The fluxes calculated by the 05R code are compared, as a function of distance, in Fig. 2 with the scattered flux computed by Beach *et al.* One notes first that the 05R results are consistent with each other. The low 05R fluxes at distances greater than 6 mfp (mean free paths) demonstrate the characteristic Monte Carlo systematic error mentioned above and are caused by an insufficient number of neutrons penetrating to distances far from the source. The high values of 05R results compared with those of Beach *et al.* at the origin are no doubt due to the contribution of a few neutrons having very small values of μ in Eq. 1.

The angular distributions of scattered neutrons at 0, 0.5, 1, and 5 mfp from the source plane are compared with the results of Beach *et al.* in Figs. 3-6, respectively. The 05R results are averages over a 0.1 interval in μ, plotted at the midpoint of the interval. Noticeable in the data for the mixture of light scatterers is the large contribution in the 0 to 0.1 interval adjacent to the source plane due to the contributions of low-μ neutrons. The semianalytic result, of course, goes to infinity at the source plane. In all cases of 05R results are consistent. Agreement with the semianalytic results is good to 1 mfp, and not really poor even at 5 mfp. At this depth, of course, the agreement is considerably better for positive μ than for negative μ, since so few neutrons penetrate deeply into the medium and are scattered back toward the origin.

The error bars shown on some of the points are consistent for both media and represent the standard deviation computed from the relation

$$\sigma = \sqrt{\frac{\frac{1}{N}\sum_{1}^{N} W^2 - \left(\frac{1}{N}\sum_{1}^{N} W\right)^2}{N-1}},$$

where W = the neutron weight and N = the total number of source neutrons.

A second test of the anisotropic-scattering selection technique was the calculation of the multiplication constant for one-velocity neutrons in infinite slabs, infinite cylinders, and spheres of media having isotropic scattering in the laboratory system. Exact results for such problems have been tabulated by Carlson and Bell[4]. The number of secondaries per collision was arbitrarily taken as 1.1 for the comparison.

Three calculations were performed for each of the configurations. The first was a strictly one-velocity problem with isotropic scattering in the laboratory system. This was intended to evaluate the accuracy of the Monte Carlo method in computing a multiplication constant. The second considered a scattering medium having a mass of 15 000 with isotropic scattering in the center-of-mass system but introduced the neutrons in a fission spectrum. This calculation, by comparison with the first, tested the equivalence of the constant cross-section one-velocity and multivelocity cases on 05R. The third calculation was the test of the anisotropic scattering treatment. The medium was a half-and-half mixture of scatterers having masses of 2 and 3, with each having a P_8 approximation to the center-of-mass distribution which yielded an isotropic angular distribution in the laboratory system. At least 20 iterations of 400 histories each were performed in each calculation, with the first five being discarded in the computation of the multiplication constant to permit spatial convergence of the source distribution.

The results of the calculations are compared with the exact results in Table II. The calculations testing the anisotropic-scattering selection technique, those for the $(A = 2) + (A = 3)$ mixture, are consistent with the other 05R results and are in agreement with the exact results.

The consistency of the anisotropic-scattering medium results obtained with the Monte Carlo calculations and the demonstrated agreement with semianalytic and exact results indicate that Coveyou's selection technique is appropriate and has been properly incorporated into the 05R code.

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[4]B. G. CARLSON and G. I. BELL, "Solution of the Transport Equation," P/2386, *Proc. U. N. Intern. Conf. Peaceful Uses Atomic Energy, 2nd,* Geneva, (1958).

The Albedo Problem

In a recent note, Rafalski[1] has considered the problem of computing the probability that a neutron will be reflected (the albedo) if it is perpendicularly incident on a semi-infinite half-space. His method of solution consisted of introducing an approximation into the integral transport equation describing the problem and led to a simple analytic result for the albedo. We show that the application of the variational method to this problem also leads to a simple analytic expression for the albedo and that this expression is significantly more accurate. Exact formulations

[1]P. RAFALSKI, *Nucl. Sci. Eng.*, 19, 378 (1964).

of this albedo problem are given by Chandrasekhar[2] and Davison[3].

Following Rafalski, we consider the one-velocity transport problem of a semi-infinite halfspace with absorption and isotropic scattering occupying the space $0 \leq z \leq \infty$. We generalize the problem by allowing the neutron flux incident at $z = 0$ to have an arbitrary distribution $B(\mu)$, where μ is the cosine of the angle between the z axis and the velocity vector of the neutron. Consider the functional

$$F[\phi,\phi^*] = \int_0^\infty dx \int_{-1}^1 d\mu[(1-c)\phi(z,\mu) - \phi^*(z,\mu)H\phi(z,\mu)] - \int_0^1 d\mu\mu\phi^*(0,\mu)[\phi(0,\mu) - B(\mu)], \quad (1)$$

where H is the integro-differential transport operator,

$$H = \mu\frac{\partial}{\partial z} + 1 - \frac{c}{2}\int_{-1}^1 d\mu', \quad (2)$$

c is the mean number of secondaries for each collision, $\phi(z,\mu)$ is the directional flux and $\phi^*(z,\mu)$ is the adjoint directional flux. The spatial coordinate z is measured in units of mean free paths, i.e., in units of $1/\Sigma$, where Σ is the macroscopic collision cross section. The first variation of Eq. (1) is

$$\delta F[\phi,\phi^*] = -\int_0^\infty dz \int_{-1}^1 d\mu[H\phi(z,\mu)]\delta\phi^*(z,\mu) - \int_0^\infty dz \int_{-1}^1 d\mu[H^*\phi^*(z,\mu) - (1-c)]\delta\phi(z,\mu) + \int_{-1}^0 d\mu\mu\phi^*(0,\mu)\delta\phi(0,\mu) - \int_0^1 d\mu\mu[\phi(0,\mu) - B(\mu)]\delta\phi^*(0,\mu). \quad (3)$$

Because of the independence and arbitrariness of these four variations, $\delta F = 0$ implies

$$H\phi(z,\mu) = 0, \ (-1 \leq \mu \leq 1), \quad (4)$$

$$\phi(0,\mu) = B(\mu), \ (0 < \mu \leq 1), \quad (5)$$

and

$$H^*\phi^*(z,\mu) = (1-c), \ (-1 \leq \mu \leq 1), \quad (6)$$

$$\phi^*(0,\mu) = 0, \ (-1 \leq \mu < 0). \quad (7)$$

Equations (4) and (5) describe the problem under consideration, and Eqs. (6) and (7) describe the associated adjoint problem. Further, if the solutions of Eqs. (4) through (7) are inserted into Eq. (1), we find

$$F[\phi,\phi^*] = \int_0^\infty dz \int_{-1}^1 d\mu(1-c)\phi(z,\mu). \quad (8)$$

This is just the absorption rate in the halfspace which, by neutron conservation, is the product of the incoming current J_{in} and $(1 - A)$, where A is the albedo and

$$J_{in} = \int_0^1 d\mu\mu B(\mu). \quad (9)$$

Thus the functional, Eq. (1), is both the Lagrangian for the problem and yields second order errors in the albedo for first order errors in the flux and adjoint flux.

As trial functions, we choose the asymptotic distributions which are bounded at infinity, i.e.

$$\phi(z,\mu) = \frac{Ke^{-\nu z}}{1 - \mu\nu}, \quad (10)$$

$$\phi^*(z,\mu) = \frac{K^*e^{-\nu z}}{1 + \mu\nu} + 1, \quad (11)$$

where ν is a positive quantity satisfying the transcendental equation

$$\frac{2\nu}{c} = \ln\left(\frac{1+\nu}{1-\nu}\right), \quad (12)$$

and K and K^* are constants to be determined. Substituting Eqs. (10) and (11) into Eq. (3), performing the angular integrations, and setting the coefficients of δK and δK^* equal to zero, we find

$$K = \frac{-2\nu^2\Gamma}{\ln(1-\nu^2)} J_{in}, \quad (13)$$

$$K^* = \frac{2[\nu - \ln(1+\nu)]}{\ln(1-\nu^2)}, \quad (14)$$

where we have defined

$$\Gamma = \frac{\int_0^1 d\mu \frac{\mu B(\mu)}{1+\mu\nu}}{\int_0^1 d\mu\mu B(\mu)}. \quad (15)$$

If we now substitute Eqs. (10) and (11), with K and K^* given above, into the functional, Eq. (1), equate the result to $J_{in}(1 - A)$, and solve for the albedo A, we find the simple result

$$A = \frac{2\Gamma}{\ln(1-\nu^2)}[\ln(1+\nu) - \nu]. \quad (16)$$

In particular, if the incident flux is a beam normal to the surface, i.e., $B(\mu) = \delta(1 - \mu)$, Eq. (16) yields

[2] S. CHANDRASEKHAR, *Radiative Transfer*, Dover, New York, (1960).

[3] B. DAVISON and J. B. SYKES, *Neutron Transport Theory*, Oxford, (1958).

$$A(\text{beam}) = \frac{2}{(1+\nu)\ln(1-\nu^2)}\,[\ln(1+\nu) - \nu]. \quad (17)$$

From Rafalski's paper, his result for a normal beam is

$$A(\text{Rafalski}) = 1 - \frac{(1-c)}{1 - \frac{c}{2}\left[1 + \frac{\ln(1+\nu)}{\nu}\right]}\,. \quad (18)$$

Equation (18) can be simplified by using Eq. (12). The result is

$$A(\text{Rafalski}) = \frac{\ln(1+\nu) - \nu}{\ln(1-\nu) + \nu}\,. \quad (19)$$

In this form it is clear that our result is different from that of Rafalski. Table I compares these two expressions for the albedo, Eqs. (17) and (19), with the exact result. If the incident flux is isotropic, i.e., $B(\mu) = 1$, Eq. (16) yields

$$A(\text{isotropic}) = \frac{-4}{\nu^2\ln(1-\nu^2)}\,[\ln(1+\nu) - \nu]^2\,. \quad (20)$$

Table II compares Eq. (20) with the exact results given by Maynard[4]. We see that in both cases we find excellent agreement between Eq. (16) and the exact results. Since the anisotropy of a general $B(\mu)$ lies between these two cases, we can conclude that Eq. (16) is probably quite accurate for all $B(\mu)$.

The functional analogous to Eq. (1) for a finite system occupying the space $0 \leq z \leq a$ is

$$F[\phi,\phi^*] = \int_0^a dz \int_{-1}^1 d\mu\,[(1-c)\phi(z,\mu) - \phi^*(z,\mu)\,H\phi(z,\mu)] - \int_0^1 d\mu\mu\,\phi^*(0,\mu)[\phi(0,\mu) - B(\mu)] + \int_{-1}^0 d\mu\mu\,\phi^*(a,\mu)\phi(a,\mu)\,. \quad (21)$$

TABLE I

1 - A (Normal Beam)

c	Rafalski	Eq. (17)	Exact
0	1.000	1.000	1.000
0.25	0.951	0.954	0.955
0.35	0.924	0.929	0.930
0.45	0.890	0.900	0.902
0.55	0.848	0.864	0.865
0.65	0.793	0.817	0.820
0.75	0.720	0.754	0.752
0.85	0.611	0.658	0.660
0.95	0.409	0.462	0.464
0.98	0.280	0.328	0.327
0.99	0.207	0.247	0.247
1.00	0.	0.	0.

[4]C. W. MAYNARD, *Nucl. Sci. Eng.*, **6**, 174 (1959).

TABLE II

1 - A (Isotropic)

c	Eq. (20)	Exact
0	1.000	1.000
0.10	0.980	0.978
0.20	0.957	0.954
0.30	0.929	0.926
0.40	0.896	0.893
0.50	0.856	0.853
0.60	0.808	0.805
0.70	0.746	0.743
0.80	0.660	0.658
0.90	0.523	0.522
1.00	0.	0.

The Euler-Lagrange equations and subsidiary conditions of Eq. (21) are again Eqs. (4) through (7) with the additional boundary conditions at $z = a$,

$$\phi(a,\mu) = 0,\ (-1 \leq \mu < 0)\,, \quad (22)$$

$$\phi^*(a,\mu) = 0,\ (0 < \mu \leq 1)\,. \quad (23)$$

Thus Eq. (21) is a proper Lagrangian for the finite albedo problem. As was the infinite system Lagrangian, Eq. (21) is stationary about $J_{\text{in}}P$, where P is the absorption probability, but for a finite system $(1 - P)$ is the sum of the albedo and the transmission probability. Hence this functional will not yield a stationary value for the albedo. A functional which is both a Lagrangian for the finite albedo problem and yields a stationary value for the albedo is

$$F[\phi,\phi^*] = -\int_0^a dz \int_{-1}^1 d\mu\phi^*(z,\mu)H\phi(z,\mu) - \int_0^1 d\mu\mu\phi^*(0,\mu)\,[\phi(0,\mu) - B(\mu)] - \int_{-1}^0 d\mu\mu\,[\phi(0,\mu) - \phi^*(a,\mu)\phi(a,\mu)]\,. \quad (24)$$

The Euler-Lagrange equations and boundary conditions of this functional are

$$H\phi(z,\mu) = 0,\ (-1 \leq \mu \leq 1)\,, \quad (25)$$

$$\phi(0,\mu) = B(\mu),\ (0 < \mu \leq 1)\,, \quad (26)$$

$$\phi(a,\mu) = 0,\ (-1 \leq \mu < 0)\,, \quad (27)$$

and

$$H^*\phi^* = 0,\ (-1 \leq \mu \leq 1)\,, \quad (28)$$

$$\phi^*(0,\mu) = 1,\ (-1 \leq \mu < 0)\,, \quad (29)$$

$$\phi^*(a,\mu) = 0,\ (0 < \mu \leq 1)\,. \quad (30)$$

Clearly this functional is stationary about $J_{\text{in}}A$. Hence Eq. (24) is a proper functional to use for the finite albedo problem.

For a large, but finite, system one would expect good results from again using asymptotic distributions (in this instance the sum of growing and decaying asymptotic exponentials) as trial functions. However, in a small system the asymptotic distributions would not become established and their use as trial functions would probably lead to large errors. Since in this situation one would expect the directional and adjoint directional fluxes to be relatively flat (in space), a more appropriate trial function might be

$$\phi(z,\mu) = \sum_{n=0}^{N} \phi_n(\mu)\, z^n \ , \qquad (31)$$

with an analogous adjoint trial function. In this case, one allows the variational method to determine the angular dependences of the trial functions. This general approach to transport problems has been discussed elsewhere[5].

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[5]G. C. POMRANING and M. CLARK, Jr., *J. Nucl. Energy, A/B*, **18**, 191, (1964).

Neutron Scattering by Polyethylene*

FREQUENCY SPECTRUM

Crystalline polyethylene is known to be formed by very long, kinked and only weakly interacting chains of CH_2 radicals[1,2]. Therefore its frequency spectrum is radically different from the one corresponding to a three-dimensional crystal. In fact, analyzing its normal modes of vibration in terms of plane waves $e^{i\vec{k}\vec{r}}$, the corresponding frequencies can only depend on the projection of the wave vector $\vec{k}$ on a direction parallel to the chains (at least to the extent that the interaction between neighboring chains can be neglected). In other words, for any direction of $\vec{k}$, the frequency ω depends only on the phase difference θ between the vibration of corresponding elements of two neighboring radicals of the same chain. This dependence, as calculated by Lin and Koenig[1], is shown in Fig. 1 where the nine different branches (corresponding to the three atoms in each radical) can be assigned to the following vibrational modes:

T	C-C-C-C torsion
B	C-C-C bending
S	C-C stretching
R	CH_2 rocking
Tw	CH_2 twisting
W	CH_2 wagging
Ib	H-C-H bending
Ss	H-C-H symmetric stretching
As	H-C-H antisymmetric stretching.

Only two of these branches go to $\omega = 0$ for $\theta = 0$ and can thus be considered as acoustical modes. The remaining ones are optical branches. This again shows very clearly the difference with a three-dimensional crystal for which the number of acoustical branches always is three.

We shall consider only the optical part of Lin and Koenig's frequency distribution since the acoustical part is perturbed, at least near $\omega = 0$, by the weak coupling between neighboring chains. Because of this, at very low frequencies one must recover the typical ω^2 behavior of a Debye crystal. Since a frequency spectrum is defined as the fraction of modes per unit frequency interval, in our case we have

$$f(\omega) = c \sum_i \frac{d\theta_i(\omega)}{d\omega},$$

where c is a normalization constant and the sum is over all branches crossing the frequency ω. Hence $f(\omega)$ becomes singular at all those points where $\frac{d\omega}{d\theta} = 0$. A histogram of the spectrum obtained in this manner, but leaving out the C-C stretching branch as well as the acoustical branches, is shown in Fig. 2. The reason for leaving out the S

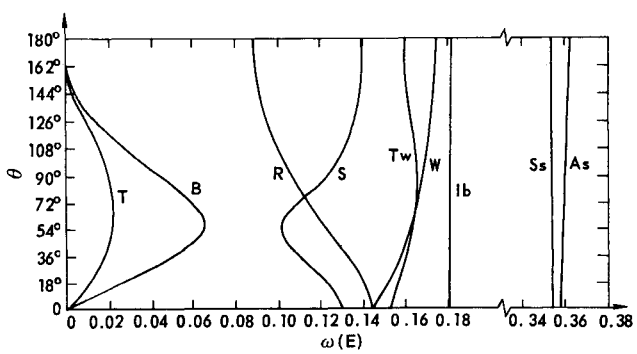

Fig. 1. Frequency dependence of the vibrational phase difference between neighboring CH_2 groups (Lin and Koenig).

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[1]TUNG PO LIN and J. L. KOENIG, *J. Molec. Spectr.*, **9**, 228 (1962).

[2]M. TASUMI and T. SHIMANOUCHI, *J. Molec. Spectra.*, **9**, 261 (1962).