes neutrons to be preferentially added at lower energies, causing a downward shift in the energy spectrum. In many calculations where it is desired to know not only the critical state of the system but also the spectrum that the system would have if it were critical, these spectral shifts are undesirable. Moreover, such shifts are insignificant when the k eigenvalue formulation is used.

A third advantage of k eigenvalue formulation lies in the physical interpretations of the eigenvalue and the iterative technique derived from it. The technique is a powerful method for carrying out criticality calculations. Also, k may be interpreted as the asymptotic ratio of the number of neutrons in one generation and the number in the next.

1.5 The Adjoint Transport Equation

For each of the foregoing forms of the transport equation a related adjoint equation may be formulated. Solutions for such adjoint equations may serve a variety of purposes. For fixed source problems they may be used to expedite certain classes of calculations, particularly when Monte Carlo methods are used. For eigenvalue problems probably the most extensive use of adjoint solution is in perturbation theory estimates for changes in the neutron multiplication caused by small changes in material properties.

In this section we first discuss the properties of adjoint operators and develop an adjoint equation for non-multiplying systems. After demonstrating some uses of the resulting adjoint equation, we turn to the criticality problem in order to formulate an adjoint equation for a multiplying system and demonstrate its use for calculating perturbations in the multiplication.

1.5.1 Non-multiplying Systems

To begin, suppose that we have an operator H and any pair of functions ζ and ζ^+ that meet appropriate boundary and continuity conditions. For real-valued functions the adjoint operator H^+ is defined by the identity

$$\left\langle \zeta^+ H\zeta \right\rangle = \left\langle \zeta H^+ \zeta^+ \right\rangle \qquad \text{Eq.(1-71)}$$

where $\langle\ \rangle$ signifies integration over all of the independent variables. If $H = H^+$, the operator is said to be self-adjoint; otherwise it is non-self-adjoint.

For the time-independent non-multiplying transport problem, given by Eq. 1-63, the transport operator may be given by

$$H\zeta = [\hat{\Omega}\cdot\vec{\nabla} + \sigma(\vec{r},E)]\zeta(\vec{r},\hat{\Omega},E) - \int dE' \int d\Omega' \sigma_s(\vec{r},E'\to E,\hat{\Omega}'\cdot\hat{\Omega})\zeta(\vec{r},\hat{\Omega},E') \qquad \text{Eq.(1-72)}$$

and the integration over the independent variable is

$$\langle \cdot \rangle = \int dV \int d\Omega \int dE \qquad \text{Eq.(1-73)}$$

The spatial domain of the problem V is bounded by a surface Γ across which we shall assume that no particles enter (i.e., vacuum boundary conditions). Hence the functions upon which H operates are constrained to satisfy

$$\zeta(\vec{r},\hat{\Omega},E) = 0, \qquad \hat{n}\cdot\hat{\Omega} < 0, \ \ \vec{r} \in \Gamma \qquad \text{Eq.(1-74)}$$

where $\hat{n}$ is the outward normal. In addition, for $\hat{\Omega}\cdot\vec{\nabla}\zeta$ to be finite, ζ must be continuous in the direction of particle travel.

To determine the form of the adjoint transport operator, we multiply Eq. 1-72 by a function $\zeta^{+}(\vec{r},\hat{\Omega},E)$ and manipulate the result in order to move $\zeta(\vec{r},\hat{\Omega},E)$ to the left of the operator.

First, we have

$$\begin{aligned}\left\langle \zeta^{+} H\zeta \right\rangle = \int dV \int dE \int d\Omega\, \zeta^{+}(\vec{r},\hat{\Omega},E)\times[\hat{\Omega}\cdot\vec{\nabla}\zeta(\vec{r},\hat{\Omega},E) + \sigma(\vec{r},E)\zeta(\vec{r},\hat{\Omega},E)] \\ - \int dE' \int d\Omega' \sigma_s(\vec{r},E'\to E,\hat{\Omega}'\cdot\hat{\Omega})\zeta(\vec{r},\hat{\Omega},E')\end{aligned} \qquad \text{Eq.(1-75)}$$

For the streaming term we use the fact that $\hat{\Omega}\cdot\vec{\nabla} = \vec{\nabla}\cdot\hat{\Omega}$, and integrate the identity

$$\vec{\nabla}\cdot(\hat{\Omega}\zeta^{+}\zeta) = \zeta^{+}\hat{\Omega}\cdot\vec{\nabla}\zeta + \zeta\hat{\Omega}\cdot\vec{\nabla}\zeta^{+} \qquad \text{Eq.(1-76)}$$

over V to obtain

$$\int d\Gamma\, \hat{n}\cdot\hat{\Omega}\zeta^{+}\zeta = \int dV \zeta^{+}\hat{\Omega}\cdot\vec{\nabla}\zeta + \int dV \zeta\hat{\Omega}\cdot\vec{\nabla}\zeta^{+} \qquad \text{Eq.(1-77)}$$

where the divergence theorem has been applied to reduce the expression on the left to a surface integral. We note, however, that the boundary condition specified by Eq. 1-74 causes the integrant to vanish for $\hat{\Omega}\cdot\hat{n} < 0$. We reduce the function ζ^{+} to have the boundary condition

$$\zeta^{+}(\vec{r},\hat{\Omega},E) = 0, \qquad \hat{n}\cdot\hat{\Omega} \geq 0, \ \ \vec{r} \in \Gamma \qquad \text{Eq.(1-78)}$$

causing the surface integral to vanish for all $\hat{\Omega}$. Thus

$$\int dV \zeta^{+}\hat{\Omega}\cdot\vec{\nabla}\zeta = -\int dV \zeta\hat{\Omega}\cdot\vec{\nabla}\zeta^{+} \qquad \text{Eq.(1-79)}$$

In the collision term of Eq. 1-75 we simply note that $\zeta^+\sigma\zeta = \zeta\sigma\zeta^+$, while in the scattering term we interchange dummy variables *E* and *E'* as well as $\hat{\Omega}$ and $\hat{\Omega}'$ to obtain

$$\begin{aligned}&\int d\Omega\int dE\zeta^+(\vec{r},\hat{\Omega},E)\int d\Omega'\int dE\sigma_s(\vec{r},E'\to E,\hat{\Omega}'\cdot\hat{\Omega})\zeta(\vec{r},\hat{\Omega}',E')\\&\quad=\int d\Omega\int dE\zeta(\vec{r},\hat{\Omega},E)\int d\Omega'\int dE\sigma_s(\vec{r},E\to E',\hat{\Omega}\cdot\hat{\Omega}')\zeta^+(\vec{r},\hat{\Omega}',E')\end{aligned} \qquad \text{Eq.(1-80)}$$

Substituting the three preceding expressions into Eq. 1-75 we have

$$\begin{aligned}\left\langle\zeta^+H\zeta\right\rangle&=\int dV\int d\Omega\int dE\zeta(\vec{r},\hat{\Omega},E)\times[\hat{\Omega}\cdot\vec{\nabla}\zeta^+(\vec{r},\hat{\Omega},E)+\sigma(\vec{r},E)\zeta^+(\vec{r},\hat{\Omega},E)]\\&\quad-\int dE'\int d\Omega'\sigma_s(\vec{r},E\to E',\hat{\Omega}\cdot\hat{\Omega}')\zeta^+(\vec{r},\hat{\Omega}',E')\end{aligned} \qquad \text{Eq.(1-81)}$$

Hence Eq. 1-71 will be satisfied provided we define the adjoint transport operator as

$$H^+\zeta^+=[-\hat{\Omega}\cdot\vec{\nabla}+\sigma(\vec{r},E)]\zeta^+(\vec{r},\hat{\Omega},E)-\int dE'\int d\Omega'\sigma_s(\vec{r},E\to E',\hat{\Omega}\cdot\hat{\Omega}')\zeta^+(\vec{r},\hat{\Omega}',E') \qquad \text{Eq.(1-82)}$$

To illustrate the use of this adjoint identity suppose we solve a transport problem with a known external source distribution q_{ex},

$$H\psi = q_{ex} \qquad \text{Eq.(1-83)}$$

where ψ meets the boundary conditions of Eq. 1-74. Suppose further that we would like to know the response of a small detector with a total cross-section σ_d and a volume V_d, represented by the reaction rate localized at point $\vec{r}_d$,

$$R = V_d\int dE\sigma_d(E)\phi(\vec{r}_d,E) \qquad \text{Eq.(1-84)}$$

We define the adjoint 1-problem as

$$H^+\psi^+ = \sigma_d V_d\delta(\vec{r}-\vec{r}_d) \qquad \text{Eq.(1-85)}$$

where the adjoint flux ψ^+ is required to satisfy the boundary condition of Eq. 1-78. Now multiply Eq. 1-83 by ψ^+ and integrate over the independent variables to obtain

$$\left\langle\psi^+H^+\psi\right\rangle=\left\langle\psi^+q_{ex}\right\rangle \qquad \text{Eq.(1-86)}$$

Similarly, multiply Eq. 1-85 by ψ and integrate to yield

$$\left\langle\psi H^+\psi^+\right\rangle=\left\langle\psi\sigma_d V_d\delta(\vec{r}-\vec{r}_d)\right\rangle=R \qquad \text{Eq.(1-87)}$$

Taking the difference of these two expressions yields

$$\left\langle\psi^+H\psi\right\rangle-\left\langle\psi H^+\psi^+\right\rangle=\left\langle\psi^+q_{ex}\right\rangle-R \qquad \text{Eq.(1-88)}$$

Replace ζ and ζ^+ with ψ and ψ^+ in the adjoint identity, Eq. 1-81. The left-hand side of Eq. 1-88 then vanishes to yield the desired result:

$$R = \left\langle \psi^+ q_{ex} \right\rangle \qquad \text{Eq.(1-89)}$$

From this illustration, we see that the detector response is just given by the volume integral of the adjoint weighted source distribution. In particular, if we assume that the particles are emitted at $\vec{r}_0$ in direction $\hat{\Omega}_0$ at energy E_0 at a rate of one per second,

$$q_{ex} = \delta(\vec{r} - \vec{r}_0)\delta(E - E_0)\delta(\hat{\Omega} \cdot \hat{\Omega}_0) \qquad \text{Eq.(1-90)}$$

and obtain

$$R = \psi^+(\vec{r}_0, \hat{\Omega}_0, E_0) \qquad \text{Eq.(1-91)}$$

This provides us with a physical interpretation of the adjoint flux defined by Eq. 1-85: it is just the importance of particles produced at $\vec{r}_0, \hat{\Omega}_0, E_0$ to the detector response. The concept of particle importance is elaborated elsewhere for a broad range of neutronics problems.

The foregoing methodology has widespread applications, particularly in Monte Carlo calculations.

The foregoing formalism may be applied by slight modification to external surface source of particles, or to calculate distributions of particles leaving the problem domain. For example, suppose that $q_{ex} = 0$ within V but that particles enter the volume across Γ. Then we would have

$$H\psi = 0 \qquad \text{Eq.(1-92)}$$

with the boundary condition

$$\psi(\vec{r}, \hat{\Omega}, E) = \tilde{\Psi}(\vec{r}, \hat{\Omega}, E), \qquad \hat{\Omega} \cdot \hat{n} < 0, \ \vec{r} \in \Gamma \qquad \text{Eq.(1-93)}$$

where $\tilde{\Psi}$ is known as distribution of incoming particles. Using Eq. 1-85 for the adjoint, with ψ^+ satisfying Eq. 1-78 on the boundary, we can again carry out the same procedure used to obtain Eq. 1-88 with $q_{ex} = 0$:

$$\left\langle \psi^+ H\psi \right\rangle - \left\langle \psi H^+ \psi^+ \right\rangle = -R \qquad \text{Eq.(1-94)}$$

Now, however, the boundary condition, Eq. 1-93, prevents Eq. 1-71 from holding. Rather, by careful inspection of Eq. 1-77 and Eq. 1-81 it is clear that

$$\left\langle \psi^+ H\psi \right\rangle - \left\langle \psi H^+ \psi^+ \right\rangle = \int d\Gamma \int dE \int_{\hat{n} \cdot \hat{\Omega} < 0} d\Omega \, \hat{n} \cdot \hat{\Omega} \psi^+ \tilde{\Psi} \qquad \text{Eq.(1-95)}$$

Hence the desired detector response

$$R = \int d\Gamma \int dE \int_{\hat{n}\cdot\hat{\Omega}<0} d\Omega \left|\hat{n}\cdot\hat{\Omega}\right| \psi^{+} \tilde{\Psi} \qquad \text{Eq.(1-96)}$$

is an integral of the adjoint flux over that part of the surface for which the known distribution of incoming particles is nonzero.

1.5.2 Multiplying Systems

For multiplying systems a fission neutron term must also be included in the adjoint equations. For time-independent problems we define the fission operator as

$$G\zeta = \chi(E) \int dE' \nu\sigma_f(\vec{r},E') \int d\Omega' \zeta(\vec{r},\hat{\Omega}',E') \qquad \text{Eq.(1-97)}$$

The adjoint operator is then defined by

$$\left\langle \zeta^{+} G\zeta \right\rangle = \left\langle \zeta\, G^{+}\zeta^{+} \right\rangle \qquad \text{Eq.(1-98)}$$

By using the same technique as that applied to the scattering operator earlier, it is easily shown that

$$G^{+}\zeta^{+} = \nu\sigma_f(\vec{r},E) \int dE' \chi(E') \int d\Omega' \zeta(\vec{r},\hat{\Omega}',E') \qquad \text{Eq.(1-99)}$$

The technique of the preceding subsection may be generalized to treat subcritical systems where an external source gives rise to a time-independent solution; one simply replaces H and H^{+} by H-G and H^{+}-G^{+} respectively. A more frequent use of the adjoint equation is in estimating changes in reactivity by perturbation theory. Before illustrating the use of perturbation theory, however, we must briefly examine some properties of homogeneous equations.

For the multiplication eigenvalue problem, Eq. 1-70 may be written in operator notation as

$$H\psi - \frac{1}{k} G\psi = 0 \qquad \text{Eq.(1-100)}$$

where ψ is taken to be the fundamental mode solution, $\psi > 0$ for $\vec{r} \in V$, obeying the vacuum boundary conditions. Likewise the adjoint equation is

$$H^{+}\psi^{+} - \frac{1}{k} G^{+}\psi^{+} = 0 \qquad \text{Eq.(1-101)}$$

where ψ^{+} is the fundamental mode solution $\psi^{+} > 0$ for $\vec{r} \in V$, obeying the boundary conditions of Eq. 1-78. If we multiply Eq. 1-100 by ψ^{+}, Eq. 1-101 by ψ, and integrate the difference over the independent variables, then

$$\left\langle \psi^{+} H\psi \right\rangle - \left\langle \psi H^{+}\psi^{+} \right\rangle - \frac{1}{k}\left\langle \psi^{+} G\psi \right\rangle + \frac{1}{k^{+}}\left\langle \psi G^{+}\psi^{+} \right\rangle = 0 \qquad \text{Eq.(1-102)}$$

After simplifying this expression with identities, Eq. 1-71 and Eq. 1-98, we have

$$\left(\frac{1}{k}-\frac{1}{k^+}\right)\left\langle \psi^+ G\psi\right\rangle = 0 \qquad \text{Eq.(1-103)}$$

It is easily shown in Eq. 103 that if ψ^+ and ψ^+ are positive, the integral on the left will not vanish. Thus for this equation to hold the eigenvalues of the transport equation and its adjoint must be equal:

$$k = k^+ \qquad \text{Eq.(1-104)}$$

We are now prepared to use the adjoint operators to calculate changes in reactivity, where reactivity is defined by

$$\rho = \frac{k-1}{k} \qquad \text{Eq.(1-105)}$$

For small changes, δk, in k, we have

$$\delta\rho = \frac{\delta k}{k_0^2} \qquad \text{Eq.(1-106)}$$

where k_0 is unperturbed value.

For the unperturbed rector we define the fundamental mode equations as

$$H_0\psi_0 - \frac{1}{k_0}G_0\psi_0 = 0 \qquad \text{Eq.(1-107)}$$

$$H_0^+\psi_0^+ - \frac{1}{k_0^+}G_0^+\psi_0^+ = 0 \qquad \text{Eq.(1-108)}$$

Let Eq. 1-100 be used to represent the perturbed state. Then for small changes we represent the perturbations by

$$\begin{aligned} H &= H_0 + \delta H, & G &= G_0 + \delta G \\ k &= k_0 + \delta k, & \psi &= \psi_0 + \delta\psi \end{aligned} \qquad \text{Eq.(1-109)}$$

Substituting these expressions into Eq. 1-100, we have

$$\left(H_0 + \delta H\right)\left(\psi_0 + \delta\psi\right) - \frac{1}{\left(k_0 + \delta k\right)}\left(G_0 + \delta G\right)\left(\psi_0 + \delta\psi\right) = 0 \qquad \text{Eq.(1-110)}$$

For small perturbations we may disregard terms of order δ^2. Thus, using

$$\frac{1}{(k_0+\delta k)}=\frac{1}{k_0(1+\delta k/k_0)}\approx\frac{1}{k_0}\left(1-\frac{\delta k}{k_0}\right) \qquad \text{Eq.(1-111)}$$

and regrouping, we obtain from Eq. 1-110

$$-\frac{\delta k}{k_0^2}G_0\psi_0\approx\left(H_0-\frac{1}{k_0}G_0\right)\psi_0+\left(\delta H-\frac{1}{k_0}\delta G\right)\psi_0+\left(H_0-\frac{1}{k_0}G_0\right)\delta\psi \qquad \text{Eq.(1-112)}$$

where δ^2 terms are deleted. Comparing this expression with Eq. 1-107, we see that first term on the right vanishes. Moreover, if we multiply by ψ_0^+ and integrate over the independent variables, we have

$$-\frac{\delta k}{k_0^2}\left\langle\psi_0^+G_0\psi_0\right\rangle\approx\left\langle\psi_0^+(\delta H-k_0^{-1}\delta G)\psi_0\right\rangle+\left\langle\psi_0^+(H_0-k_0^{-1}G_0)\delta\psi\right\rangle \qquad \text{Eq.(1-113)}$$

We may now use the properties of the adjoint operators to eliminate the last term. If in Eq. 1-71 and Eq. 1-98 we take $\zeta=\delta\psi$ and $\zeta^+=\delta\psi_0^+$, then we obtain

$$\left\langle\psi_0^+(H_0-k_0^{-1}G_0)\delta\psi\right\rangle=\left\langle\delta\psi(H_0^+-k_0^{-1}G_0^+)\psi_0^+\right\rangle \qquad \text{Eq.(1-114)}$$

which , according to Eq. 1-108, must vanish. Hence

$$\frac{\delta k}{k_0^2}=\frac{\left\langle\psi_0^+(k_0^{-1}\delta G-\delta H)\psi_0\right\rangle}{\left\langle\psi_0^+G_0\psi_0\right\rangle} \qquad \text{Eq.(1-115)}$$

This is powerful result, for it allows us to estimate many different small reactivity changes using only two unperturbed solutions, ψ_0 and ψ_0^+, and the cross-section changes that appear as δH and δG.