22.54 Neutron Interactions and Applications
(Spring 2002)

Lecture Notes on Neutronics of Multiplying Media

This is a set of notes for the four lectures on neutron interactions in a reactor system in which a neutron population can change as a result of capture and fission reactions, in addition to scattering. We will discuss the concept of criticality as a way of describing any self-sustaining chain reaction which, in principle, can be just as well chemical in nature, and focus on the fundamental understanding of neutron diffusion and slowing down, and the interplay between materials constants (expressed through cross sections) and geometric factors (system size and shape) in determining criticality. The four lectures are:

Lec 14. Neutronics of Multiplying Media – criticality, moderation, leakage
Lec 15. Elements of Neutron Diffusion Theory
Lec 16. Neutron Slowing Down
Lec.17. The Two-Group Two-Region Reactor

As a start the following references are recommended for supplemental reading:

J. Lemarsh, *Introduction to Nuclear Reactor Theory*
K. M. Case, F. deHoffmann, G. Placzek, *Introduction to The Theory of Neutron Diffusion*, vol. 1, LASL, 1953.

I. Some Basic Notions of Neutron Multiplication

Consider a homogeneous beam of neutrons having a distribution of energies. Define distribution function n(E) such that

$$n(E)dE = \text{expected no, of neutrons with energies in dE about E per cm}^3 \quad (1)$$

Suppose we ask how many neutrons in a certain energy range will cross an area during a time interval Δt. Call this number

$$\phi(E)dEA\Delta t \equiv n(E)dE[Av\Delta t] \quad (2)$$

since all the neutrons in a certain volume $Av\,\Delta t$ will cross during Δt. Thus we have defined in a physically intuitive way the neutron "flux"

$$\phi(E) \equiv vn(E) \quad (3)$$

with n(E) being the number density. Clearly, the interpretation of $\phi(E)$ is that it is the expected number of neutrons with energies in dE about E crossing a unit area per unit

time. Dimensionally, n(E) is no. per cm^3 per eV, while $\phi(E)$ is no. per cm^2 per eV per sec. Both are therefore distributions in E, while n(E) is also a distribution in position.

Since we are always interested in neutron reactions, we imagine the neutron beam is directed at a thin target of surface area A and thickness d. The rate at which neutrons in dE about E are incident upon the target is $\phi(E)\,\mathrm{dEA}$. Now let the interaction (reaction) rate be denoted as $[\phi(E)\,\mathrm{dEA}]\mathrm{P(d,E)}$, which means by this we define P(d,E) as the interaction probability (and therefore dimensionloess). It will be convenient to take out the dependence on target thickness by writing $P(d,E) = d\Sigma(E)$, where

$$\Sigma(E) \equiv \text{ interaction probability per unit path length (for short paths)} \qquad (4)$$

The fact that P can be taken to be simply directly proportional to the target thickness is valid only for thin targets where one has the situation of only one interaction or none most of the time. The interaction rate then becomes

$$\Sigma(E)\phi(E)dEV$$

The product $\Sigma(E)\phi(E)$, or the spatial-dependent form $\Sigma(\underline{r},E)\phi(\underline{r},E)$, appears frequently in reactor physics discussions; it is often called the 'collision density'. Despite this nomenclature, we should keep in mind that it is a distribution function in energy and space, and is also a rate.

We have previously introduced the macroscopic cross section $\Sigma(\underline{r},E)$ to represent the target property that is most relevant to the consideration of neutron interaction in a material medium. Recall that $\Sigma = N\sigma$, where N is nuclear density, the number of target nuclei per cm3, and $\sigma(E)$ is the microscopic cross section. When the medium is not homogeneous, then nuclear density can vary position in which case N becomes position dependent. In any event, the spatial and energy dependence of Σ is separable.

For problems of neutronics of multiplying systems, we need to take into account several types of reactions. This can be expressed by writing a decomposition of the total cross section as a sum of scattering, capture, and fission cross sections, and the term absorption is used to denote the sum of capture and fission.

$$\sigma_t(E) = \sigma_s(E) + \sigma_a(E) \qquad (5)$$

$$\sigma_a(E) = \sigma_c(E) + \sigma_f(E) \qquad (6)$$

The basic reason that reactor physics has its own unique flavor (and this is the reason for us to study it) is that the materials which make up a nuclear reactor have characteristic cross sections that make each reaction important at low or high neutron energies, but usually not both. For a thermal reactor with uranium fuel, the fission cross section of U^{235} is large (several hundred barns) at thermal energy but about 1 barn at the energy

where fission neutrons come off. In contrast the capture cross section $\sigma(n,\gamma)$ of U^{238} can be quite large in the resonance energy region (between thermal and fast), and is also non-negligible at thermal energy. The scattering cross section, to a first approximation, can be taken to be just a constant throughout the entire energy range of interest. Combining these variations with the fact that neutrons emitted from a fission reaction have a distribution peaked around 2 MeV, we have the situation of maintaining a chain reaction where neutrons are introduced into the system at high energy, but they need to slow down to thermal energy where the probability of their causing further fission reactions is the greatest. This then is the essence of the fundamental problem of criticality in all of reactor physics.

The Fission Reaction

While we will refer the students to any standard text on nuclear reactor theory, such as the very readable text by J. Lemarsh cited above, for a discussion of the various neutron interactions relevant to the operation of a nuclear reactor system, we note here a few basic facts about the fission event in recognition of the important role of neutrons in nuclear power production.

A typical fission reaction in U^{235} induced by a thermal neutron is:

$$^{235}_{92}U + n \rightarrow {}^{95}_{42}Mo + {}^{139}_{57}La + 2n$$

From mass balance we have (1 amu = 931 MeV)

$$\begin{aligned} M(U) + M(n) &= 236.133 \text{ amu} \\ M(Mo) + M(La) + 2M(n) &= \underline{235.918} \end{aligned}$$

mass difference $\Delta = 0.215$ amu or about 200 MeV

The distribution of this energy is:

kinetic energies of fission fragments	168 MeV
fission product decay	
γ	7
β	8
neutrinos	12
prompt γ	7
kinetic energies of fission neutrons	5
	~ 207

All the energies except those of the neutrinos are recoverable in the form of heat. In addition, each parasitic absorption (capture) of a neutron leads to capture γ whose

energies ~ 12 MeV are also recoverable. Thus the total energy recoverable is ~ 207 MeV.

In contrast, for D-D fusion reaction, $4H^1 \rightarrow He^4$, 4M(H) = 4.13258, M(He) = 4.0038, Δ ~ 26.7 MeV. It may seem that fission is the better energy source since more energy is released per reaction. However, because there is so much more hydrogen than uranium in the world, fusion power, when feasible, would be the ultimate source of energy.

We know from the binding energy curve that when a nucleus with mass A ~ 240 breaks into two fragments, A1 and A2, the total binding energy BE after the reaction is greater than that before. So <u>energy must be supplied</u> in order to make the reaction go. Such energy can be provided in several ways, such as, neutron capture, photofission by capture of γ, and charged particle reaction. It is known experimentally that photofission is a threshold event, the minimum excitation energy required being:

Th232	U233	U235	U238	Pu239
5.9	5.5	5.75	5.85	5.5 MeV

In view of such data, a question for the student is: If fission is a threshold reaction, how then can thermal neutrons induce fission?

Some facts worth keeping in mind about neutron-induced fission:

The mass distribution of fission fragment mass is not symmetric; an empirical rule is that the most probable charge distribution is that proton deficiency is the same in the two fragments, with the two peaks centered at A ~ 94 and 142.

Some of the neutrons emitted from fission appear with significant time delays, up to seconds because β decay processes can be quite slow. The role of delayed neutrons is critical in reactor control under normal operations; without delayed neutrons the population of neutrons from one generation to the next will change exponentially.

Energy distribution of fission neutrons follows the so-called Watts spectrun which peaks at ~ 0.7 MeV with average energy at ~ 1.9 MeV.

Average number of neutrons emitted per fission event (ν) varies somewhat from one fissile nucleus to another. It is mildly energy dependent. For U^{235} $\nu = \nu$(thermal) + constant x E (MeV), with ν(thermal) = 2.43 and constant = .1346 MeV^{-1}

Criticality

A simple way of stating the criticality problem is to consider how one might estimate the critical condition to maintain a self-sustained fission chain reaction. This example is quite instructive in showing the role of different types of neutron interactions, and the interplay between materials properties and geometric factors.

Suppose we separate all neutrons into either the fast (F) or high-energy group or the thermal (T) group. We begin by introducing a fast neutron into the homogenized (no spatial variation) reactor, and then follow all the contributions to the next generation of neutrons that it can possibly make (much like what one would do in MCNP).

Four things can happen to the neutron as it move through the reactor, it can escape from the reactor (fast leakage) contributing nothing to the next generation, undergo a fission reaction (fast fission) contributing $\nu P_{NFL} P_{FF}$, undergo a capture reaction contributing nothing, or undergo a scattering interaction. The contribution of the fourth event is a little or more complicated to estimate. We will assume that any scattering of a fast neutron will cause it to become a thermal neutron (we can come back to examine this later on). Then three things can happen to this thermal neutron, it can escape from the reactor as a thermal neutron (thermal escape), undergo a capture reaction (thermal capture), or undergo a fission reaction (thermal fission). The first two events contribute nothing to the next generation while the third gives $\nu P_{NFL} P_{FS} P_{NTL} P_{TF}$.

For the various probabilities, we can estimate those pertaining to reactions using the corresponding Σ, while leaving aside the non-escape probabilities to be discussed later.

$$P_{FF} = \frac{\Sigma_{FF}}{\Sigma_{FA} + \Sigma_{FS}}, \qquad P_{FS} = \frac{\Sigma_{FS}}{\Sigma_{FA} + \Sigma_{FS}}, \qquad P_{TF} = \frac{\Sigma_{TF}}{\Sigma_{TA}} \tag{7}$$

If we add up all the contributions to the next generation, the sum k is then the multiplication constant of the reactor. That is every succeeding generation is multiplied by a factor k. From the above scenario, we see there are two contributions to k, one from fast fission and the other from thermal fission. All other processes represent loss of neutron with no further contribution. Thus,

$$k = \nu P_{NFL} [P_{FF} + P_{NTL} P_{FS} P_{TF}] \tag{8}$$

In terms of k we can now define what we mean by a critical reactor, namely, k = 1. For k > 1, the neutron population increases by a factor k for every generation, so the reactor is said to be 'supercritical', whereas for k < 1, the system is 'subcritical' and cannot maintained a self-sustained chain reaction. In the supercritical case, how quickly the

reactor 'runs away' (neutron flux increases too quickly for the control system to maintain the reactor in a safe operating state) is a major concern. We will come back to discuss this situation before too long.

The multiplication constant k is perhaps the most fundamental quantity in reactor physics calculations. It is conventional to recast it into a form that separates out the spatial effects of neutron escaping from the system from the materials effects of various reactions. We rewrite k as

$$k = k_\infty P_{NFL} P_{NTL} \tag{9}$$

$$k_\infty = \nu \frac{P_{FF} + P_{NTL} P_{FS} P_{TF}}{P_{NTL}}$$

$$= \eta f p \varepsilon \tag{10}$$

with

$$\eta = \nu P_{TF} \tag{11}$$

$$p = P_{FS} \tag{12}$$

$$\varepsilon = 1 + \frac{P_{FF}}{P_{NTL} P_{TF} P_{FS}} \tag{13}$$

In reactor physics terminology, k_∞ is known as the infinite-medium multiplication constant, and it is given by the four-factor formula as shown. Here η is the average number of neutrons emitted per fission event, the thermal utilization factor f denotes the probability that the absorption of a thermal neutron takes place in the fuel rather than anywhere else (since we have only fuel in the present simple example, f = 1), p is the resonance escape probability, referring to the fact that in slowing down from fast to thermal energy the neutron must avoid any resonance absorption reaction, and ε is called the fast fission factor because it is the sum of fast and thermal fission contributions. We see also that the multiplication constant is just the product of k_∞ and the two non-escape probabilities.

To get a feel for the various numbers one can consult a figure such as Fig. 9-5 on p. 305 of Lemarsh, showing the variation of ε, f, p and k_∞ for a homogeneous mixture of 2% enriched uranium as fuel and H_2O as moderator over a range fuel to moderator ratios (x). Although not shown, the value $\eta(U^{235})$ is a constant at ~ 2.06. Since ε increases only slightly with x, the value of k_∞ is determined mostly by the competition between f and p. It is reasonable that with increasing x thermal utilization will initially increase rapidly but the effects then saturates, whereas resonance escape probability does not show the saturation and thus causes k_∞ to decrease when f starts to saturate. The peak value of k_∞

at about 1.25 sets the limit on the product of the two non-leakage probabilities if the reactor is to be critical.

II. Neutron Transport Concepts -- An Introduction

The most fundamental equation in reactor physics is the neutron transport equation which we have encountered before (Lecture 2). This equation has as its solution the time-dependent distribution function for neutrons in configuration-velocity (phase) space. A knowledge of this distribution function is sufficient to solve almost all problems of interest in reactor theory; most of the time one does not need to know the function itself, only integrals over some of the phase-space coordinates such as velocity direction, energy, or position.

We give a brief derivation of the transport equation to show that it is nothing more than just a balance relation. Define

$n(\underline{r},\underline{v},t)d^3rd^3v \equiv$ expected no. of neutrons in d^3r about $\underline{r}$ with velocities in d^3v about $\underline{v}$ at time t

Instead of the vector variable $\underline{v}$, it is often more convenient to use the scalar variable E and a two-dimensional vector $\underline{\Omega}$, v = (vx, vy, vz) $\rightarrow (v,\theta.\varphi) \rightarrow (E,\theta,\varphi)$.
Correspondingly, $d^3v = v^2 dv d\Omega$, with $d\Omega = \sin\theta d\theta d\varphi$, and

$n(\underline{r},\underline{v},t)d^3rd^3v \equiv n(\underline{r},E,\underline{\Omega},t)d^3rdEd\Omega$ = expected no. neutrons in d3r about r with energies in dE about E and going in directions in $d\Omega$ about $\underline{\Omega}$ at time t.

Consider a subsystem of volume V and surface S. Suppose we want to calculate the change in the number of neutrons in V with energies in dE about E and direction in $d\Omega$ about $\underline{\Omega}$ during a time interval Δt. This is given by

$$\iint_V [n(\underline{r},E,\Omega,t+\Delta t) - n(\underline{r},E,\Omega,t)]d^3rdEd\Omega \text{ = Gains - Losses} \qquad (14)$$

For gains we have two contributions.

(1) Fission and external source

$$\frac{\nu f(E)dEd\Omega}{4\pi} \iiint_{V,\underline{\Omega}',E'} \Sigma_f(E')\phi(\underline{r},E',\underline{\Omega}',t)dE'd\Omega'd^3r\Delta t + \int_V S(\underline{r},E,\underline{\Omega},t)d^3rdEd\Omega\Delta t \quad (15)$$

where f(E) is the fission spectrum, and S is the external source distribution.

(2) Scattering

$$\iiint_{V,E',\underline{\Omega}'} \Sigma_s(E')\phi(\underline{r},E',\underline{\Omega}',t)d^3rdE'd\Omega'\Delta tF(E'\underline{\Omega}'\to E\underline{\Omega})dEd\Omega \qquad (16)$$

where $F(E'\underline{\Omega}'\to E\underline{\Omega})dEd\Omega$ = conditional probability that given a neutron scattered at E', $\underline{\Omega}'$, it will be in dE about E and $d\Omega$ about $\underline{\Omega}$.

For losses there are also two terms, one for collisions and the other convective flow.

(3) Collisions

$$\int_V \Sigma_t(E)\phi(\underline{r},E,\underline{\Omega},t)d^3rdEd\Omega\Delta t$$

(4) Net Flow Outward

$$\int_S \underline{\Omega}\cdot\hat{n}vn(\underline{r}_s,E,\underline{\Omega},t)dsdEd\Omega\Delta t \;=\; \int_V d^3r\underline{\Omega}\cdot\underline{\nabla}\phi(\underline{r},E,\underline{\Omega},t)dEd\Omega\Delta t \qquad (17)$$

where $\hat{n}$ is the outward normal at $\underline{r}_s$, and the divergence theorem, $\int_S d\underline{s}\cdot\underline{F} = \int_V d^3r\underline{\nabla}\cdot\underline{F}$, has been applied.

Putting together the gains and losses, dividing by Δt, and taking the limit of $\Delta t\to 0$, we can write the balance as $\int_V [\;] = 0$. Since V can be any arbitrary part of the system, the integrand [ ] must vanish identically if the integral is to vanish for any V. Thus,

$$\frac{\partial n(\underline{r},E,\underline{\Omega},t)}{\partial t} = \frac{\nu f(E)}{4\pi}\int_{E',\underline{\Omega}'} dE'd\Omega'\Sigma_f(E')\phi(\underline{r},E',\underline{\Omega}',t) + S(\underline{r},E,\underline{\Omega},t) \qquad (18)$$

$$+\int_{E',\underline{\Omega}'} dE'd\Omega'\Sigma_s(E')\phi(\underline{r},E',\underline{\Omega}',t)F(E'\underline{\Omega}'\to E\underline{\Omega}) - \Sigma_t(E)\phi(\underline{r},E,\underline{\Omega},t) - \underline{\Omega}\cdot\underline{\nabla}\phi(\underline{r},E,\underline{\Omega},t)$$

This is what is known as the neutron transport equation for a homogeneous medium. For a heterogeneous system we simply let $\Sigma(E)\to\Sigma(\underline{r},E)$. Notice that this is a linear equation because we have ignored the neutron-neutron interaction (the mean free path for such events is 10^8 cm or greater). Sometimes the neutron transport equation is also called the Boltzmann equation; one should be careful in doing this since the Boltzmann equation in kinetic theory of gases treats explicitly the collisions among the particles and is in general nonlinear.

The transport equation is an integro-differential equation in 7 variables. While it is much too complicated for us to attempt any kind of solution directly, either as a boundary-value

or initial-value problem, all the equations in reactor theory that we will encounter all can be derived from the transport equation in one approximation or another.

Neutron Current

The term current has been used to denote a stream of particles flowing in a certain direction; it frequently appears in discussions of scattering of a particle beam or some kind of transport process. To be precise, one should begin with the definition in terms of the neutron flux ϕ which, as we have just seen, is the solution to the neutron transport equation. Let

$$\underline{J}(\underline{r},E,t) \equiv \int_{\underline{\Omega}} \underline{\Omega}\phi(\underline{r},E,\underline{\Omega},t)d\Omega$$

$$= \int_{\underline{\Omega}} \underline{v}n(\underline{r},E,\underline{\Omega},t)d\Omega \qquad (19)$$

Recall the meaning of a particle flux as
$vn(\underline{r},E,\underline{\Omega},t)dEd\Omega\Delta tdA\cos\theta$

= expected no. in dE about E and dΩ about $\underline{\Omega}$ crossing dA during Δt (20)

Let $J_+(\underline{r},E,t)dEdA\Delta t$

= expected no. in dE about E crossing dA during Δt from '-' to '+' in the sense of a normal $\hat{n}$

$$= \int_{\hat{n}\cdot\underline{\Omega}\geq 0} \hat{n}\cdot\underline{\Omega}\phi(\underline{r},E,\underline{\Omega},t)dEd\Omega\Delta tdA \qquad (21)$$

or,

$$J_+(\underline{r},E,t) = \int_{\hat{n}\cdot\underline{\Omega}\geq 0} \hat{n}\cdot\underline{\Omega}\phi(\underline{r},E,\underline{\Omega},t)d\Omega \qquad (22)$$

Similarly, those going in the opposite direction become

$$J_-(\underline{r},E,t) = \int_{\hat{n}\cdot\underline{\Omega}\leq 0} (-\hat{n}\cdot\underline{\Omega})\phi(\underline{r},E,\underline{\Omega},t)d\Omega \qquad (23)$$

We can define the vector $\underline{J}(\underline{r},E,t)$ such that

$$\hat{n}\cdot\underline{J}(\underline{r},E,t) = J_+(\underline{r},E,t) - J_-(\underline{r},E,t) = \hat{n}\cdot\int_{\underline{\Omega}} \underline{\Omega}\phi(\underline{r},E,\underline{\Omega},t)d\Omega \qquad (24)$$

which is consistent with (19), and allows us to interpret

$$\hat{n}\cdot\underline{J}(\underline{r},E,t)dEdA\Delta t$$
$$= \text{ net no. neutrons in dE about E crossing dA from '-' to '+' during } \Delta t \qquad (25)$$

The difference between $\hat{n}\cdot\underline{J}$ and J_+ is the word net.

III. One-Speed Transport Equation

Suppose we are not particularly interested in the variation of the neutron distributions in time or energy. We can then eliminate these variables by going to a reduced distribution. To eliminate t we simply require the system to be stationary, i.e., $\partial n/\partial t = 0$. To eliminate E we can assume all the neutrons have the same energy, say E_o. This is equivalent to taking

$$\phi(\underline{r},E,\underline{\Omega}) = \phi(\underline{r},\underline{\Omega})\delta(E-E_o) \qquad (26)$$

$$F(E'\underline{\Omega}'\to E\underline{\Omega}) = F(\underline{\Omega}'\to\underline{\Omega})\delta(E-E_o) \qquad (27)$$

$$f(E) = \delta(E-E_o) \qquad (28)$$

$$\Sigma(E) = \Sigma \text{, a constant} \qquad (29)$$

Here $\delta(x)$ is the Dirac delta function – it is zero everywhere except at the point where its argument vanishes, and there its value is infinite. Some properties of $\delta(x)$ are:

$$\int_{a-\varepsilon}^{a+\varepsilon}\delta(x-a)dx = 1, \qquad \int_{a-\varepsilon}^{a+\varepsilon} f(x)\delta(x-a)dx = f(a) \qquad (30)$$

$$\delta(x) = \delta(-x), \qquad x\delta(x) = 0, \qquad \delta(ax) = \frac{1}{a}\delta(x) \qquad (31)$$

Inserting (26) – (29) into the transport equation (18) and integrating over E, we get

$$[\Sigma_t + \underline{\Omega}\cdot\underline{\nabla}]\phi(\underline{r},\underline{\Omega}) = \frac{\nu\Sigma_f}{4\pi}\int_{\underline{\Omega}'} d\underline{\Omega}'\phi(\underline{r},\underline{\Omega}') + S(\underline{r},\underline{\Omega}) + \Sigma_s\int_{\underline{\Omega}'} d\Omega'\phi(\underline{r},\underline{\Omega}')F(\underline{\Omega}'\to\underline{\Omega}) \qquad (32)$$

This is the one-speed, time-independent transport equation. It can be simplified further if we restrict our attention to a slab system (system is infinite in two directions and finite in the third, or x, direction). Let the angle between $\underline{\Omega}$ and the x-axis be the polar angle θ. Then,

$$\underline{\Omega}\cdot\underline{\nabla}\phi = \mu\frac{\partial\phi}{\partial x} + \sin\theta\cos\varphi\frac{\partial\phi}{\partial y} + \sin\theta\sin\varphi\frac{\partial\phi}{\partial z} \tag{33}$$

We then integrate over y and z, and the azimuthal angle φ to obtain

$$[\mu\frac{\partial}{\partial x} + \Sigma_t]\phi(x,\mu) = \frac{\nu\Sigma_2}{2}\int_{-1}^{1} d\mu'\phi(x,\mu') + \Sigma_s\int_{-1}^{1} d\mu'\phi(x,\mu')F(\mu_o) + S(x,\mu) \tag{34}$$

where

$$\phi(x,\mu) = \iint dydz\int_0^{2\pi} d\varphi\phi(xyz\mu\varphi) \tag{35}$$

and $\mu = \cos\theta$, and we have put $F(\underline{\Omega}'\to\underline{\Omega}) = F(\underline{\Omega}\cdot\underline{\Omega}') \equiv \frac{1}{2\pi}F(\mu_o)$. Eq.(34) is the one-speed transport equation for a slab. It is the simplest transport equation which one can consider. It is however still as rigorous as the original transport equation since we have no approximations in the reduction. Eq.(34) can be solved in an infinite-medium problem or in problems involving boundaries. These solutions are useful mainly for checking approximate solutions and also in cases where energy dependence is of no interest.

IV. The P_1 Approximation in Transport Theory

Eq. (34) is still an integro-differential equation that cannot be solved easily. One of the most common methods of extracting a more tractable description of transport is to expand the distribution function in a series of angular functions and then truncate the series. This is reminiscent of what the use of partial wave expansion as a means of reducing the Schroedinger equation to a more manageable form. For this discussion we can ignore the fission without any loss of generality. We write

$$\phi(x,\mu) = \sum_{\ell=0}^{\infty}\frac{2\ell+1}{2}\phi_\ell(x)P_\ell(\mu) \tag{36}$$

$$F(\mu_o) = \sum_{\ell=0}^{\infty}\frac{2\ell+1}{2}F_\ell P_\ell(\mu_o) \tag{37}$$

where $P_\ell(\mu)$ is the ℓth order Legendre polynomial. This expansion leads to an infinite set of coupled equations for the functions

$$\phi_\ell(x) = \int_{-1}^{1} d\mu P_\ell(\mu)\phi(x,\mu) \tag{38}$$

$$F_\ell = \int_{-1}^{1} d\mu P_\ell(\mu) F(\mu) \tag{39}$$

The first two such equations are

$$\frac{d\phi_1(x)}{dx} + \Sigma_t \phi_o(x) = \Sigma_s F_o \phi_o(x) + S_o(x) \tag{40}$$

$$\frac{2}{3}\frac{d\phi_2(x)}{dx} + \frac{1}{3}\frac{d\phi_o(x)}{dx} + \Sigma_t \phi_1(x) = \Sigma_s F_1 \phi_1(x) \tag{41}$$

If somehow we are justified in ignoring the term containing $\phi_2(x)$, then we would have a closet set of equations with which we solve for the flux coefficients, ϕ_o and ϕ_1,

$$\frac{d\phi_1(x)}{dx} + (\Sigma_t - \Sigma_s F_o)\phi_o(x) = S_o(x) \tag{42}$$

$$\frac{1}{3}\frac{d\phi_o(x)}{dx} + (\Sigma_t - \Sigma_s F_1)\phi_1(x) = 0 \tag{43}$$

The truncation of the Legendre polynomial expansion at ℓ=1 is called the P_1 approximation. In general, retaining the N+1 terms in the series leads to a coupled set of N+1 equations – the P_N approximation.

The two scattering kernel coefficients which appear in the P_1 equations have quite simple meanings,

$$F_o = \int_{-1}^{1} d\mu F(\mu) = 1 \qquad \text{(particle conservation)} \tag{44}$$

$$F_1 = \int_{-1}^{1} d\mu \mu F(\mu) = <\mu> \tag{45}$$

An immediate consequence of the P_1 approximation is that we obtain a relation between the current and the gradient of the flux from (43),

$$\phi_1(x) = -\frac{1}{3}[\Sigma_t - \Sigma_s <\mu>]^{-1} \frac{d\phi_o(x)}{dx} \tag{46}$$

where ϕ_0 and ϕ_1 are the neutron flux distribution in position space (position flux) and the neutron net current, respectively. Such a relation defines a transport coefficient, in this case, the neutron diffusion coefficient,

$$D = [3(\Sigma_t - \Sigma_s < \mu >)]^{-1} \tag{47}$$

Eq.(46) is the P1 approximation to the Fick's law of diffusion, generally written as

$$\underline{J} = -D\underline{\nabla}\phi \tag{48}$$

This relation is also well known in the kinetic theory of gases, with one difference. In neutron transport, the diffusion coefficient has dimension of cm, whereas in kinetic theory its dimension would be cm^2/sec. This distinction arises from a factor of the thermal speed, that is, in kinetic theory one uses number density rather than flux.

If absorption is weak, $\Sigma_a / \Sigma_t << 1$, the diffusion coefficient simplifies to

$$D \approx \frac{1}{3\Sigma_s(1 - < \mu >)} \equiv \frac{1}{3\Sigma_{tr}} \tag{49}$$

with Σ_{tr} being an effective 'transport cross section'. Since $< \mu >$ is average of the cosine of the scattering angle in LCS, it would have a larger value if the scattering were preferentially biased in the forward direction. Then D and the net current would increase as one would intuitively expect. On the hand, if the medium has a large scattering cross section, D would decrease since the neutron would be scattered more frequently thus impeding its forward progress. These simple physical interpretations apply to neutron diffusional transport as well as particle diffusion in general. Another remark is that we can go back to the transport equation without making the P1 approximation, and derive a Fick's law relation between the current and the flux gradient. This however would take us beyond the scope of the present discussion.

V. Neutron Diffusion Theory

When one is interested only in the spatial distribution of the neutrons and not in the direction of their travel, we can simplify the transport equation by eliminating (integrating out) the $\underline{\Omega}$ dependence. When we integrate (18) over $\underline{\Omega}$, we get an equation with two unknowns,

$$\phi(\underline{r}, E, t) = \int d\Omega \phi(\underline{r}, E, \underline{\Omega}, t) \tag{50}$$

$$\underline{J}(\underline{r}, E, t) = \int d\Omega \underline{\Omega} \phi(\underline{r}, E, \underline{\Omega}, t) \tag{51}$$

Now we invoke Fick's law, (40), to eliminate J, thus obtaining

$$\frac{1}{v}\frac{\partial\phi(\underline{r},E,t)}{\partial t} = [D(E)\nabla^2 - \Sigma_t(E)]\phi(\underline{r},E,t) + S(\underline{r},E,t) +$$

$$\nu f(E)\int dE'\Sigma_f(E')\phi(\underline{r},E',t) + \int dE'\Sigma_s(E')\phi(\underline{r},E',t)F(E'\to E) \qquad (52)$$

To reduce further, we will again consider only steady-state solutions, and integrate over all energy, arriving at

$$[\overline{D}\nabla^2 + (\nu\overline{\Sigma}_f - \overline{\Sigma}_a)]\phi(\underline{r}) = -S(\underline{r}) \qquad (53)$$

where

$$\phi(\underline{r}) = \int dE\phi(\underline{r},E) \qquad (54)$$

$$\overline{D} \equiv \frac{\int dED(E)\phi(\underline{r},E)}{\int dE\phi(\underline{r},E)} \qquad (55)$$

and a similar expression like (55) for $\overline{\Sigma}$. In writing (53) we have made use of the statement of neutron conservation,

$$\int dEF(E'\to E) = 1 \qquad (56)$$

We should also keep in mind that in (53) we are assuming that the external source is time-independent, and more significantly that $\overline{D}$ is independent of position, which would be the case if $\phi(\underline{r},E)$ were separable in $\underline{r}$ and E (generally, this is not true).

Eq.(53) is a simple, in the sense that all the coefficients are constants, second order differential equation. The problem of solving for the position flux $\phi(\underline{r})$ is now analogous to solving the Schroedinger equation for the wave function, and all the mathematical machinery developed in quantum mechanics is thus applicable to nuclear reactor theory. We will next discuss the appropriate boundary conditions which one should apply in neutron diffusion; to keep the notations simple we will drop the overhead bar on the material constants with implicit understanding that they are energy averaged quantities.

Boundary Conditions

The boundary conditions to be imposed on $\phi(\underline{r})$ are quite similar, with perhaps one exception, to those imposed on the wave function in solving the Schroedinger equation. Because we are dealing with a physical quantity, the neutron distribution in space, $\phi(\underline{r})$ must be positive and finite everywhere or zero. Also the distribution must reflect the symmetry of the problem, such as $\phi(x) = \phi(-x)$ in a slab system with x = 0 being at the center of the slab. Then there are the usual boundary conditions at a material interface,

where flux and currents must be continuous since there are no sources or sinks at such interfaces. All these conditions have counterparts in solving the wave equation.

The one boundary condition which requires some discussion is the statement of no re-entrant current across the boundary between a medium and vacuum. Let this surface be located at the position x = x_o in a slab geometry. The physical condition is $J_-(x_o) = 0$. We can calculate this using the definition of J_- given in (23). By assuming isotropic scattering in LCS, no absorption, and slowly varying flux, one finds

$$J_-(x_o) = \frac{\phi(x_o)}{4} + \frac{D}{2}\left(\frac{d\phi}{dx}\right)_{x_o} \tag{57}$$

or

$$\left(\frac{d\phi}{dx}\right)_{x_o} = -\frac{1}{2D}\phi(x_o) \tag{58}$$

Eq.(58) is not really a bona-fide condition on $\phi(x_o)$ because the gradient $d\phi/dx$ is not known. To find another relation between the flux and gradient, we interpret the latter as a finite difference,

$$\left(\frac{d\phi}{dx}\right)_{x_o} = -\frac{\phi(x_o) - \phi(x')}{x' - x_o} \qquad x' > x_o \tag{59}$$

where we use the negative sign because we know the gradient must be negative. Now we choose x' such that we know the value of the flux at this position. How is this possible? Suppose we choose x' to be the distance where the flux linearly extrapolates from x = x_o to zero. Calling this distance x' = x_o + d, we then have from (59)

$$\left(\frac{d\phi}{dx}\right)_{x_o} = -\frac{1}{d}\phi(x_o) \tag{60}$$

Combining this with (58) we obtain for the extrapolated distance d = 2D. Conventionally one often applies the simpler mathematical (and approximate) condition of

$$\phi(x_o + 2D) = 0 \tag{61}$$

instead of the physical condition of no re-entrant current. One can use transport theory to do a better calculation of the extrapolated distance d, which is 2D or $2/3\Sigma_{tr}$ in simple diffusion theory. The result, when there is no absorption, is $0.71/\Sigma_{tr}$, the difference is generally not so significant.

Diffusion Kernels (Green's Functions)

One can solve the neutron diffusion equation for the flux shape corresponding to various localized sources. This is tantamount to the standard problem of finding the Green's function for a point source and then integrating the result to obtain solutions for other simple source distributions. Since this kind of calculations is well described in the standard references, we will give only some of the results here.

Consider a plane source at x = 0 in an infinite medium which emits isotropically s_o neutrons/cm^2/sec. The diffusion equation reads

$$\left[\frac{d^2}{dx^2} - \kappa^2\right]\phi_{pl}(x) = 0 \qquad x \neq 0 \tag{62}$$

with $\kappa^2 = \Sigma_a / D > 0$ (κ is real). The solution for the case of plane source is

$$\phi_{pl}(x) = \frac{s_o}{2D\kappa} e^{-\kappa|x|} \tag{63}$$

Suppose now instead of a plane source we have a point source at the origin emitting s_o neutrons/sec. The equation becomes

$$(\nabla^2 - \kappa^2)\phi_{pt}(r) = 0 \qquad r \neq 0 \tag{64}$$

with solution

$$\phi_{pt}(r) = \frac{s_o}{4\pi r D} e^{-\kappa r} \tag{65}$$

Comparison of (63) and (65) suggests that the two kernels are related, and that one can be obtained from the other. This connection is actually quite general and follows directly from the property of the Green's function. Since the diffusion equation is linear, one can superpose the contributions from different point sources to make the solution to any distributed source,

$$\phi(\underline{r}) = \frac{1}{s_o}\int d^3 r' \, s(\underline{r}')\phi_{pt}(|\underline{r} - \underline{r}'|) \tag{66}$$

Applying this to the plane source distribution, one obtains

$$\phi_{pl}(x) = \int_{-\infty}^{\infty} dz \delta(z) \int_0^{\infty} \rho d\rho \int_0^{2\pi} d\varphi \phi_{pt}(\sqrt{x^2 + \rho^2}) \tag{67}$$

where the integral is written out in cylindrical coordinates with x being the perpendicular distance from the source plane. Carrying out the integrations, one finds

$$\phi_{pl}(x) = 2\pi \int_x^\infty d\gamma \gamma \phi_{pt}(\gamma) \tag{68}$$

which one can verify is consistent with (63) and (65). One can invert (68) by differentiating to give

$$\phi_{pt}(r) = -\frac{1}{2\pi}\left[\frac{d\phi_{pl}(x)}{dx}\right]_{x=r} \tag{69}$$

The relation (68) also helps us to understand why is point source kernel is singular at the origin and yet the plane source kernel is not singular anywhere.

The Concept of Buckling in Criticality

We now return to the problem of criticality and show how diffusion theory can be used to estimate the nonescape probabilities that appear in the multiplication constant. To do this it is instructive to ask what could be a measure of the reactor size besides the bare system dimensions. Recall that the extrapolated boundary condition, such as (61), expresses the idea of an extrapolated distance as an incremental length beyond the actual system boundary. Thus it is not surprising that a useful geometric measure of system size should involve the extrapolated distance. How does this come about naturally in the context of boundary conditions for solving the diffusion equation? We will examine this connection through the example of a critical spherical reactor, a system in which the materials properties and the geometric size are in balance such that its multiplication constant is unity.

Consider a spherical reactor of radius R composed of materials for which all the cross sections, scattering, absorption, and fission, are nonzero, and there is no external source. The diffusion equation for this system is

$$(\nabla^2 + \alpha^2)\phi(\underline{r}) = 0 \qquad r \le R \tag{70}$$

with $\alpha^2 = (\nu\Sigma_f - \Sigma_a)/D$ >0. (Note $\alpha^2 \le 0$ means at best k_∞ = 1, and any finite system must therefore be subcritical, i.e., cannot maintain a non-zero steady state flux in the absence of a source.). The physical solution of (70), after applying the condition of finite flux at the origin, is just

$$\phi(\underline{r}) = A\frac{\sin \alpha r}{r} \tag{71}$$

We also can conclude that A must be positive and that αR must be $\le \pi$. We can apply one more boundary condition, that at the reactor surface r = R. Since (70) is a homogeneous equation, we know that we will not be able to determine A. Thus the

condition at R has to impose a constraint on α, the only other constant left in the description. (The analogy with energy quantization in quantum mechanics when solving the wave equation for a certain shape of the potential should be quite apparent at this point.)

We have already seen that the proper boundary condition for a material-vacuum interface is no re-entrant current, $J_-(R) = 0$. In diffusion theory this is approximately

$$\frac{\phi(R)}{4} + \frac{D}{2}\hat{n}\cdot\nabla\phi\Big|_{r=R} = 0, \qquad \text{or} \quad \frac{R}{\phi}\frac{d\phi}{dr}\Big|_{r=R} = -\frac{R}{2D} \tag{72}$$

Applying this to (71) gives

$$1 - \alpha R\cot\alpha R = \frac{R}{2D} \tag{73}$$

The solution to (73), $\alpha_o R$, is seen to depend on the magnitude of the ratio R/2D, close to zero if R << 2D and close to π if R >> 2D. The latter is the more physically common situation for any interesting value of D, i.e., reactor material. So we write $\alpha_o R = \pi - \varepsilon$, with ε being small. The left hand side of (73) then becomes

$$1 - \alpha_o R\cot\alpha_o R \approx 1 + \frac{\pi - \varepsilon}{\varepsilon} = \frac{\pi}{\varepsilon} = \frac{\pi}{\pi - \alpha_o R} \tag{74}$$

and since R>>2D, (73) can be rearranged to give

$$\alpha_o \approx \frac{\pi}{\tilde{R}} \equiv B_g \tag{75}$$

with $\tilde{R}$ being the 'extrapolated' radius,

$$\tilde{R} \equiv R + 2D \tag{76}$$

Thus we arrive at the same result as in the case of the slab reactor before, one can apply the surface boundary condition as $\phi(\tilde{R}) = 0$, rather than $J_-(R) = 0$. Eq. (75) also serves to introduce the quantity B_g, called 'geometric buckling' in reactor physics, presumably because it has to do with the shape ("buckling") of the flux and it depends only on the size (geometry) of the system.

The implication of (75) is that in order for the critical spherical reactor to have a physical solution satisfying the boundary conditions in diffusion theory, the constant α has to have the value specified by (75). However, recall that in writing the diffusion equation

(70), the constant α already was defined by the materials properties. We will rewrite this definition as

$$\alpha^2 = \frac{\nu\Sigma_f - \Sigma_a}{D} \equiv B_m^2 \tag{77}$$

thereby introducing the quantity B_m, 'materials buckling', in analogy with the geometric buckling. Therefore, the only way to satisfy both the materials constraint, represented by (70) and (77), and the system size constraint, represented by (71) and (75), is to require

$$B_m^2 \equiv B_g^2 \tag{78}$$

which we can regard as the condition for system criticality, the balance between materials properties and system size. To see what this relation can lead to, we rewrite it as

$$\Sigma_a \left(\frac{\nu\Sigma_f}{\Sigma_a} - 1 \right) = DB_g^2 \tag{79}$$

or,

$$\frac{\eta f}{1 + L^2 B_g^2} = 1 \tag{80}$$

with $\nu\Sigma_f / \Sigma_a \equiv \eta f$ and $L^2 \equiv D / \Sigma_a$, L being called the diffusion length. We purposely write (80) in the form of a critical condition, explicitly showing the multiplication constant $k = k_\infty P_{NL}$ having the value of unity. With this identification we can pick off an expression for the non-leakage probability,

$$P_{NL} \equiv \frac{1}{1 + L^2 B_g^2} \tag{81}$$

Eq.(81) is useful because it provides a quick estimate, in the context of simple diffusion theory, of the non-escape probability that appears in the multiplication constant. Going back to (78), we see that another way to interpret the balance condition is the requirement

$$\nu\Sigma_f - \Sigma_a = DB_g^2 \tag{82}$$

The left hand side represents the effective cross section for 'neutron gain', whereas the right hand side represents the 'neutron loss', with DB_g^2 playing the role of a 'leakage cross section'. This observation makes it possible to compare the effects of neutron interactions, in the sense of scattering and reactions measured in the form of macroscopic cross sections (or the mean free path), with those of neutron diffusion, in the sense of diffusion and surface boundary condition in terms of D and the geometric buckling, on

the same basis. An appreciation of this simple equivalence is a primary reason that we can give for studying neutron diffusion theory.