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AN APPROXIMATE CALCULATION OF THE NEUTRON FLUX IN A THICK SHIELD CONTAINING SOME HEAVY ELEMENTS, WITH THE AID OF CERTAIN RECURRENT RELATIONS BETWEEN THE COEFFICIENTS IN A LEGENDRE SERIES EXPANSION

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REACTOR TECHNOLOGY DIVISION

Reactor Physics Department

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ABSTRACT

The penetration of neutrons through a thick shield is analysed with the aid of the Boltzmann equation. If this is written in the form for a plane source

$$\left(\mu \frac{\partial}{\partial z} + \sigma\right) F = \frac{\overline{Q}}{4\pi} + \frac{\sigma}{4\pi} \sum (2n+1)\ C_n\ F_n\ P_n\ (\mu)$$

corresponding to the expansion of the flux nv in Legendre functions

$$F = \frac{1}{4\pi} \sum (2n+1)\ F_n\ P_n\ (\mu)$$

the Boltzmann equation is equivalent to an infinite set of equations in F_n. For the special case in which the coefficients C_n are independent of the distance z, methods are developed for calculating F_n numerically in terms of the discrete and continuous spectrum of the homogeneous system. If the shield contains some heavy elements, an approximate calculation for the high energy region can be made in which C_n is determined by the elastic scattering from these elements. The calculations are shortened by a systematic use of the recurrence relations.

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In the case of a shield material containing some heavy elements whose nuclei scatter neutrons chiefly in a forward direction, a large number of spherical harmonics may be required to represent the neutron flux at any point of the shield. The analysis of the problem with the aid of determinants of large order may be less useful than a method of calculation based directly on the recurrence relations between the coefficients, and the purpose of this paper is the development of formulas convenient for the solution of a reduced form of the Boltzmann equation of the problem. Some extensions of formulas of Verde and Wick[1/] are derived, and a numerical calculation with the aid of the continuous spectrum of the system of equations is outlined.

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Introduction

If the flux nv per unit solid angle and per unit log energy interval is expanded in a Legendre series

$$F = \frac{1}{4\pi} \sum_{n=0}^{\infty} (2n+1)\, F_n\, P_n\,(\mu)$$

1/ Some stationary distributions of neutrons in an infinite medium, P.R. 71, 852-864 (1947); cf. G. C. Wick, Space distribution of slow neutrons, P.R. 75, 738-756 (1949); also R. E. Marshak, Reviews of Modern Physics 19, 185-238 (1947).

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the Boltzmann equation for the problem with a plane source of neutrons can be written[2/]

$$(1) \quad \left(\mu \frac{\partial}{\partial z} + \sigma\right) F = \frac{\overline{Q}}{4\pi} + \frac{\sigma}{4\pi} \sum_{n=0}^{\infty} (2n+1) \; C_n \, F_n \, P_n(\mu)$$

Here $F = nv$, σ is the total cross section of the material, z is a distance from the plane source, u is the cosine of the angle between the neutron velocity and the z-axis; and C_n is a coefficient which may depend on energy, (and on distance in general) and is defined by the various scattering functions of those nuclei which scatter elastically, as well as on the energy distribution; hydrogen and possibly other light elements are sometimes assumed to function as absorbers for an energy region where σ is considerably increased after the energy loss associated with one average collision. Here C_n is calculated from the elastic scattering functions for the heavy elements only, and is essentially independent of z in this approximate treatment.

Introducing a Fourier transformation with respect to z, which replaces $\partial/\partial z$ by $-k\sigma = p$, and replacing F_n by its transform G_n, one obtains from (1)

$$(2) \quad (1 - k\mu)\, G = \frac{Q}{4\pi\sigma} + \frac{1}{4\pi} \sum (2n+1)\, C_n \, G_n \, P_n(\mu)$$

2/ See ORNL-424, equation (3)

If each side is multiplied by $P_n(\mu)$ and the result integrated over the unit sphere, the result is

$$(3)\quad (2n+1)\,G_n - k\left[n\,G_{n-1} + (n+1)\,G_{n+1}\right] = \delta_{no}\,Q/\sigma + (2n+1)\,C_n\,G_n$$

Let $h_n = 1 - C_n$, $\lambda = 1/k$, $G_n = 0$, $n < 0$. Then

$$(4)\quad (2n+1)\lambda\,h_n\,G_n - \left[n\,G_{n-1} + (n+1)\,G_{n+1}\right] = \lambda\,\delta_{no}\,Q/\sigma \quad n = 0,\ 1,\ 2\ \ldots$$

Consider a set of homogeneous equations

$$(5)\quad (2n+1)\,\bar{\lambda}\,\bar{h}_n\,\bar{G}_n - \left[n\,\bar{G}_{n-1} + (n+1)\,\bar{G}_{n+1}\right] = 0, \quad n = 0,\ 1\ \ldots$$

Multiply (4) by $\bar{G}_n$, (5) by G_n, and subtract the latter product; we obtain

$$(6)\quad (2n+1)(\lambda h_n - \bar{\lambda}\,\bar{h}_n)\bar{G}_n\,G_n - n\,(G_{n-1}\,\bar{G}_n - \bar{G}_{n-1}\,G_n) + (n+1)(G_n\bar{G}_{n+1} - \bar{G}_n\,G_{n+1})$$

$$= \lambda\,\delta_{no}\,\bar{G}_n\,Q/\sigma\ .$$

Adding the first N + 1 equations, one finds

$$(7)\quad \sum_{0}^{N}(2n+1)(\lambda h_n - \bar{\lambda}\,\bar{h}_n)G_n\,\bar{G}_n + (N+1)(G_N\,\bar{G}_{N+1} - \bar{G}_N\,G_{N+1}) = \lambda\,\bar{G}_o\,Q/\sigma.$$

<u>The solution for a finite number N + 1 of equations</u>

It is assumed that N is arbitrarily large, and that $G_{N+1} = 0$. For $Q = 0$, $h_n = \bar{h}_n$, $\lambda \neq \bar{\lambda}$, from (7) two distinct solutions satisfy

the orthogonality relation

$$\sum_{n=0}^{N} (2n+1)\, h_n\, G_n\, \bar{G}_n = 0 \quad .$$

Hence roots $\bar{\lambda}$ are real if h_n is > 0. Also from (6), with λ arbitrary, but only the first $m + 1$ equations or the last $N-m$ satisfied,

$$(9) \qquad \sum_{n=0}^{m} (2n+1)\, h_n\, \bar{G}_n^{\,2} - (m+1)\, \bar{G}_m^{\,2} \frac{d}{d\lambda}\left(\frac{\bar{G}_{m+1}}{\bar{G}_m}\right) = 0 \; .$$

$$\sum_{n=m+1}^{N} (2n+1)\, h_n\, \bar{G}_n^{\,2} + (m+1)\, \bar{G}_m^{\,2} \frac{d}{d\lambda}\left(\frac{\bar{G}_{m+1}}{\bar{G}_m}\right) = 0 \; .$$

If $h_n = \bar{h}_n$ and G_n represents the solution for the non-homogeneous equations, from (7)

$$(10) \qquad \sum_{n=0}^{N} (2n+1)\, h_n\, \bar{G}_n\, G_n = \frac{\lambda \bar{G}_o\, Q/\sigma}{\lambda - \bar{\lambda}}$$

Let G_n have a representation in terms of the eigenvectors $(G_n^{(r)})$, $r = 1 \ldots N + 1$

$$G_n = \sum_r a_r\, G_n^{(r)}$$

From the orthogonality of distinct eigenvectors, it results that

$$a_r = \frac{\lambda}{\lambda - \lambda_r} \frac{\bar{G}_o^{(r)}\, Q/\sigma}{\sum_0^N (2n+1)\, h_n\, G_n^{(r)2}}$$

$$\frac{\lambda}{\lambda - \lambda_r} = \frac{\sigma k_r}{p - p_r}, \quad p_r = -\sigma k_r \; , \; \lambda = k^{-1} \quad .$$

The inverse Fourier transformation gives the result

$$(11)\quad F_n(z) = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} e^{pz}\, G_n(p)\, dp = \sum_r G_n^{(r)} \int_{-i\infty}^{i\infty} \frac{\sigma k_r\, e^{pz}\; G_o^{(r)}\; Q/\sigma dp}{(p - p_r)\sum_m (2m+1)\; h_m\; G_m^{(r)2}}$$

$$= \sum_r \frac{Q\; G_o^{(r)}\; G_n^{(r)}\; k_r\; e^{-k_r\,\sigma z}}{\sum_m (2m+1)\; h_m\; G_m^{(r)2}}$$

Besides the value or values corresponding to the discrete spectrum ($\lambda > 1$) the values on the continuous spectrum ($\lambda < 1$) may be important. The constants C_n become negligibly small in practice for $n > n_o$, and for $h = 1$, the recurrence equations for $\lambda < 1$ have solutions, $P_n(\lambda)$, $Q_n(\lambda)$, the Legendre functions of the first and second kind. For large n, 1/ $\lambda = \cos\theta$,

$$(12)\quad P_n(\cos\theta) \cong \left(\frac{2}{\pi \sin\theta}\right)^{\frac{1}{2}} \frac{\Gamma(n+1)}{\Gamma\left(n+\frac{3}{2}\right)} \sin\left[\left(n+\tfrac{1}{2}\right)\theta + \pi/4\right]$$

$$Q_n(\cos\theta) \cong \left(\frac{\pi}{2\sin\theta}\right)^{\frac{1}{2}} \frac{\Gamma(n+1)}{\Gamma\left(n+\frac{3}{2}\right)} \cos\left[\left(n+\tfrac{1}{2}\right)\theta + \pi/4\right]$$

1/ Hobson, Spherical and Elliptical Harmonics, p. 297.

Also,

$$\frac{\Gamma(n+1)}{\Gamma\left(n+\frac{3}{2}\right)} \cong \left(n+\tfrac{1}{2}\right)^{-\frac{1}{2}} \quad .$$

If the values of G_n $(n \leq n_o + 1)$ are determined for small $1-\lambda$, (only small values of $1-\lambda$ are required for large distances from the source, and power series in terms of powers of $1-\lambda$ can be calculated without difficulty), the solution for $n > n_o$ can be found from the conditions

$$(13) \qquad G_{n_o} = A\sqrt{\frac{\pi}{2}}\, P_{n_o}(\lambda) + B\sqrt{\frac{2}{\pi}}\, Q_{n_o}(\lambda)$$

$$G_{n_o+1} = A\sqrt{\frac{\pi}{2}}\, P_{n_o+1}(\lambda) + B\sqrt{\frac{2}{\pi}}\, Q_{n_o+1}(\lambda) \quad .$$

$$Q_n(\lambda) = \tfrac{1}{2}\int_{-1}^{1} \frac{P_n(t)\,dt}{\lambda - t}$$

$$= P_n(\lambda)\cdot \tfrac{1}{2}\ln\left(\frac{1+\lambda}{1-\lambda}\right) + \sum_{m=0}^{M} a_m (1-\lambda)^m$$

where the Cauchy principal value is chosen. Hence

$$G_n(\lambda) \cong \left[\left(n+\tfrac{1}{2}\right)\sin\theta\right]^{-\frac{1}{2}} \left(A^2+B^2\right)^{\frac{1}{2}} \sin\left[n\theta + \frac{\theta}{2} + \frac{\pi}{4} + \tan^{-1}\frac{B}{A}\right]$$

and for N large,

$$\sum_{n_1}^{N} (2n+1)\, G_n^2 \cong \frac{A^2+B^2}{\sin\theta}\left[N - \frac{\cos(N\theta + 2\alpha)\sin(N+1)\theta}{\sin\theta}\right]$$

$$\alpha = \frac{\theta}{2} + \frac{\pi}{4} + \tan^{-1}\frac{B}{A}$$

$$\cong \frac{N}{\sin\theta}\left(A^2 + B^2\right) .$$

(The first equation (9) gives this also).

The density of the roots of $G_N = 0$ is found from the asymptotic expression; we have approximately

$$\sin(N\theta + \alpha) = \sin(N\theta' + \alpha) ,$$

$$N(\theta' - \theta) = \pi, \quad \Delta\theta = \pi/N$$

$$\lambda = \cos\theta ,$$

$$\Delta\lambda = -\sin\theta\,\Delta\theta = -\sqrt{1-\lambda^2}\,\Delta\theta$$

$$= -\sqrt{(1-\lambda^2)}\,\pi/N .$$

Then

$$\rho(\lambda) = \left|\frac{1}{\Delta\lambda}\right| = \frac{N}{\pi\sin\theta}$$

and

$$\sum_{0}^{N} (2n+1)\, h_n\, G_n^{\,2} \cong \pi\rho(\lambda)\,(A^2 + B^2)$$

Hence

$$F_n(z) = Q \sum \frac{\Delta\lambda_r \rho(\lambda_r)\, G_o^{(r)} G_n^{(r)} k_r\, e^{-k_r \sigma z}}{\pi \rho(\lambda_r)(A^2 + B^2)} \qquad \Delta\lambda_r = -\frac{\Delta k_r}{k_r^2}$$

$$\cong \frac{Q}{\pi} \int_1^{\bar{k}} \frac{G_o(k) G_n(k)\, e^{-k\sigma z}}{(A^2 + B^2)} \frac{dk}{k} + Q \sum_r{}' \frac{G_o^{(r)}\, G_k^{(r)} k_r\, e^{-k_r \sigma z}}{\sum_m (2m+1)\, h_m\, G_m^{(r)2}}$$

The second integral represents the contribution of the discontinuous spectrum.

For the calculation of the functions Q_n one has the relations

$$\lambda Q_o - Q_1 = 1 \qquad Q_o = \tfrac{1}{2} \ln \frac{1+\lambda}{1-\lambda}$$

$$n\, Q_{n-1} - (2n+1)\lambda Q_n + (n+1)\, Q_{n+1} = 0. \qquad n = 1, 2, 3, \ldots.$$

Calculation of C_n.

If the elastic scattering as function of the angle for a given scattering nucleus is of the form

$$\sigma_s\, f(\mu)\, d\Omega, \quad \mu = \cos\theta, \quad \text{evidently}$$

$$2\pi \int_{-1}^{1} f(\mu)\, d\mu = 1$$

For scattering which is highly concentrated in the forward direction, approximately

$$f(\mu) \doteq \frac{\alpha}{2\pi} e^{-\alpha(1-\mu)}$$

The constants $c_n^{(M)}$ are defined by (c. f. ORNL-424)

$$c_n^{(M)} = 2\pi \int_{-1}^{1} f(\mu)\, P_m(\mu)\, d\mu$$

Now if the total cross section, the reaction cross section and the transport cross section are known, we have

(18) $$\frac{\sigma_{tr} - \sigma_r}{\sigma_{tot} - \sigma_r} = \int_{-1}^{1} f(\mu)(1-\mu) \Big/ \int_{-1}^{1} f(\mu)\, d\mu$$

$$= \frac{1}{\alpha} - 2\left(e^{-2\alpha} + e^{-4\alpha} + e^{-6\alpha} + \right)$$

Hence α can be determined from these cross sections, which will be taken from the curves of Feshbach and Weisskopf, (Physical Review, 76, p. 1551, (1949)).

We have

(19) $$f(\mu) = \frac{\alpha e^{-\alpha}}{2\pi} \sqrt{\frac{\pi}{2\alpha}} \sum_m (2m+1)\, I_{m+\frac{1}{2}}(\alpha)\, P_m(\mu)\,.$$

$$c_n^{(M)} = 2\alpha_M e^{-\alpha M} f_n(\alpha_M), \quad f_n(\alpha) = \sqrt{\frac{\pi}{2\alpha}}\, I_{n+\frac{1}{2}}(\alpha)$$

A useful recursion formula is

$$I_{v-1}(z) - I_{v+1}(z) = \frac{2v}{z} I_v(z), \qquad v = n + \tfrac{1}{2}$$

For several scatterers,

$$(20) \qquad C_n = \sum_M \frac{\sigma_s^{(M)}}{\sigma} c_n^{(M)}$$

If a single heavy element is present the coefficients c_n^M may be computed from the recursion formula for $I_v(\alpha)$ and the relations

$$(21) \qquad I_{-\frac{1}{2}}(z) = \sqrt{\frac{2}{\pi z}} \cosh z, \qquad I_{\frac{1}{2}}(z) = \sqrt{\frac{2}{\pi z}} \sinh z$$

$$c_n = 2\sqrt{\frac{\pi\alpha}{2}}\, e^{-\alpha} I_{n+\frac{1}{2}}(\alpha)$$

$$c_{n-1} - c_{n+1} = \frac{2n+1}{\alpha} c_n \qquad n = 1, 2, 3 \ldots\ldots$$

$$c_o = 2e^{-\alpha} \sinh \alpha, \quad c_1 = 2e^{-\alpha}\left[\cosh \alpha - \frac{1}{\alpha}\sinh \alpha\right]$$

<u>Discussion</u>

The calculation of the discrete spectrum is carried through by setting up equations (5) with $\bar{G}_0 = 1$; trial values of λ are used until a value is found such that $\bar{G}_n$ becomes a positive function of n up to n = N, ($N \sim 12$ in one application). When the trial value is too small, $\bar{G}_n$ becomes negative; if too large, after an initial decrease $\bar{G}_n$ starts increasing, contrary to the requirement that $G_n \to 0, n \to \infty$.

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When a continuous source distribution is present, the calculation is required for several values of the energy, after which the functions $F_n(z)$ given in equation (11) are to be summed or integrated over the energy distribution.

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