APPENDIX C

MOMENTS METHOD
FOR NEUTRONS

The moments method has been extensively applied to the calculation of neutron densities in shields, and we shall treat this application here. This application has the same advantages and disadvantages as in problems involving photons. Of the various terms of the Boltzmann equation, only the scattering integral for neutrons differs from that for photons. The scattering integrals differ for several reasons: First, neutron scattering is largely isotropic in the center-of-mass system, whereas photon scattering is rather anisotropic. Second, reasonably simple analytical expressions exist for the energy dependence of gamma ray scattering, whereas only very complicated graphical, empirical data exist describing the energy dependence of neutron scattering. Third, the dependence of gamma ray scattering upon atomic properties is provided by relatively simple analytic expressions, whereas each nuclide must be considered separately in determining neutron scattering.

The moments method for neutron attenuation proceeds exactly like that for gamma rays. Since neutrons of different speeds are now being taken into account, the flux depends upon the speed of the neutrons, and the scattering integral includes an integral over all possible speeds of the incident neutrons. In place of Eq. (5.1.1), we then have

\[ \Omega \cdot \nabla \phi(r, v, \Omega) + \sigma_t(r, v) \phi(r, v, \Omega) = \tau(r, v, \Omega) + S(r, v, \Omega), \]  

\[ \text{where the scattering integral } \tau(r, v, \Omega) \text{ is given by} \]

\[ \tau(r, v, \Omega) = \int \int dv' d\Omega' \sigma_s(r, \Omega' \rightarrow \Omega, v' \rightarrow v) \phi(r, v', \Omega'); \]

\[ v \text{ and } v' \text{ are the speeds of the scattered and incident neutrons, and the other notation is as before. The quantity } \sigma_s(r, \Omega' \rightarrow \Omega, v' \rightarrow v) \text{ is the} \]
probability that a neutron of speed $v'$ going a unit distance in the
direction $\Omega'$ is scattered to produce a neutron of speed $v$ per unit
speed going in the direction $\Omega$ per unit solid angle. The probability
$\sigma_s(r, \Omega' \to \Omega, v' \to v)$ may be expressed as the product of the prob­
ability $\sigma_s(r, v')$ that a neutron of speed $v'$ in going a unit distance is
scattered and the probability $F(v', v, \theta_0)$ that the scattered neutron has
a speed $v$ per unit speed and is scattered through an angle $\theta_0$ in the
laboratory system per unit solid angle, the scattering being induced by
a neutron of speed $v'$. This latter probability $F(v', v, \theta_0)$ is in turn the
product of the probability $f(v', \theta_0)$ that the neutron is scattered through
the angle $\theta_0$ into a unit solid angle and the probability

$$\delta[\cos \theta_0 - g(v', v)] \left[ \frac{d(\cos \theta_0)}{dE} \right] \left[ \frac{dE}{dv} \right]$$

that the neutron scattered into a unit speed has a speed $v$. By Eq. (B.40)

$$g(v', v) = \frac{1 - M}{2} \frac{v'}{v} + \frac{1 + M}{2} \frac{v}{v'} .$$

The Dirac delta function expresses the deterministic constraint
between $v, v'$, and $\theta_0$ imposed by the laws of energy and momentum
conservation, the quantities $v, v'$, and $\theta_0$ being regarded as independent
above. The product $[d(\cos \theta_0)/dE][dE/dv]$ of derivatives merely provides
the transformation needed between a unit increment in $g$ and a unit
speed. Finally, for reasons that appear below, it is convenient to use the
angle $\theta_c$ of scattering in the center-of-mass system, instead of that $\theta_0$
in the laboratory system. Accordingly,

$$f(v', \theta_0) = f(v', \theta_c) \frac{d(\cos \theta_c)}{d(\cos \theta_0)} .$$

By combining all these independent probabilities together, we have

$$\sigma_s(r, \Omega' \to \Omega, v' \to v) =$$

$$\sigma_s(r, v') f(v', \theta_c) \frac{d(\cos \theta_c)}{d(\cos \theta_0)} \delta[\cos \theta_0 - g(v', v)] \left[ \frac{d(\cos \theta_0)}{dE} \right] \left[ \frac{dE}{dv} \right] ,$$

so that

$$\sigma_s(r, v', v) = \sigma_s(r, v') f[v', \theta_c(g)] P(g) \frac{(M + 1)^2}{2ME'} v$$

(C.4)
upon using Eqs. (5.1.5) and (B.12). We may now expand the flux in Legendre polynomials as in Eq. (5.1.5). Proceeding as from Eq. (5.1.1) to (5.1.11), we find for one dimensional geometry that

\[
\frac{l}{(2l + 1)} \frac{\partial \phi_{l+1}(z, v)}{\partial z} + \left( \frac{l + 1}{2l + 1} \right) \frac{\partial \phi_{l+1}(x, v)}{\partial x} + \sigma_l(z, v) \phi_l(z, v) = \int dv' \, \sigma_s(z, v, v') \phi_l(x, v') + S_l(z, v), \tag{C.5}
\]

where the notation is as in Chap. 5.

In our subsequent work, the limits of the scattering integral frequently come into consideration. It simplifies these limits if the cosine of the angle \(\theta\) through which the neutron is scattered in the center-of-mass system is used as the independent variable, instead of the speed \(v'\) of the incident neutron in the laboratory system. Equation (B.12) provides the necessary transformation.

Next, we introduce the flux per unit energy to replace the flux per unit speed. We then find

\[
\frac{l}{(2l + 1)} \frac{\partial \phi_{l-1}(z, E)}{\partial z} + \left( \frac{l + 1}{2l + 1} \right) \frac{\partial \phi_{l+1}(z, E)}{\partial z} + \sigma(z, E) \phi_l(z, E)

= S_l(z, E) + \int d(cos \theta_e) \, P_l(g) \frac{E'}{E} f(E', \theta_e(g)) \sigma_s(z, E') \phi_l(z, E'). \tag{C.6}
\]

Finally, we multiply both sides of this equation with \(z^l\) and integrate from \(-\infty\) to \(+\infty\). With the definition (5.7.5) of the moments and the condition (5.7.13), we find that

\[
\frac{l}{(2l + 1)} \sigma_0 \phi_{l-1,l-1}(E) + \left( \frac{l + 1}{2l + 1} \right) \sigma_0 \phi_{l-1,l+1}(E) - \sigma(v) \phi_{l,l}(E)

+ S_{l,l}(E) + \int d(cos \theta_e) \, P_l(g) \frac{E'}{E} f(E', \theta_e(g)) \sigma_s(E') \phi_{l,l}(E') = 0, \tag{C.7}
\]

where \(\sigma\) and \(\sigma_s\) are independent of position. In this expression the scattering integral is the chief source of difficulty.

Three approximations have been used to treat the scattering integral. In the first, the energy loss of the neutrons at collisions is neglected, in which case the scattering integral reduces to \(\sigma_s(E)\phi_{l,l}(E)\). This approximation is good for the small contributions to moderation due to oxygen when hydrogen is present; when hydrogen is absent, then the approximation is valid for nuclides heavier than iron.
In the second approximation, the scattering integral is expanded in powers of $M^{-1}$. We leave the details of the development as an exercise for the reader. The result is

$$\tau_{i,l}(M) = \sigma_s(E) \phi_{i,l}(E) \left[ \phi_{l}(E) + \frac{l(l + 1)}{2(l + 1)} \left[ \phi_{l-1}(E) - \phi_{l+1}(E) \right] \right] + \frac{4\pi}{M} \times$$

$$\int \frac{d^4 E}{E} f(E',\theta'_s,\phi_s) E' \phi_{i,l}(E') \left[ P_l(\mu) - \frac{lP_{l-1}(\mu) + (l + 1) P_{l+1}(\mu)}{2l + 1} \right].$$

(C.8)

Certaine has developed a more accurate method of dealing with the scattering integral (References 1–3). The method consists of approximating the energy dependent part of the integrand by a sequence of continuous straight line segments. The integral over each such segment can be computed analytically; to this end, recurrence relations for, and starting values of, two different quantities must be developed. The complete integral is then the sum of the subintegrals whose integrands have been approximated by straight lines and whose values have been computed analytically. In other words, the method is very closely akin to Simpson's approximation.

We shall describe only one complete variation of Certaine's method to a degree sufficient to enable the reader to use and understand it. Other variations may be found in References 1–3. Although the algebra is quite tedious, the method is really quite straightforward. This method is applicable to even the lightest nuclides, whereas the other two described above are not. One of the difficulties is that for large $l$, $P_l(E)$ oscillates rapidly.

Certaine's method starts by expanding the collision transfer probability in Legendre polynomials:

$$f(E',\theta_s,\phi_s) = \sum_{l=0}^{\infty} \frac{(2l' + 1)}{2} \phi_{l'}(E) P_l(\mu),$$

(C.9)

where $\mu = \cos \theta'_s$ and $\phi_{l'}(E)$ are the expansion coefficients. The moment of the scattering integral $\tau$ is then given by

$$\tau_{i,l} = \sum_{l'=0}^{\infty} \frac{(2l' + 1)}{2} \int_{-1}^{1} d\mu \phi_{l'}(E) P_l(\mu) \sigma_s(E) \frac{E'}{E} \phi_{i,l}(E').$$

(C.10)

In order to execute Certaine's method, we subdivide the total energy interval from which an incident neutron can produce a scattered neutron
of energy $E$. Because the average lethargy gain of a neutron upon scattering is independent of the lethargy of the incident neutron, we choose subintervals so that they are of equal length $\Delta$ in lethargy. If the lethargy of the scattered neutron is $u$, then the lethargy of the incident neutron may be as high as $u$ or as low as $u - 2 \ln(M + 1)/(M - 1)$. Let us next define the $K$th subinterval by the relation

$$u_{K+1} \leq u - 2 \ln(M + 1)/(M - 1) < u_K.$$

The cosine of the scattering angle in the center-of-mass system then satisfies the relation

$$\mu_0 = 1.$$ 

Further, the lethargy $u_k$ of the $k$th subinterval is given by

$$u_k = u - k\Delta.$$ (C.12)

The part of the integrand of the scattering integral $\tau$ dependent upon the energy of the incident neutron is then approximated by a series of continuous straight line segments:

$$\phi_l(E') \approx \frac{U_{k+1} \Delta}{\Delta} \sum_{k=0}^{K+1} \sum_{l=0}^{K+1} \epsilon_\epsilon(E') \sigma_{l,k} \phi_j,l,k,$$

where

$$U_k = u' - u_k.$$ (C.13)

If this approximation is substituted into the scattering integral, we find that

$$\tau_{l',l,0} = \sum_{k=0}^{K+1} \sum_{l'=0}^{K+1} \epsilon_\epsilon(E') \sigma_{l',k} \phi_j,l,k \tau_{l',l,k},$$ (C.14)

where

$$\tau_{l',l,k} = \frac{(2l' + 1)}{2\Delta} \left[ (1 - \delta_{k,K+1}) \int_{\mu_{k+1}}^{\mu_k} d\mu U_{k+1}(\mu) P_l(\mu) P_l(\mu) \right]$$

$$+ \left[ (1 - \delta_{k,0}) \int_{\mu_{k-1}}^{\mu_k} d\mu U_{k-1}(\mu) P_l(\mu) P_l(\mu) \right].$$ (C.15)

The quantity $U_k$ may be regarded as a function of $\mu$ by (B.12),

$$U_k(\mu) = \ln \left[ \frac{M^2 + 2M\mu + 1}{M^2 + 2M\mu_k + 1} \right].$$ (C.16)
If we knew the \( L_{l,i',k} \), then the moments of the scattering integral could be found and the scattering integral itself computed. From this, we can find the moments of the neutron flux from the relation

\[
\frac{l\sigma_0}{(2l + 1)} \phi_{j-1,i-1,i} + \frac{(l + 1)}{(2l + 1)} \sigma_0 \phi_{j-1,i+1,i} - \sigma_0 \phi_{j,i,i} + S_{j,i,i} + \sum_{l'=0}^{\infty} \sum_{k'=0}^{K+1} g_{l',k,k+i} \sigma_{g,k+i} L_{l',i',k+i} \phi_{j,i',k+i} = 0 \tag{C.17}
\]

by numerical analysis. One starts from the lethargy of the source, which is the lowest lethargy and works upward.

The quantities \( L_{l,i',k} \) must be evaluated. This can be done by means of the recurrence relation

\[
L_{l+1,i',k} = \left( \frac{2l + 1}{l + 1} \right) \sum_{j=0}^{\infty} M_{l',j} L_{l,j,k} - \frac{l}{l + 1} L_{l-1,i',k} \tag{C.18}
\]

where

\[
M_{l',j} = \frac{(2l' + 1)}{2} \int_{-1}^{1} d\mu \ P_{l'}(\mu) P_j(\mu) g \tag{C.19}
\]

and by means of a relation to be given later for \( L_{0,i',k} \) that gives its value explicitly. The relation (C.18) follows directly from the definitions (C.15) and (C.19). It is first noted from Eq. (C.19) that

\[
\frac{(2l' + 1)}{2} g P_{l'}(\mu) = \sum_{j=0}^{\infty} \frac{(2j + 1)}{2} M_{l',j} P_j(\mu).
\]

This result may be used to reduce integrals of the form found in Eq. (C.15)

\[
\frac{(2l' + 1)}{2} \int_{\mu_{k+1}}^{\mu_k} d\mu \ U_k(\mu) P_{l'}(\mu) P_{l+1}(g)
\]

\[
= \left( \frac{2l + 1}{l + 1} \right) \sum_{j=0}^{\infty} M_{l',j} \left( \frac{2j + 1}{2} \right) \int_{\mu_{k+1}}^{\mu_k} d\mu \ U_k(\mu) P_j(\mu) P_l(g)
\]

\[
- \left( \frac{l}{l + 1} \right) \left( \frac{2l' + 1}{2} \right) \int_{\mu_{k+1}}^{\mu_k} d\mu \ U_k(\mu) P_{l'}(\mu) P_{l-1}(g).
\]

Application of the present result to Eq. (C.15) proves the recurrence (C.18).
The $\mathcal{M}_{l',j}$ must be evaluated. Various relations exist for the computation of these quantities. A recurrence relation

$$\mathcal{M}_{l',j+1} = \left(\frac{2j + 1}{j + 1}\right) \left[\left(\frac{l' + 1}{2l' + 1}\right) \mathcal{M}_{l'+1,j} + \left(\frac{l'}{2l' - 1}\right) \mathcal{M}_{l'-1,j}\right] - \left(\frac{j}{j + 1}\right) \mathcal{M}_{l',j-1} \quad (C.20)$$

facilitates the calculation of the $\mathcal{M}_{l',j}$. This result is quickly shown by applying the recurrence relation (D.8) for $m = 0$ twice to the definition (C.19). In addition, we need to know that

$$\nu = -\frac{1}{2} - \frac{1}{4}$$

(C.21)

to calculate $\mathcal{M}_{l',j}$. This result follows immediately from the generating function (D.2) for Legendre polynomials, the orthogonality relation (D.7) for $m = 0$ for these polynomials, the recurrence relation (D.8) for them, and, of course, the definition (C.19).

We return to the evaluation of the $L_{l',l',k}$. So far we have found a recurrence relation (C.18) to evaluate these quantities, and we have evaluated the that occur in this recurrence relation by means of Eqs. (C.20) and (C.21). We need the further relations

$$L_{0,l',k} = \frac{2 - \delta_{k0}}{4M} (2l' + 1) (l + M)^2 \sum_{l=0}^{l'} B_{l,l'} \sum_{j=0}^{l} j! (l-j)! \left[\frac{(1 + M)^2}{2M} e^{-x^2} \right]^j g_x[\Delta(j + 1)], \quad \text{if } k < K, \quad (C.22)$$

and

$$L_{0,0',k} = \frac{2l' + 1}{2} (M - 1)^2 \sum_{l=0}^{l'} B_{l,0'} \sum_{j=0}^{l} j! (l-j)! \left[\frac{(M - 1)^2}{2M} \right]^j g_x[\Delta(j + 1)], \quad \text{if } k = K \text{ or } K + 1, \quad (C.23)$$

where

$$g_0(x) = (e^{-x} - 1 + x)/x^2,$$

$$g_1(x) = (e^{x} - x)/x^2,$$

$$g_x(x) = [1 - 2e^{x} + e^{(q+1)x} + (q - 1)x]/x^2,$$

$$g_{x+1}(x) = (e^{x} - 1 - qx)/x^2; \quad (C.24)$$
\[ b = -\frac{(M^2 + 1)}{2M} \]  \hspace{1cm} (C.25)

\[ q = \frac{2}{A} \ln \left( \frac{M + 1}{M - 1} \right) - K \]  \hspace{1cm} (C.26)

\[ B_{l, l'} = 0, \quad \text{if } l' - l < 0 \text{ or odd} \]  \hspace{1cm} (C.27)

\[ = -\frac{(-)^{l'-l/2}(l' + l)!}{2^l \left( \frac{l' - l}{2} \right)! \left( \frac{l' + l}{2} \right)! l!}, \quad \text{if } l' - l \geq 0 \text{ and even.} \]  \hspace{1cm} (C.28)

The proof of these relations is straightforward and tedious, and follows from Eq. (C.15). The expression

\[ \int_{\alpha_k}^{b_k} d\mu \ U_k(\mu) \mu^l = \frac{(\mu^{l+1} - b^{l+1})}{(l + 1)} U_k(\mu) \bigg|^{b_k}_{\alpha_k} - \sum_{j=0}^{l} \frac{l! b^{l-j} d^{l+1}}{j!(l - j)! (j + 1)^2} \bigg|^{b_k}_{\alpha_k}, \]  \hspace{1cm} (C.29)

where

\[ d = (1 + 2M\mu + M^2)/2M, \]  \hspace{1cm} (C.30)

may be deduced by integrating the left-hand side once by parts and by substituting the expansion

\[ \mu^{l+1} = [d + b]^{l+1} = \sum_{j=0}^{l+1} \frac{(l + 1)! d^j b^{l+1-j}}{j!(l + 1 - j)!}. \]

into the result. The observations

\[ U_k(\mu_k) = 0, \]
\[ U_{k+1}(\mu_k) = \pm \Delta, \]
\[ U_K(-1) = -q\Delta, \]  \hspace{1cm} (C.31)
\[ U_{K+1}(-1) = \Delta(1 - q), \]
\[ d^{l+1}(\mu_k) = \left[ \frac{(1 + M^2)}{2M} \right]^{j+1} e^{-k\Delta(j+1)}, \]
\[ d^{l+1}(\pm 1) = \left[ \frac{(1 \pm M^2)}{2M} \right]^{j+1} \]

follow from Eqs. (C.12), (C.16), (C.26), and (C.30).

\[ P_i(\mu) = \sum_{l' = j}^{l'} B_{l, l'} \mu^{l'} \]
\[ j = 0, \quad \text{if } l' \text{ is even}, \]  \hspace{1cm} (C.32)
\[ j = 1, \quad \text{if } l' \text{ is odd}, \]
follows from the definition (D.1) of Legendre polynomials.

\[ \frac{(±1)^{l+1} - b^{l+1}}{l + 1} = \sum_{j=0}^{l} \frac{l!}{(j + 1)! (l - j)!} \left[ \frac{(M ± 1)^2}{2M} \right]^{j+1} \]  

(C.33)

may be used to write Eq. (C.29) more compactly for the case \( a_k = \mu_1, b_k = 1 \). The conclusions (C.22) and (C.23) are the consequence of introducing the definitions (C.24) into the result (C.29) for various pairs \((a_k, b_k)\),\(^1\) of multiplication of the results by \( B_{l',l} \), of summing over \( l \), and by use of the observations (C.31) through (C.33).

We have now completed our work. The moments may be found from Eq. (C.17), the scattering integrals may be found from Eq. (C.14), and quantities \( L_{l,l'}, k \), \( M_{l',j} \), \( M'_{l'}, 0 \) and \( L_{0,l',k} \) from Eqs. (C.15), (C.20), (C.21), (C.22), and (C.23). The concepts are simple; the execution tedious.

References


\(^1\) The pairs used are \((\mu_1, 1), (\mu_{k+1}, \mu_2), (\mu_{k-1}, \mu_2), (\mu_{K-1}, \mu_K), (-1, \mu_K)\) and \((\mu_K, -1)\).