

22.54 Neutron Interactions and Applications (Spring 2004)

Lecture 10 (3/17/05)

Neutron Diffusion

References --

J. R. Lamarsh, *Introduction to Nuclear Reactor Theory* (Addison-Wesley, Reading, 1966)

To study neutron diffusion we go back to the neutron transport equation and obtain an equation only in the spatial variable. We first eliminate the $\underline{\Omega}$ dependence by integrating the transport equation over $\underline{\Omega}$, getting an equation with two unknowns,

$$\phi(\underline{r}, E, t) = \int d\Omega \phi(\underline{r}, E, \underline{\Omega}, t) \quad (10.1)$$

$$\underline{J}(\underline{r}, E, t) = \int d\Omega \underline{\Omega} \phi(\underline{r}, E, \underline{\Omega}, t) \quad (10.2)$$

Then we invoke Fick's law to eliminate \underline{J} , thus obtaining

$$\frac{1}{v} \frac{\partial \phi(\underline{r}, E, t)}{\partial t} = [D(E)\nabla^2 - \Sigma_r(E)]\phi(\underline{r}, E, t) + S(\underline{r}, E, t) + \nu f(E) \int dE' \Sigma_f(E') \phi(\underline{r}, E', t) + \int dE' \Sigma_s(E') \phi(\underline{r}, E', t) F(E' \rightarrow E) \quad (10.3)$$

To reduce further, we consider only steady-state solutions, and integrate over all energy to arrive at

$$[\overline{D}\nabla^2 + (\nu\overline{\Sigma}_f - \overline{\Sigma}_a)]\phi(\underline{r}) = -S(\underline{r}) \quad (10.4)$$

where

$$\phi(\underline{r}) = \int dE \phi(\underline{r}, E) \quad (10.5)$$

$$\bar{D} \equiv \frac{\int dE D(E) \phi(\underline{r}, E)}{\int dE \phi(\underline{r}, E)} \quad (10.6)$$

and a similar expression like (10.6) for the macroscopic cross section $\bar{\Sigma}$. The overhead denotes energy average weighed by the flux as indicated in (10.6) (see also (8.17)). In writing (10.4) we have made use of the statement of neutron conservation,

$$\int dE F(E' \rightarrow E) = 1 \quad (10.7)$$

We need to keep in mind that in (10.4) we are also assuming that the external source is time-independent, and more significantly that \bar{D} is independent of position, which would be the case if $\phi(\underline{r}, E)$ were separable in \underline{r} and E (this is not true in general).

Eq.(10.4) is a second-order differential equation with constant coefficients. Since the *Schrödinger* equation, in the case of constant potential, is also of this form, it is worthwhile to make note of the analogy between the problem of neutron diffusion and the problem of a particle confined in a potential well, particularly in the role of the boundary conditions. To keep the notations simple we will drop the overhead bar on the material constants with the understanding that they are to be regarded as energy averaged quantities.

Boundary Conditions

The boundary conditions to be imposed on $\phi(\underline{r})$ are quite similar to those imposed on the wave function in solving the *Schrödinger* 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; 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 $x = x_0$ in a slab geometry. The physical condition is $J_-(x_0) = 0$. While the definition of J_- given in Eq. (8.10), is perfectly correct, we can evaluate J_- according to its physical meaning and by making the assumptions that the scattering is isotropic in LCS, the medium is non absorbing, and the flux is slowly varying. Then J_- is approximately given by the following integral (see Fig. 1),

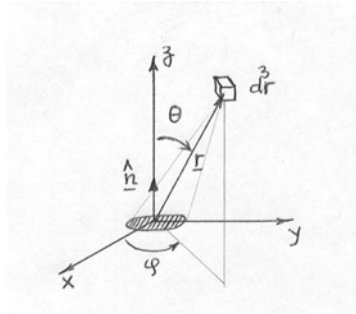


Fig. 1. The geometrical set up for estimating the current of neutrons crossing a unit area A at the origin (with normal \hat{n}) after scattering isotropically in the volume element d^3r about \underline{r} . (Adapted from Lamarsh, p. 126.)

$$\hat{z} \cdot \underline{J}_- = \int_{uhs} \Sigma_s \phi(\underline{r}) \left(\frac{A \cos \theta}{4\pi r^2} \right) e^{-\Sigma_t r} d^3r \quad (10.8)$$

where the integral extends over the upper half space (uhs) of the medium because we are interested in all those neutrons which can cross the unit area A from above (in the direction opposite to the unit normal). The part of the integrand in the parenthesis is fraction of neutron going through the unit area A if there were no collisions along the way, with A being subtended at an angle θ from the elemental volume d^3r at \underline{r} . The fact that neutrons can collide on the way to the unit area is taken into account by the factor $\exp(-\Sigma_t r)$. To carry out the indicated integral we need to know $\phi(\underline{r})$. Since we have assumed the flux is slowly varying we can expand about the origin (the location of the unit area) and keep only the first term in the expansion,

$$\phi(\underline{r}) \square \phi(0) + \underline{r} \cdot \underline{\nabla} \phi \Big|_o \quad (10.9)$$

Then,

$$J_-^z(0) = \frac{\Sigma_s}{4\pi} \int_{\varphi=0}^{2\pi} d\varphi \int_{\theta=0}^{\pi/2} \cos\theta \sin\theta d\theta \int_0^{\infty} dr e^{-\Sigma_t r} [\phi_o + x(\partial\phi/\partial x)_o + y(\partial\phi/\partial y)_o + z(\partial\phi/\partial z)_o] \quad (10.10)$$

where we have taken $A = 1$. Writing out the Cartesian component x , y and z in terms of the spherical coordinates (r, θ, φ) , $x = r \sin\theta \cos\varphi$, $y = r \sin\theta \sin\varphi$ and $z = r \cos\theta$, we find the φ -integration renders the terms containing x or y equal to zero. The term containing z can be easily integrated to give (after shifting the unit area from being at the origin as in Fig. 1 to a slab geometry with the unit area on the surface at $x = x_o$)

$$J_-(x_o) = \frac{\phi(x_o)}{4} + \frac{D}{2} \left(\frac{d\phi}{dx} \right)_{x_o} \quad (10.11)$$

or

$$\left(\frac{d\phi}{dx} \right)_{x_o} = -\frac{1}{2D} \phi(x_o) \quad (10.12)$$

Eq.(10.12) 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,

$$\left(\frac{d\phi}{dx} \right)_{x_o} = -\frac{\phi(x_o) - \phi(x')}{x' - x_o} \quad x' > x_o \quad (10.13)$$

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 $x = x_0$ to zero. Calling this distance $x' = x_0 + \delta$ (see Fig. 2), we then have from (10.13)

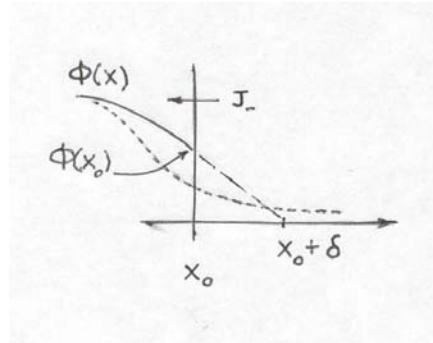


Fig. 2. Schematic of the extrapolated boundary condition, with δ being the distance beyond the actual boundary where a linear extrapolation of the flux at $x = x_0$ would vanish. The dotted curve shows the variation of the flux that would be obtained from transport theory. (Adapted from Lamarsh, p. 135.)

$$\left(\frac{d\phi}{dx} \right)_{x_0} = -\frac{1}{\delta} \phi(x_0) \quad (10.14)$$

Combining this with (10.9) we obtain for the extrapolated distance $\delta = 2D$.

Conventionally instead of the physical condition of no re-entrant current, one often applies the simpler mathematical (and approximate) condition of

$$\phi(x_0 + 2D) = \phi(\tilde{x}_0) = 0 \quad (10.15)$$

where $\tilde{x}_0 = x_0 + 2D$. Eq.(10.15) is called the extrapolated boundary condition; it is commonly adopted because of its simplicity. One can use transport theory to do a better calculation of the extrapolated distance δ . We have seen that in simple diffusion theory this turns out to be $2D$, or $2/3\Sigma_{tr}$. The transport theory result, when there is no absorption, is $0.71/\Sigma_{tr}$. The rather small difference between diffusion theory and transport theory should not be taken to mean that the flux near the surface is always

accurately given by diffusion theory. As can be seen in Fig. 2, diffusion theory typically overestimates the flux at the surface relative to transport theory.

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_0 neutrons/cm²/sec. The diffusion equation reads

$$\left[\frac{d^2}{dx^2} - \kappa^2 \right] \phi_{pl}(x) = 0 \quad x \neq 0 \quad (10.16)$$

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

$$\phi_{pl}(x) = \frac{s_0}{2D\kappa} e^{-\kappa|x|} \quad (10.17)$$

where we have applied the source condition,

$$[AJ(x)]_{x \rightarrow x_0} = D[d\phi(x)/dx]_{x \rightarrow x_0} = s_0/2 \quad (10.18)$$

with A being a unit area. Eq.(10.18) is simply the statement that if s_0 is the number of neutrons emitted per unit area per sec by the plane, then half of the neutrons would come out in the +x direction.

Suppose now instead of a plane source we have a point source at the origin emitting s_0 neutrons/sec. The equation becomes

$$(\nabla^2 - \kappa^2)\phi_{pt}(r) = 0 \quad r \neq 0 \quad (10.19)$$

with solution

$$\phi_{pt}(r) = \frac{S_o}{4\pi r D} e^{-\kappa r} \quad (10.20)$$

Comparison of (10.17) and (10.20) 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,

$$\phi(\underline{r}) = \frac{1}{S_o} \int d^3r' s(\underline{r}') \phi_{pt}(|\underline{r} - \underline{r}'|) \quad (10.21)$$

Applying this to the plane source distribution, one obtains

$$\phi_{pt}(x) = \int_{-\infty}^{\infty} dz \delta(z) \int_0^{\infty} \rho d\rho \int_0^{2\pi} d\phi \phi_{pt}(\sqrt{x^2 + \rho^2}) \quad (10.22)$$

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

$$\phi_{pt}(x) = 2\pi \int_x^{\infty} d\gamma \gamma \phi_{pt}(\gamma) \quad (10.23)$$

which one can verify is consistent with (10.17) and (10.20). One can invert (10.23) by differentiating to give

$$\phi_{pt}(r) = -\frac{1}{2\pi} \left[\frac{d\phi_{pt}(x)}{dx} \right]_{x=r} \quad (10.24)$$

The relation (10.23) also helps us to understand why the point source kernel is singular at the origin and yet the plane source kernel is regular everywhere.

The Concept of Buckling in Nuclear Reactor Criticality

(We recommend the student to first study Chap11 before reading this section, since the concept of criticality is discussed in detail in Chap11.)

We now turn 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 (10.15), 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

$$(\nabla^2 + \alpha^2)\phi(\underline{r}) = 0 \quad r \leq R \quad (10.25)$$

with $\alpha^2 = (v\Sigma_f - \Sigma_a)/D > 0$. (Note $\alpha^2 \leq 0$ means at best $k_\infty = 1$, and any finite system must therefore be subcritical, i.e., the system cannot maintain a non-zero steady state flux in the absence of a source.). The physical solution to (10.25), after applying the condition of finite flux at the origin, is just

$$\phi(r) = A \frac{\sin \alpha r}{r} \quad (10.26)$$

We also can conclude that A must be positive and that αR must be $\leq \pi$. We can apply one more boundary condition, that at the reactor surface $r = R$. Since (10.26) 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

$$\frac{\phi(R)}{4} + \frac{D}{2} \hat{n} \cdot \nabla \phi \Big|_{r=R} = 0, \quad \text{or} \quad \frac{R}{\phi} \frac{d\phi}{dr} \Big|_{r=R} = -\frac{R}{2D} \quad (10.27)$$

Applying this to (10.26) gives

$$1 - \alpha R \cot \alpha R = \frac{R}{2D} \quad (11.28)$$

The solution to (10.28), $\alpha_o R$, is seen to depend on the magnitude of the ratio $R/2D$, close to zero if $R \ll 2D$ and close to π if $R \gg 2D$. 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 (10.28) then becomes

$$1 - \alpha_o R \cot \alpha_o R \approx 1 + \frac{\pi - \varepsilon}{\varepsilon} = \frac{\pi}{\varepsilon} = \frac{\pi}{\pi - \alpha_o R} \quad (10.29)$$

Noting that

$$\alpha_o = (\pi - \varepsilon) / R = (\pi / R)(1 - \varepsilon / \pi) \square (\pi / R)(1 + \varepsilon / \pi)^{-1} \quad (10.30)$$

From (10.29) and (10.28) we also have

$$\frac{\pi}{\varepsilon} = \frac{R}{2D}, \text{ or } R\varepsilon / \pi = 2D \quad (10.31)$$

Combining (10.30) and (10.31) we thus obtain

$$\alpha_o \sim \pi / \tilde{R} \equiv B_g \quad (10.32)$$

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

$$\tilde{R} \equiv R + 2D \quad (10.33)$$

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. (10.32) 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 (10.32) 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 (10.32). However, recall that in writing the diffusion equation (10.25), the constant α already was defined by the materials properties. We will rewrite this definition as

$$\alpha^2 = \frac{\nu\Sigma_f - \Sigma_a}{D} \equiv B_m^2 \quad (10.34)$$

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 (10.25) and (10.32), and the system size constraint, represented by (10.29) and (10.32), is to require

$$B_m^2 \equiv B_g^2 \quad (10.35)$$

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

$$\Sigma_a \left(\frac{\nu \Sigma_f}{\Sigma_a} - 1 \right) = DB_g^2 \quad (10.36)$$

or

$$\frac{\eta f}{1 + L^2 B_g^2} = 1 \quad (10.37)$$

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 (10.37) 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,

$$P_{NL} \equiv \frac{1}{1 + L^2 B_g^2} \quad (10.38)$$

Eq.(10.38) 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 (10.36), we see that another way to interpret the balance condition is the requirement

$$\nu\Sigma_f - \Sigma_a = DB_g^2 \quad (10.39)$$

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.