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SOME ANALYTICAL SOLUTIONS OF THE SLOWING DOWN PROBLEM IN HYDROGEN

L. Dresner
A. Simon

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SOME ANALYTICAL SOLUTIONS OF THE SLOWING DOWN PROBLEM IN HYDROGEN

L. Dresner A. Simon

Abstract

Two situations are presented for which the slowing down problem in an infinite, hydrogenous medium can be solved explicitly in the P_1, B_1, and Selengut-Goertzel approximations. One case is for all cross sections constant, the other for a nonabsorbing hydrogen whose scattering cross section varies as v^3. The results are discussed in detail.

SOME ANALYTICAL SOLUTIONS OF THE SLOWING DOWN PROBLEM IN HYDROGEN

L. Dresner A. Simon

Introduction

Because the continuous slowing down model is inapplicable to moderation by hydrogen, Selengut and Goertzel[1] introduced an approximate method which correctly accounts for the neutron energy distribution after scattering. Their method, however, computes neutron leakage by the usual age-diffusion theory. This approximation has the well-known consequence that the age in water is overestimated.[2] The most elementary approximation to the Boltzmann equation in which the age is given correctly is the P_1 approximation.[3] For large reactors, in which only the second moment of the slowing down distribution is significant, the P_1 approximation ought to represent an improvement over the Selengut-Goertzel method. In small reactors, in which several moments of the slowing down distribution are important, this may not necessarily be true. In particular, the slowing down density in the P_1 approximation becomes negative for large bucklings for certain assumed variations of the cross sections with energy.[4] This pathologic behavior is due to the attempt to represent the highly anisotropic angular distribution of the flux in a small reactor with only the first two Legendre polynomials.[4] There is another approximation to the Boltzmann equation, called the B_1,[2] in which terms of order P_1 or P_o in the angular distribution of scattered neutrons

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1. G. Goertzel, Criticality of Hydrogen Moderated Reactors, TAB-53 (July, 1950).
2. H. Hurwitz and P. F. Zweifel, Jour. App. Phys. 26, 923 (1955).
3. R. E. Marshak, Rev. Mod. Phys. 19 201 (1947).
4. A. Simon, Neutron Slowing Down by Hydrogen in the Consistent P_1 Approximation, ORNL-2098 (July, 1956). Note that there is a misprint in Eq. (23) of this paper. The denominator of the last term in this equation should be $(\Sigma_A + \Sigma_S)^2$ rather than $(\Sigma_T + \Sigma_S)^2$.

in the lab system are retained. Terms of all orders, P_ℓ, in the angular expansion of the neutron flux are retained, however, so that even quite anisotropic fluxes can be represented. This improves the accuracy of the approximation and results in a positive slowing down density for all values of the buckling.

In a previous note[4] one of us considered several problems in which analytic solutions for the Fourier transform of the slowing down density exist in both the P_1 and Selengut-Goertzel approximations. From a study of these solutions some insight into the behavior of the two approximations was obtained. It is the purpose of this note to study two problems in which analytic solutions in the P_1, B_1, and Selengut-Goertzel approximations exist.

Summary of Previous Results

The one-dimensional energy dependent Boltzmann equation with an isotropic, monoenergetic neutron source whose spatial dependence is of the form e^{-ikx} is

$$-ik\mu N(\mu ku) + \Sigma_t(u)N(\mu ku)$$

$$= \sum_j \int d\Omega' \int_{u-\epsilon_j}^{u} du' \Sigma_{sj}(u')K_j(u',U,\mu_o)N(\mu' ku') + \frac{\delta(u)}{4\pi} \qquad (1)$$

where

μ = cosine of the angle between the neutron velocity and the x-axis,

N = neutron flux in the lethargy interval du, solid angle $d\Omega = d\phi d\mu$; all fluxes, however, are independent of ϕ, the azimuthal angle,

Σ_t = total cross section,

Σ_{sj} = scattering cross section of the jth species,

$K_j(u,U,\mu_o)$ = probability of scattering from lethargy u to lethargy u + U through an angle arccos μ_o,

ϵ_j = maximum lethargy loss per collision with the jth species.

The Boltzmann equation can be expressed as a coupled set of equations in lethargy by expanding the flux and scattering kernels in Legendre polynomials, viz.:

$$N(\mu ku) = \sum_{\ell=0}^{\infty} \frac{2\ell + 1}{4\pi} N_\ell(ku)P_\ell(\mu) \tag{2a}$$

$$K_j(uU\mu_o) = \sum_{\ell=0}^{\infty} \frac{2\ell + 1}{4\pi} K_{j\ell}(uU)P_\ell(\mu_o) \tag{2b}$$

The coupled equations which result from multiplying Eq. (1) by $P_\ell(\mu)$ and integrating are

$$\Sigma_t(u)N_\ell(ku) - ik \frac{\ell}{2\ell + 1} N_{\ell-1}(ku) - ik \frac{\ell + 1}{2\ell + 1} N_{\ell+1}(ku)$$

$$= \sum_j \int_{u-\epsilon_j}^{u} \Sigma_{sj}(u')K_{j\ell}(u'U)N_\ell(ku')du' + \mathcal{S}(u)\delta_{\ell 0} \tag{3}$$

where U = u - u'. The P_ℓ approximation results from setting $N_{\ell+1}$ and higher equal to zero.

Another procedure is to substitute the expansions (2) into Eq. (1), divide by $\Sigma_t - ik\mu$ and then multiply by $P_\ell(\mu)$ and integrate. This

procedure leads to the coupled equations

$$\Sigma_t(u)N_\ell(ku) = \sum_{m=o}^{\infty} (2m + 1)A_{\ell m}$$

$$\times \left[\sum_j \int_{u-\epsilon_j}^{u} du' \Sigma_{sj}(u')K_{jm}(u'U)N_m(ku') + \delta(u)\delta_{mo} \right] \qquad (4)$$

where

$$A_{\ell m} = \frac{1}{2} \int_{-1}^{+1} \frac{P_\ell(\mu)\, P_m(\mu)}{1 - \frac{ik}{\Sigma_t}\mu} d\mu,$$

and $U = u - u'$.

The $A_{\ell m}$ satisfy the recurrence relation

$$\frac{(2\ell + 1)}{\eta} A_{\ell m} - (\ell + 1)A_{\ell+1\ j} - \ell\, A_{\ell-1\ j} = \frac{\delta_{j\ell}}{\eta}$$

where

$\eta = ik/\Sigma_t$,

$A_{oo} = (\Sigma_t/k)\arctan(k/\Sigma_t)$, and from this value and Eq. (5) all the $A_{\ell m}$ can be obtained.

The B_ℓ approximation results from setting $K_{\ell+1}$ and higher equal to zero. It is noteworthy that for a scattering kernel for which $K_{\ell+1}$ and higher are precisely zero the B_ℓ approximation is exact, whereas <u>no</u> P_ℓ approximation for any ℓ is exact.

If we specialize the nuclear species to hydrogen and some infinitely heavy absorbing and scattering (but non-moderating) material and require hydrogen to have isotropic scattering in the center-of-mass system, then for hydrogen

$$K_\ell(u',U) = e^{-U} P_\ell(e^{-U/2}) \tag{6a}$$

and for the heavy scatterer

$$K_\ell(u',U) = \delta(U) \langle P_\ell(\mu) \rangle \tag{6b}$$

where the average in (6b) is with respect to the angular distribution of the heavy scatterer. With these kernels the P_1 equations become

$$\left[\Sigma_a(u) + \Sigma_{SH}(u)\right] N_o(ku) - ikN_1(ku)$$

$$= \int_o^u \Sigma_{SH}(u')e^{u'-u} N_o(ku')du' + \delta(u) \tag{7a}$$

$$\Sigma_t(u)N_1(ku) - \frac{ik}{3} N_0(ku) = \int_o^u \Sigma_{SH}(u')e^{\frac{3}{2}(u'-u)} N_1(ku')du' \tag{7b}$$

where Σ_a is the absorption cross section, and $\Sigma_t = \Sigma_{SH} + \Sigma_{SM}(1-\bar{\mu}) + \Sigma_a$ and the subscripts H and M refer to hydrogen and to the heavy scatterer, respectively.

Interestingly, the B_1 equations can be manipulated into precisely the form given by Eqs. (7a) and (7b). All the quantities except Σ_t have the same meaning as in Eqs. (7a) and (7b). In the B_1 approximation

$$\Sigma_t = \frac{k^2}{3\Sigma} \cdot \frac{\arctan(k/\Sigma)}{(k/\Sigma) - \arctan(k/\Sigma)} - \bar{\mu}\Sigma_{SM} \tag{8}$$

where $\Sigma = \Sigma_a + \Sigma_{SH} + \Sigma_{SM}$.

If Eq. (7b) is differentiated it can be reduced to a first order, linear differential equation in N_1. It is therefore possible to solve for N_1 explicitly in terms of N_o and substitute in Eq. (7a). The resulting equation for N_o in both P_1 and B_1 approximations is

$$\left(\Sigma_a^{(u)} + \Sigma_{SH}^{(u)} + \frac{k^2}{3\Sigma_t^{(u)}}\right) N_o(ku)$$

$$+ \frac{k^2}{3\Sigma_t^{(u)}} \int_o^u \frac{\Sigma_{SH}(u')}{\Sigma_t(u')} N_o(ku')\, e^{\int_u^{u'} \left(\frac{3}{2} - \frac{\Sigma_{SH}(u'')}{\Sigma_t(u'')}\right) du''} du'$$

$$- \int_o^u du' \Sigma_{SH}(u') e^{u'-u} N_o(ku') du' = \delta(u) \qquad (9)$$

The relation of the Selengut-Goertzel approximation to the P_1 (or B_1) equations is as follows: If in the integral on the right-hand side of Eq. (7b) we approximate $\Sigma_{SH}(u')N_1(ku')$ by $\Sigma_{SH}(u)N_1(ku)$, i.e., if we assume $\Sigma_{SH}(u')N_1(ku')$ changes slowly with lethargy, then Eq. (7b) reduces to

$$N_1(ku) = \frac{ik}{3\Sigma_{tr}(u)} N_o(ku)$$

where $\Sigma_{tr}(u) = \Sigma_a(u) + \frac{1}{3}\Sigma_{SH}(u) + (1 - \bar{\mu})\Sigma_{SM}(u)$. Equation (10) is the usual diffusion theoretic relation between flux and current. Equation (7a) then becomes

$$\frac{k^2}{3\Sigma_{tr}(u)} N_o(ku) + \left[\Sigma_a(u) + \Sigma_{SH}(u)\right] N_o(ku)$$

$$= \int_o^u \Sigma_{SH}(u')e^{u'-u} N_o(ku')du' + \delta(u) \qquad (11)$$

which is the Selengut-Goertzel approximation. A modified Selengut-Goertzel approximation has been suggested by Hurwitz and Zweifel[2] in which $\Sigma_{tr} = \Sigma_t - 2/3\,\Sigma_{SH} - \bar{\mu}\Sigma_{SM}$ and Σ_t is given by Eq. (8).

Constant Cross Sections

The solutions of the P_1 and Selengut-Goertzel equations in the case of constant cross sections has been given by Simon[4] and is written below for the sake of completeness. The Fourier transformed slowing down density in the P_1 approximation is:

$$q(k,u) = \frac{\Sigma_{SH}}{\Sigma_a + \Sigma_{SH} + \frac{k^2}{3\Sigma_t}} (r_1 - r_2)^{-1}$$

$$\times \left\{ \left(\frac{3}{2} - \frac{\Sigma_{SH}}{\Sigma_t} + r_1\right) e^{r_1 u} - \left(\frac{3}{2} - \frac{\Sigma_{SH}}{\Sigma_t} + r_2\right) e^{r_2 u} \right\} \qquad (12a)$$

where

$$r_{1,2} = \frac{1}{2}\left(\frac{\Sigma_a}{\Sigma_t} + \frac{\Sigma_{SH}}{\Sigma_t} + \frac{k^2}{3\Sigma_t^2}\right)^{-1}$$

$$\times \left\{ - \left[\frac{5}{2}\ \frac{k^2}{3\Sigma_t^2} + \frac{\Sigma_a}{\Sigma_t}\left(\frac{5}{2} - \frac{\Sigma_{SH}}{\Sigma_t}\right) + \frac{\Sigma_{SH}}{\Sigma_t}\left(\frac{3}{2} - \frac{\Sigma_{SH}}{\Sigma_t}\right)\right]\right.$$

$$\pm \left[\frac{1}{4}\left(\frac{k^2}{3\Sigma_t^2}\right)^2 + \frac{k^2}{3\Sigma_t^2}\left(\frac{\Sigma_a}{\Sigma_t}\left(\frac{1}{2} - \frac{\Sigma_{SH}}{\Sigma_t}\right) + \frac{\Sigma_{SH}}{\Sigma_t}\left(\frac{3}{2} - \frac{5\Sigma_{SH}}{\Sigma_t}\right)\right)\right.$$

$$\left.\left. + \left(\frac{\Sigma_a}{2\Sigma_t} + \frac{3}{2}\ \frac{\Sigma_s}{\Sigma_t} - \frac{\Sigma_a + \Sigma_s}{\Sigma_t} \cdot \frac{\Sigma_s}{\Sigma_t}\right)^2\right]^{1/2}\right\} \qquad (12b)$$

The same quantity in the Selengut-Goertzel approximation is

$$q(ku) = \frac{\Sigma_{SH}}{\Sigma_a + \Sigma_{SH} + \frac{k^2}{3\Sigma_{tr}}} \exp\left(- \frac{\Sigma_a + \frac{k^2}{3\Sigma_{tr}}}{\Sigma_a + \Sigma_{SH} + \frac{k^2}{3\Sigma_{tr}}}\ u\right) \qquad (13)$$

Equations (12a) and (12b) also give the correct solution for q(ku) in the B_1 approximation except that Σ_t must be reinterpreted according to Eq. (8).

Plotted in Fig. 1 is q(ku) vs k^2/Σ_{SH}^2 for a particular choice of constant cross sections. The curves must all intersect in one point whose ordinate is the resonance escape probability when $k^2 = 0$; their slopes at the origin are numerically equal to $-\Sigma_{SH}^2\ \tau$ where τ is the age to u. In this drawing it appears that the Selengut-Goertzel age is smaller than the true age and computation verifies that it is smaller by about 2%. On the other hand, if $\Sigma_a = \Sigma_{SM} = 0$ then the true age is always smaller than the

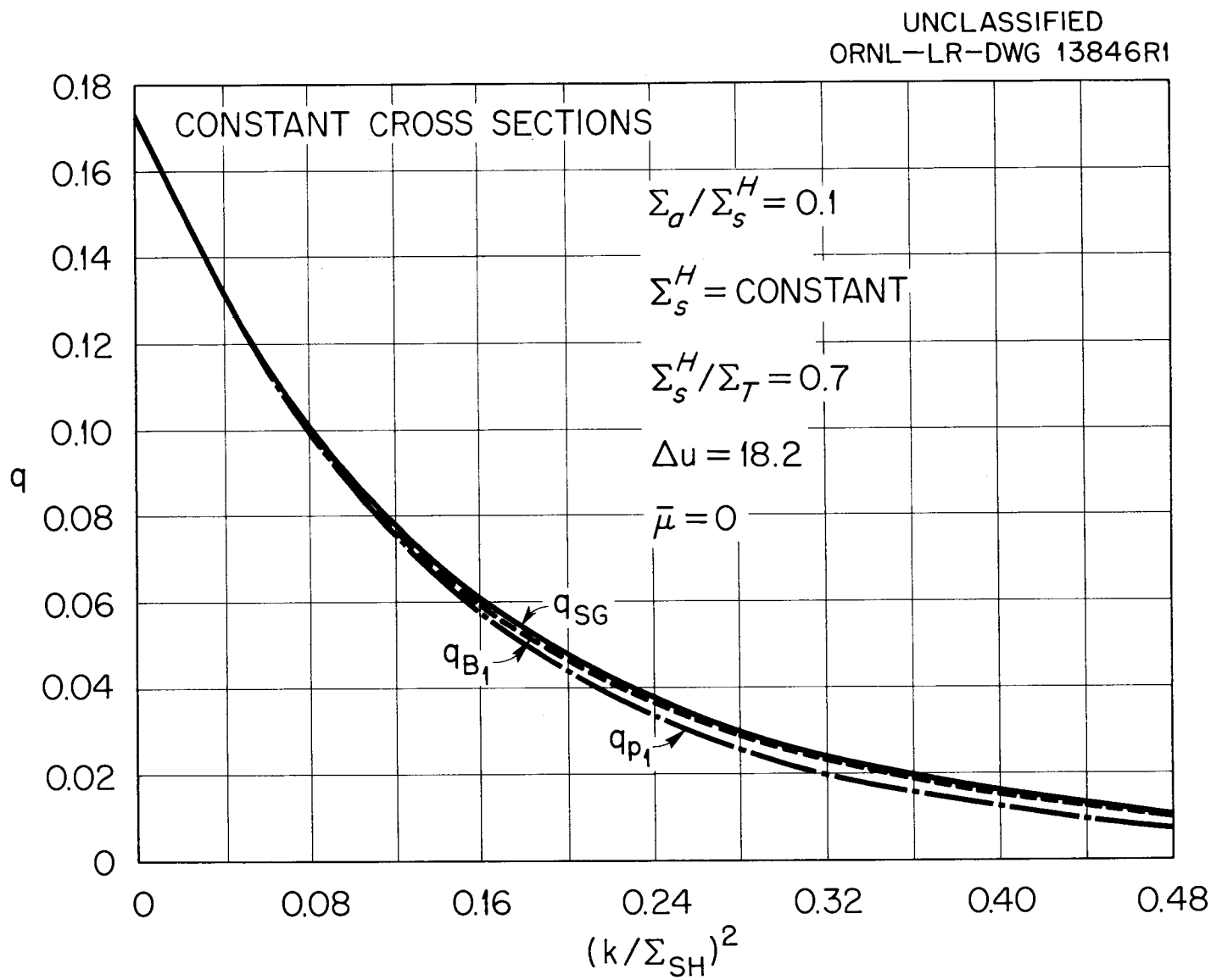

Fig. 1. Variation of Slowing Down Density with Buckling.

Selengut-Goertzel age, the latter becoming asymptotically correct for large u.[5]

In the limit of large buckling and for the case $\Sigma_a = \Sigma_{SM} = 0$ the three curves have the following asymptotic behavior

$$q(ku) \sim \frac{\Sigma_{SH}^2}{k^2} e^{-u} \qquad \text{(Selengut Goertzel)} \qquad (14a)$$

$$\sim -\frac{3\Sigma_{SH}^2}{k^2} e^{-u} \qquad (P_1) \qquad (14b)$$

$$\sim \frac{\pi}{2} \frac{\Sigma_{SH}}{k} e^{-u} \qquad (B_1) \qquad (14c)$$

It is possible to show that the asymptotic behavior of the B_1 approximation is actually the correct asymptotic behavior of the true solution of the Boltzmann equation. This can be done, e.g., directly from Eq. (1). A more physical method is as follows: q(ku) can be interpreted[6] as the fast leakage probability to lethargy u from a slab of thickness π/k of an isotropic, monoenergetic neutron source whose spatial dependence is given by $\cos(kx)$ where x is measured from the center line of the slab. If the buckling k is sufficiently large, the reactor will be so thin that only those neutrons will not leak out which are thrown below lethargy u in their first collision. The leakage is given by the current normal to the faces of the slab, and for a thin reactor is essentially due to the uncollided flux. Specifically, the leakage per unit surface from an isotropic unit plane source placed at x in the slab is

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5. L. C. Biedenharn and T. A. Welton, Some Remarks on the Slowing Down of Neutrons in Hydrogen, ORNL-2107 (Aug., 1956).
6. S. Glasstone and M. C. Edlund, Elements of Nuclear Reactor Theory, D. Van Nostrand Co., New York, p. 349 ff (1952).

$$P(x) = \frac{1}{2}\left\{E_3\left[\Sigma_{SH}\left(\frac{\pi}{2k} - x\right)\right] + E_3\left[\Sigma_{SH}\left(\frac{\pi}{2k} + x\right)\right]\right\}$$

$$= 1 - \frac{\pi\Sigma_{SH}}{2k} + 0\left[\left(\frac{\pi\Sigma_{SH}}{2k}\right)^2 \log\left(\frac{2k}{\pi\Sigma_{SH}}\right)\right] \qquad (15)$$

Hence to the lowest order the non-leakage probability is independent of x and equal to $\pi\Sigma_{SH}/2k$. Of the neutrons which collide, the fraction thrown below u on the first (and in this approximation, only) collision is $K_o(u) = e^{-u}$. Multiplying this quantity with the non-leakage probability gives Eq. (14c).

The physical reason for the correctness of the asymptotic behavior of the B_1 approximation lies in the fact, obvious from the previous paragraph, that all solutions of the slowing down problem with an isotropic, mono-energetic source and the same K_o have the same asymptotic solution. The B_1 approximation to hydrogen moderation is the <u>exact</u> solution of the slowing down problem with $K(u'U\mu_o) = (4\pi)^{-1}\,(e^{-U} + 3e^{-3U/2}\,\mu_o)$ which has the same K_o as the complete slowing down problem in hydrogen. The P_1 approximation, on the other hand, is not the <u>exact</u> solution to any slowing down problem because it lacks terms in P_2 and higher in the flux. A similar conclusion applies to the Selengut-Goertzel approximation.

The fact that the B_1 approximation must be a good solution of the slowing down problem in the limit of both small and large buckling implies that it should be quite a good approximation for all buckling. Hurwitz and Zweifel[2] have calculated some integrated fluxes, $\int_0^\infty N_o(ku)du$, in the case of constant cross sections ($\Sigma_a = \Sigma_{SM} = 0$) for $k = \Sigma_{SH}$ and $k = 5\Sigma_{SH}$. In the first case the B_1 is only 10% smaller than the exact result; the P_1 is smaller

by nearly a factor of 2. In the second case the P_1 is smaller than the exact result by nearly a factor of 10; the B_1 is still only 10% smaller.

For large k one expects the Selengut-Goertzel approximation to give a larger q(ku) than the P_1 approximation. One can see this as follows: If in Eq. (9) one sets $N_o(Ku') = N_o(ku)$ on the left-hand side on one obtains the Selengut-Goertzel approximation. For a small slab, with high leakage, however, $N_o(ku) < N_o(ku')$ if $u' < u$; hence, the Selengut-Goertzel approximation has a smaller leakage than the P_1, other things being equal. This gives the stated conclusion.

From the closer agreement of the Selengut-Goertzel with the B_1 than the P_1 and the B_1 approximation one may conjecture that for small reactors ($\sim$ 5 to 10 mean free paths in diameter) the Selengut-Goertzel is better than the P_1.

v^3 Cross Section

Another problem in which the P_1, B_1, and Selengut-Goertzel approximations may all be solved analytically is $\Sigma_a = \Sigma_{SM} = 0$, $\Sigma_{SH} \propto v^3$, the cube of the neutron velocity. We proceed as follows in the P_1 and B_1 approximations: We substitute N_1 from Eq. (7a) directly into Eq. (7b). The double integrals which arise can be reduced to single integrals by first interchanging the order of integration and then performing one of the integrations. The resulting integral equation can be reduced to a first-order linear, inhomogeneous, differential equation by the process of differentiation if $\Sigma_{SH} \propto v^3$. In the P_1 approximation this differential equation can also be obtained by Laplace transformation. The differential equation can be solved straight-forwardly and results in the following expression for q(k,u):

$$q(k,u) = 1 - \int_0^u \frac{ce^{-3x}}{A(x) + ce^{-3x}} \exp\left(\int_0^x \frac{1 - ce^{-3y}}{A(y) + ce^{-3y}}\, dy\right) dx \qquad (16)$$

where $c = k^2/3\Sigma^2_{SH}(u)$ and $A(x) = 1$ for the P_1 approximation and $A(x) = ce^{-3x}\arctan\left(\sqrt{3c}\ e^{-3x/2}\right)\left[\sqrt{3c}\ e^{-3x/2} - \arctan\left(\sqrt{3c}\ e^{-3x/2}\right)\right]^{-1}$ for the B_1 approximation. If the source energy is made high enough then $q(ku)$ becomes independent of the source energy. The physical reason is that the cross section is sufficiently large at source energy so that the neutrons slow down for a while without migrating at all. $q(ku)$ then depends on u only through c. In the case that the source energy is very high the limit of the outer integral in Eq. (16) can be replaced by ∞ which is the formal manner in which the explicit dependence of $q(ku)$ on u disappears. In this limit it is possible to express the right-hand side of Eq. (16) as a convergent series for all values of c in the P_1 approximation, which greatly facilitates numerical evaluation, viz.,

$$q(k) = 1 - \frac{1}{2}\left(\frac{c}{c+1}\right)\left[1 + \frac{1}{5}\left(\frac{c}{c+1}\right) + \frac{1.4}{5.8}\left(\frac{c}{c+1}\right)^2 + \frac{1.4.7}{5.8.11}\left(\frac{c}{c+1}\right)^3 + \ldots\right] \qquad (17)$$

The Selengut-Goertzel approximation can also be solved by reduction to a first-order linear differential equation. The result is

$$\begin{aligned} q(ku) &= e^{2u}\,(e^{3u} + 3c)^{-2/3}\,(1 + 3c)^{-1/3} \\ &\longrightarrow (1 + 3c)^{-1/3} \text{ as } u \longrightarrow \infty \end{aligned} \qquad (18)$$

Plotted in Fig. 2 is the $q(ku)$ in the P_1, B_1, and Selengut-Goertzel approximations in the case that q is independent of the source energy. In this case it is

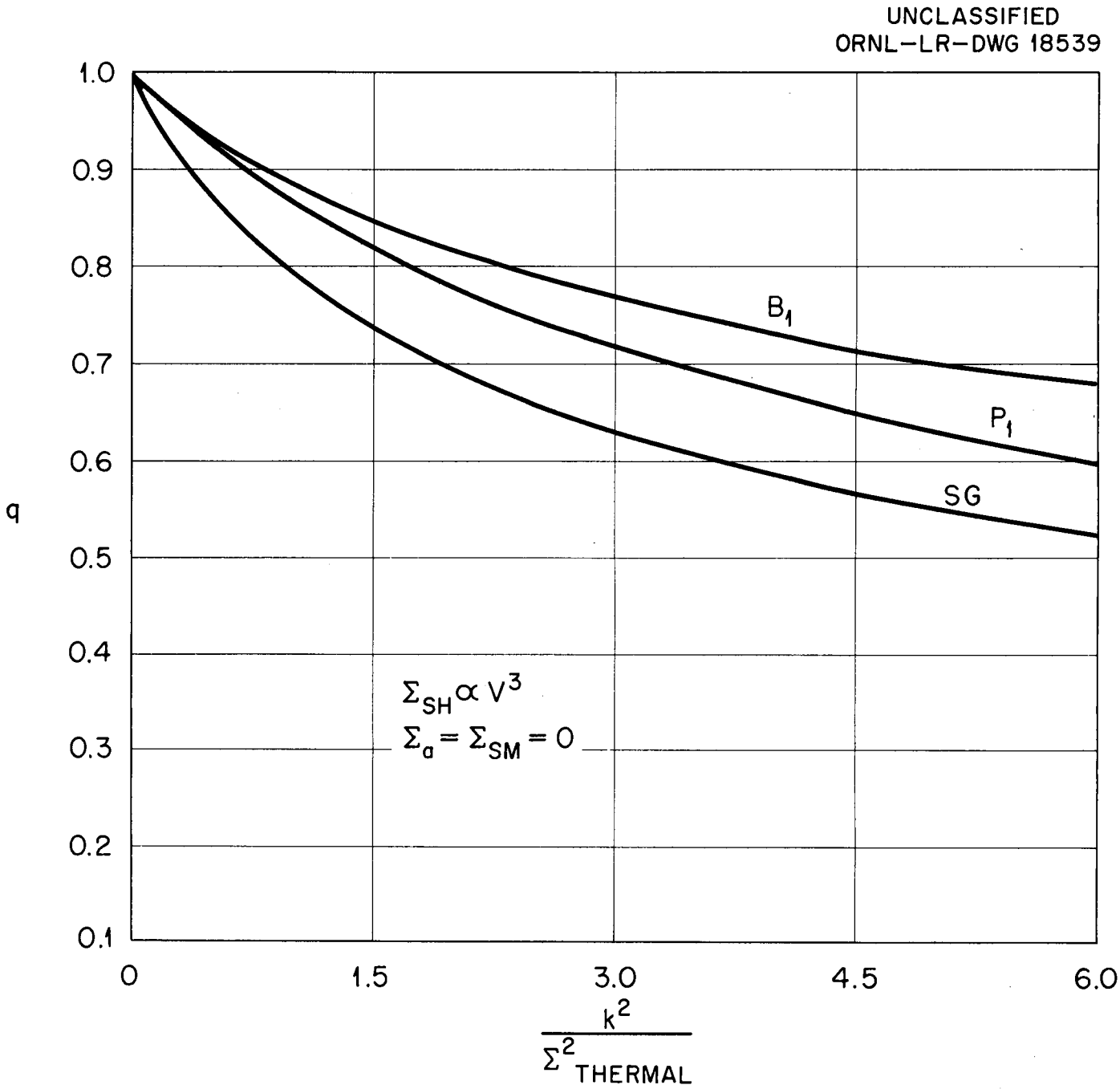

Fig. 2. Variation of Slowing Down Density with Buckling.

seen that both the P_1 and Selengut-Goertzel underestimate the B_1 value of $q(ku)$, the underestimate being larger for the Selengut-Goertzel approximation. The age in the Selengut-Goertzel approximation is greater than the exact age, calculation shows it to be $1/3\,\Sigma^2_{SH}(u)$, which is twice the exact age.