Multiple Scattering in a Semi-Infinite Medium^{*}

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The Boltzmann equation for the multiple scattering of charged particles is solved for a semi-infinite medium by means of the Laplace transformation. The sources are isotropic and distributed throughout the medium, corresponding to a thick layer of electron emitting atoms. The solution is obtained as a series in spherical harmonics and is carried as far as the P_2 coefficient. In order to obtain a solution it is necessary to assume that the transport mean free path λ is not a function of energy. As a particular evaluation of the solution the flux on the surface is examined and modified to correct for the energy dependence of λ by comparing with the corresponding solution of the age diffusion equation. The resulting spectrum is compared with an experimental case of 301.3-kev photoelectrons produced in a thick thorium converter. Using the experimental spectrometer resolution of 1.5 percent the theoretical spectrum is integrated over the window curve and a shift of the peak from the edge of the primary spectrum of 4.3 kev is obtained. Considering the errors involved this compares favorably with the experimental peak shift of 3.5 kev for a converter thickness of 25 mg/cm².

I. INTRODUCTION

IN the study of multiple scattering of charged par-ticles much has been done within the limits of the small angle approximation, that is, by exploiting the fact that the scattering is predominantly forward. However, little has been done to include the effect of the wide angle scattering in the transport process and it is precisely this effect that must be considered if any knowledge of backscattering is to be obtained.

Goudsmit and Saunderson¹ have developed the theory for the angular distribution without the small angle limitation but this does not include the spatial distribution. Snyder and Scott² studied the integro-differential Boltzmann equation but again the small angle approximation was made. Lewis³ studied the Boltzmann equation in an infinite medium and obtained the Goudsmit and Saunderson angular distribution. In addition he developed a method for obtaining the moments of the spatial distribution.

The purpose of this paper is to study the solution of the Boltzmann equation in the presence of boundaries and thereby to gain some information on the backscattering. In particular, the multiple scattering in a semi-infinite medium is examined. The method, depending on an expansion in spherical harmonics, is not well suited for such situations as incident beams but converges rapidly for spherically symmetric sources. The main difficulty with the method is that the scattering cross section is not allowed to vary as a function of the velocity. Within this limitation the energy loss is treated by considering the energy as a function of the residual range of the particle.

The general method for solution of the Boltzmann equation in a semi-infinite medium is outlined in Sec-

tion II. In Sections III and IV the problem is solved for a uniform distribution of spherically symmetric sources and the flux at the surface is calculated. In Section Van estimation is made of the correction due to the variation of the cross section with velocity. This corrected flux is applied in Section VI to an experimental example of the energy spectrum of a thick source of electron emitters.

II. GENERAL METHOD

A. Transport Equation

We consider the distribution function f(x, s, v) in the semi-infinite medium, where x is the perpendicular distance in from the surface, s the distance the particle has traveled, and v a unit vector designating the direction of motion. This function satisfies the transport equation

$$\partial f/\partial s + u\partial f/\partial x = N \int [f(x, s, \mathbf{v}') - f(x, s, \mathbf{v})]\sigma(\mathbf{v} \cdot \mathbf{v}')d\mathbf{v}',$$
 (1)

where N is the number of scattering centers per unit volume, $u = \cos\theta$ relative to the x axis, and $\sigma(\mathbf{v})$ is the differential scattering cross section. The source is treated as an "initial" condition.

The procedure followed to solve the transport equation is to expand f(x, s, v) in Legendre polynomials and to solve the resulting system of equations by means of the Laplace transformation. Since the angular dependence of f is only through $\cos\theta$ we can let

$$f(x, s, \mathbf{v}) = \sum_{l} (2l+1) f_{l}(x, s) P_{l}(u).$$

Putting this into (1) and operating with $\int_{-1}^{+1} P_{l'} du$ we get

$$2\frac{\partial f_{l'}}{\partial s} + \sum_{l} (2l+1)\frac{\partial f_{l}}{\partial x} \int_{-1}^{1} P_{l'} u P_{l} du$$
$$= N \sum_{l} (2l+1) f_{l} \int_{-1}^{1} \int P_{l'}(u)$$
$$\times [P_{l}(u') - P_{l}(u)] \sigma(\mathbf{v} \cdot \mathbf{v}') d\mathbf{v}' du.$$

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<sup>San Francisco, Camorna.
¹S. Goudsmit and J. L. Saunderson, Phys. Rev. 57, 24 (1940).
^a H. Snyder and W. T. Scott, Phys. Rev. 76, 220 (1949).
^a H. W. Lewis, Phys. Rev. 78, 526 (1950).</sup>

Using the recurrence relation for $uP_{l'}$ in the second term we obtain, for this term

$$(2l+1) \int_{-1}^{1} P_{l'} u P_{l} du = 2 \bigg\{ \frac{l'+1}{2l'+1} \delta_{l, l'+1} + \frac{l'}{2l'+1} \delta_{l, l'-1} \bigg\}.$$

For the right-hand side expand the cross section

$$\sigma(u) = \sum_{n} (2n+1)c_n P_n(u),$$

with

$$c_n = \frac{1}{2} \int_{-1}^{1} P_n \sigma du,$$

so this term becomes, using the addition theorem for $P_n(u),$

$$2\pi N \sum_{l} \sum_{n} (2l+1)(2n+1) f_{l}c_{n} \int_{-1}^{1} \int_{-1}^{1} P_{l'}(u) \\ \times [P_{l}(u') - P_{l}(u)] P_{n}(u) P_{n}(u') du du' \\ = 8\pi N f_{l'}(c_{l'} - c_{0}).$$

If we define

$$\kappa_l(s) = 2\pi N \int_{-1}^1 \sigma(u) [1 - P_l(u)] du,$$

then Eq. (1) becomes

$$(2l+1)\left(\frac{\partial}{\partial s}+\kappa_{l}(s)\right)f_{l}(x,s)$$
$$+\frac{\partial}{\partial x}[(l+1)f_{l+1}(x,s)+lf_{l-1}(x,s)]=0. \quad (2)$$

In this problem the explicit form of the κ_l is determined by the fact that we use the scattering cross section for the screened coulomb potential $V = (Ze/r)e^{-r/a}$, that is

$$\sigma(u) = C/(1 - u + 2\psi)^2, \qquad (3)$$

where $C = (Z^2 e^4)/(m^2 v^4)$ and $\psi = \hbar^2/(2amv)^2$, v being the velocity of the scattered particle. For the cases we consider here ψ is small, so for moderate values of l we have4

$$l=0, \quad \kappa_l \equiv 0$$
$$l\neq 0, \quad \kappa_l \approx \pi NCl(l+1) \left[\ln \frac{1}{\psi} + 1 - 2 \sum_{m=1}^l \frac{1}{m} \right]. \quad (4)$$

We will first assume that σ is not a function of energy, then later study the modification due to energy dependence.

B. Solution by Laplace Transformation

To solve the system of differential Eq. (2) we make the Laplace transformations

$$h_l(y, t) = \int_0^\infty \int_0^\infty f_l(x, s) e^{-xy} e^{-st} dx ds$$

Thus integrating (2) over x and s we get the system of equations (κ_l are now constants)

$$(2l+1)(t+\kappa_l)h_l(y,t)+y[(l+1)h_{l+1}(y,t)+lh_{l-1}(y,t)] = (l+1)\eta_{l+1}(t)+l\eta_{l-1}(t)+(2l+1)\gamma_l(y),$$
(5)

where the transform of the distribution function at the boundary and at the "initial time" are given by

$$\eta_l(t) = \int_0^\infty f_l(0, s) e^{-st} ds, \quad \gamma_l(y) = \int_0^\infty f_l(x, 0) e^{-xy} dx.$$
(6)

The method of solution of the system (5) was suggested by a procedure applied to neutron diffusion⁵ as well as a similar treatment of Chandrasekhar⁶ on solar radiation. To simplify the equations we take s and xin units of the transport mean free path $1/\kappa_1$. Utilizing the relation (4) for the κ_l we make the approximation

$$\kappa_l/\kappa_1 \approx \frac{1}{2}l(l+1).$$

Then Eq. (5) becomes

$$lyh_{l-1}(y, t) + \alpha_{l}(t)h_{l}(y, t) + (l+1)yh_{l+1}(y, t) = (l+1)\eta_{l+1}(t) + l\eta_{l-1}(t) + (2l+1)\gamma_{l}(y), \quad (7)$$

where $\alpha_l(l) = (2l+1)[l+\frac{1}{2}l(l+1)]$. The approximation used is to assume that the expansion in Legendre polynominals converges rapidly enough so that the series may be cut off after the nth polynomial (this is called the P_n approximation). For the problem worked out here this assumption seems to be quite good, as will be seen below.

The determinant of the system (7) in the P_n approximation is:

	$lpha_0$	у	0	0	•••	0
D =	у	α_1	2y	0	• • •	0
	0	2y	α_2	3y	•••	0
	0	0	3y	α_3	•••	0
	•	•	•	•		•
	•	•	•	•		•
		•	•	•		•
	0	0	0	0	• • •	α_n

If we define D_l as the determinant D with the lth column replaced by the inhomogeneous terms in (7), then

$$h_l(y, t) = D_l(y, t)/D(y, t).$$

We will first consider the inverse transformation in the variable y. If $I_l(x, t)$ is the function obtained in this

⁴ See reference 3, p. 528.

 ⁵ See R. E. Marshak, Revs. Modern Phys. 19, 222 (1947).
 ⁶ S. Chandrasekhar, Astrophys. J. 99, 180 (1944).

transformation, then

$$I_{l}(x, t) = (1/2\pi i) \int_{C} h_{l}(y, t) e^{xy} dy, \qquad (8)$$

where C is the usual Laplace contour [parallel to the imaginary axis and to the right of the singularities of $h_l(y)$]. This integration is easily carried out since $h_l(y)$ contains only simple poles. The only poles that might occur in the numerator $D_l(y)$ are due to the functions $\gamma_l(y)$ in the inhomogeneous terms. If the x dependence of the source is restricted to $\delta(x)$ or to a constant (i.e., surface or thick sources) then the $\gamma_l(y)$ will have at most a simple pole at y=0. Such terms can be separated out by breaking up the inhomogeneous terms in the following manner. Let

$$c_{l}(y, t) \equiv (l+1)\eta_{l+1}(t) + l\eta_{l-1}(t) + (2l+1)\gamma_{l}(y) = \psi_{l}(t) + b_{l}/y.$$
(9)

Then D_i can be broken up also, $D_i = D_i^{\psi} + D_i^{b}$, where only D_i^{b} contains any poles that are in D_i . The only term in D_i^{b} for which b_i/y has no factor y, and therefore the only term retaining the pole, is the diagonal product

$$\alpha_0\alpha_1\cdots\alpha_{l-1}(b_l/y)\alpha_{l+1}\cdots\alpha_n.$$

Since $D(0) = \alpha_0 \alpha_1 \cdots \alpha_n$, the residue of this term in h_l contributes b_l / α_l to the integral. The remaining contributions come from the roots y_i of D(y). Therefore we can write

$$I_{l}(x, t) = \sum_{i} \left\{ \frac{D_{l}(y_{i})e^{xy_{i}}}{\left[D(y)/(y-y_{i})\right]y = y_{i}} \right\} + \frac{b_{l}}{\alpha_{l}}.$$

Since D(y) can be written in the form

$$D(y) = a - by^{2} + cy^{4} - \dots (-)^{k/2} dy^{k}, \quad k = n+1 \text{ if } n \text{ odd}$$
$$= n \text{ if } n \text{ even},$$

the roots of D(y) occur in pairs $y_i = \pm y_r$. Therefore we can write

$$D(y) = a \prod_{r=1}^{k/2} \left(1 - \frac{y^2}{y_r^2} \right), \quad a = \alpha_0 \alpha_1 \cdots \alpha_n.$$

The denominator then becomes

$$\left[\frac{D(y)}{y-y_i}\right] = \pm \frac{2a}{y_r} \prod_{s \neq r} \left(1 - \frac{y_r^2}{y_s^2}\right),$$

with the (+) sign if $y_i = -y_r$ and the (-) sign if $y_i = +y_r$. Therefore the y integration gives

$$I_{l}(x, t) = \sum_{r=1}^{k/2} \frac{y_{r}}{2a \prod_{s \neq r} \left(1 - \frac{y_{r}^{2}}{y_{s}^{2}}\right)} \times \{-D_{l}(+y_{r})e^{xy_{r}} + D_{l}(-y_{r})e^{-xy_{r}}\} + \frac{b_{l}}{\alpha_{l}}.$$
 (10)

The final inverse transformation then yields the solution

$$f_l(x, s) = (1/2\pi i) \int_C I_l(x, t) e^{st} dt.$$
(11)

C. Boundary Conditions

In order to perform the integration in Eq. (11) it is necessary to determine the $\eta_l(t)$. This is done by imposing boundary conditions at x=0 and $x\to\infty$. The conditions used are

$$f(x, s, u) = 0, \quad \begin{cases} x = 0 \\ u > 0 \end{cases} \quad (all s), \quad (12)$$

f(x, s, u) bounded as $x \rightarrow \infty$.

From the first condition it follows that

$$\int_{0}^{1} P_{l}(u) f(x=0, s, u) du = 0, \text{ all } l.$$
 (13)

In the P_n approximation this condition is applied to all l up to some value m < n determined by restrictions discussed below. This is equivalent to saying each moment of u up to u^m vanishes for u > 0. Since $f = \sum_k (2k+1) f_k P_k$ this condition becomes,

at
$$x=0$$
, $f_l+\sum_{k\neq l} f_k(2k+1) \int_0^1 P_l P_k du=0$,
 $l=0, 1, \cdots, m.$ (14)

Performing the Laplace transformation in s (Eq. (6)) this condition becomes

$$\eta_l(t) + \sum_{k \neq l} \eta_k(t)(2k+1) \int_0^1 P_l P_k du = 0.$$
 (15)

These conditions give m+1 linear relations among the η_l . The number of these relations that can be used are restricted by (1) the conditions imposed at infinity and (2) an additional condition that exists among the η_l when the number of differential equations used is odd (*n* even).

(1) Restrictions Imposed at Infinity

We will now show that the conditions at infinity give as many relations among the η_l as there are pairs of roots of D(y). The condition at infinity requires that $f_l(x, s)$ be bounded. Therefore the transform of f_l in x, $I_l(y, t)$, must be bounded. Looking at Eq. (10) we see that this means

$$D_{l}(+y_{r}) = 0, \quad l = 0, 1, \dots, n;$$

$$r = 1, \dots, \frac{1}{2}(n+1) \quad \text{for } n \text{ odd} \qquad (16)$$

$$= 1, \dots, \frac{1}{2}n \qquad \text{for } n \text{ even.}$$

Each equation in (16) gives a relation among the η_i , but we must determine how many are independent.

768

For a given root y_r consider the equation $D_l = 0$ as a set of n+1 homogeneous equations in the terms c_l as defined in (9). For instance, the first equation of this set is:

It can be seen that the coefficient of c_l in this equation is the cofactor of the corresponding term in $D(y_r)$. Since interchanging the rows and columns of D leaves it unchanged, we see that the determinant of the coefficients of the c_l , which we will call $\Delta(y_r)$, is formed by replacing each element of $D(y_r)$ by its cofactor; that is Δ is the adjoint of D, or $\Delta = D'$. Now if M is a minor of D of dimensions m and M' the corresponding minor of D', then7

$$M' = (D)^{m-1} \times (\text{algebraic complement of } M)$$

Since $D(y_r) = 0$ then any minor, M', equals zero unless m=1. Therefore the rank of Δ is one. Thus there is one independent relation among the c_l . The same argument holds for all the roots y_r . Therefore there are as many relations among the c_l , and consequently among the η_l , as there are pairs of roots⁸ y_r . In the P_n approximation this number is $\frac{1}{2}(n+1)$ if n is odd and $\frac{1}{2}n$ if n is even.

(2) Restriction Imposed for n Even

In the P_n approximation the first and the last differential equation of the set each contain only one x derivitive. Thus when the number of equations used is odd (n even) the last equation can be combined with all the preceding equations for which l is even so as to eliminate all the x derivatives in the sub-set. This means that in the x, t space there exists one algebraic relation among the $I_l(x, t)$ where l is even. At x=0 this gives one relation among the η_l . This can be seen in the P_2 approximation carried out below.

From this and the discussion above it follows that the number of relations (15) that must be used is $(n+1) - \frac{1}{2}(n+1) = \frac{1}{2}(n+1)$ if *n* is odd and (n+1) $-\frac{1}{2}n-1=\frac{1}{2}n$ if *n* is even.

III. P_1 APPROXIMATION

A. Solution of Equations

We now proceed to study a specific problem in the P_1 approximation. This is to find the distribution function for a thick layer of beta-emitting sources. We therefore treat this as a semi-infinite medium with the initial condition

$$f(x, s, u) = 0, \quad x < 0$$

= $A, \quad x > 0$ (18)

This represents a spherically symmetric emission of Aelectrons per unit volume, per unit solid angle throughout the medium.

The system (2), in this approximation, becomes

$$\frac{\partial f_0/\partial s + \partial f_1/\partial x = 0}{3(\partial/\partial s + 1)f_1 + \partial f_0/\partial x = 0}.$$
(19)

From Eq. (6) the initial condition (18) becomes

$$\gamma_l = (A/y)\delta_{l0}. \tag{20}$$

Therefore the transformed system (7) is

$$th_0 + yh_1 = \eta_1 + A/y, \quad yh_0 + \alpha_1 h_1 = \eta_0,$$
 (21)

where $\alpha_1 = 3(t+1)$. The determinant

$$D(y) = t\alpha_1 - y^2 \tag{22}$$

has roots $y = \pm y_1$ where

$$y_1 = (t\alpha_1)^{\frac{1}{2}}.$$
 (23)

From Eq. (10) and the condition at $x \rightarrow \infty$ (Eq. 16) the transforms in s are

$$I_{0}(x, t) = \frac{1}{2y_{1}} \left(\alpha_{1}\eta_{1} - \frac{\alpha_{1}A}{y_{1}} + y_{1}\eta_{0} \right) e^{-xy_{1}} + \frac{A}{t},$$

$$I_{1}(x, t) = \frac{1}{2y_{1}} (t\eta_{0} + y_{1}\eta_{1} - A) e^{-xy_{1}}.$$
(24)

From the previous discussion it is apparent that only one of the conditions (15) between the η_l can be used. The one chosen is for l=1, that is

$$\eta_1 + \frac{1}{2}\eta_0 = 0.$$

This is the relation resulting from the condition that the net incoming current vanishes. Using this relation to eliminate η_1 and using relation (16) for $x \rightarrow \infty$, we get

Then

$$D_0(y_1) \equiv \alpha_1 (A/y_1 - \frac{1}{2}\eta_0) - \eta_0 y_1 = 0.$$

$$\eta_0 = -2\eta_1 = 2A/(2t + y_1).$$

Substituting these into (24), the solutions become

$$f_{0}(x, s) = A - \frac{A}{2\pi i} \int_{C} \left[\frac{3(t+1)}{t} \right]^{\frac{1}{2}} \frac{e^{-xy_{1}+st}}{2t + [3t(t+1)]^{\frac{1}{2}}} dt,$$

$$f_{1}(x, s) = \frac{-A}{2\pi i} \int_{C} \frac{e^{-xy_{1}+st}}{2t + [3t(t+1)]^{\frac{1}{2}}} dt.$$
(25)

It will be noticed that the solutions give a more general initial situation than was imposed. That is, since $y_1 \rightarrow t\sqrt{3}$ for large t, the contours must be closed to the right if $\sqrt{3}x > s$ and the integrals contribute nothing.

⁷ M. Bôcher, Introduction to Higher Algebra (Macmillan Com-¹¹ New York, 1947), p. 31. ⁸ Assuming that there are no accidental relations $y_r = y_{r'}$.



FIG. 1. Theoretical electron flux $f_1(0, s)$ at surface of semiinfinite medium in P_1 and P_2 approximations. The P_2 approximation gives the lower curve for small values of s.

Thus the initial condition is for $s < \sqrt{3}x$ rather than just for s=0. This is what should be expected since the initial distribution is unaffected until s is large enough for the particle to reach the surface. The same condition holds in the P_2 approximation as will be seen below. However, in higher approximations, there will be a series of such integrals each arising from an additional root y_r and each contributing when s is greater than some value of x determined by the value of y_r for large t.

B. Current at the Boundary

For a specific evaluation of these solutions we consider the net flux at the boundary, that is

$$f_1(0,s) = -\frac{A}{2\pi i} \int_C \frac{e^{st}dt}{2t_+ [3t(t+1)]^{\frac{1}{2}}}.$$
 (26)

A cut is placed between the branch points t=0 and t=-1, and the contour is closed to the left about these points. The integrand may be rationalized and written as follows

$$f_1(0,s) = -\frac{A}{2\pi i} \int_C \frac{2t - [3t(t+1)]^{\frac{1}{2}}}{t(t-3)} e^{st} dt.$$

Since t=3 is a root of the numerator it is not a pole and thus the first term contributes nothing. The second term can be written as two integrals along the cut and combined to give (for convenience we replace t by -t)

$$f_1(0,s) = -\frac{A}{\pi} \int_0^1 \left[\frac{3(1-t)}{t}\right]^{\frac{1}{2}} \frac{e^{-st}}{(t+3)} dt.$$
(27)

This is evaluated in the appendix and plotted in Fig. 1.

IV. P2 APPROXIMATION

A. Solution of Equations

We now carry the same problem to the next approximation. The system (2) of equations is now

$$\frac{\partial f_0}{\partial s} + \frac{\partial f_1}{\partial x} = 0,$$

$$3(\partial/\partial s + 1)f_1 + \frac{\partial f_0}{\partial x} + 2\frac{\partial f_2}{\partial x} = 0,$$

$$5(\partial/\partial s + 3)f_2 + 2\frac{\partial f_1}{\partial x} = 0.$$

$$(28)$$

The transformed system, with the same initial conditions as above, is

$$th_{0}+yh_{1}=\eta_{1}+A/y,$$

$$yh_{0}+\alpha_{1}h_{1}+2yh_{2}=\eta_{0}+2\eta_{2},$$

$$2yh_{1}+\alpha_{2}h_{2}=2\eta_{2}.$$
(29)

The roots $y = \pm y_1$ of the determinant of this system are

$$y_1 = \left[t\alpha_1 \alpha_2 / (4t + \alpha_2) \right]^{\frac{1}{2}}.$$
 (30)

The transforms in s are (using conditions (16))

$$I_{0}(x, t) = \frac{1}{2} \left[\frac{\alpha_{2}(\eta_{0} - A/t + 2\eta_{2})}{4t + \alpha_{2}} + \frac{y_{1}\eta_{1}}{t} \right] e^{-xy_{1}} + \frac{A}{t},$$

$$I_{1}(x, t) = \frac{1}{2} \left[\eta_{1} + \frac{\alpha_{2}t(\eta_{0} - A/t + 2\eta_{2})}{y_{1}(4t + \alpha_{2})} \right] e^{-xy_{1}},$$

$$I_{2}(x, t) = \left[\frac{t(\eta_{0} - A/t + 2\eta_{2})}{4t + \alpha_{2}} + \frac{\eta_{1}y_{1}}{\alpha_{2}} \right] e^{-xy_{1}}.$$
(31)

For the relations among the η_l there is first the relation (16) due to the condition at $x \rightarrow \infty$. This is

$$(4t+\alpha_2)y_1\eta_1 - \alpha_2t(\eta_0 - A/t + 2\eta_2) = 0.$$

The relation due to the use of an odd number of equations as discussed above can be seen by considering the first and third of the Eqs. (28) in the x, t space:

$$tI_0 + \partial I_1 / \partial x = A$$
, $\alpha_2 I_2 + 2 \partial I_1 / \partial x = 0$.

Therefore at x=0, we have

$$2t\eta_0 - \alpha_2\eta_2 = 2A.$$

The third relation to be used is one of the conditions (15) and as before the condition for l=1 is chosen. This is

$$4\eta_0 + 8\eta_1 + 5\eta_2 = 0.$$

Solving for the η_l from these three equations gives

$$\eta_0(t) = A (4\alpha_2 + 5y_1)/W, \eta_1(t) = -2A\alpha_2/W, \eta_2(t) = -4Ay_1/W,$$

where $W = 2\alpha_2 y_1 + t(4\alpha_2 + 5y_1)$. Putting these into (31) gives

$$f_{0}(x, s) = A - \frac{2A}{2\pi i} \int_{C} \frac{\alpha_{2} y_{1} e^{-xy_{1}+st}}{tW} dt,$$

$$f_{1}(x, s) = -\frac{2A}{2\pi i} \int_{C} \frac{\alpha_{2} e^{-xy_{1}+st}}{W} dt,$$

$$f_{2}(x, s) = -\frac{4A}{2\pi i} \int_{C} \frac{y_{1} e^{-xy_{1}+st}}{W} dt.$$

(32)

B. Current at the Boundary

As before we evaluate this solution for a special case, that is the flux at the boundary

$$f_1(0,s) = -\frac{2A}{2\pi i} \int_C \frac{\alpha_2 e^{st} dt}{2\alpha_2 y_1 + t(4\alpha_2 + 5y_1)}.$$
 (33)

For large s the integral can be evaluated for $t \rightarrow 0$. This gives

$$f_1(0, s) \approx -\frac{A}{2\pi i} \int_C \frac{e^{st}}{(3t)^{\frac{1}{2}}} dt = -\frac{A}{(3\pi s)^{\frac{1}{2}}},$$

which is the same result that is obtained in the P_1 approximation [see (26) or compare with the leading term in (A1)].

For small s the integral is treated as follows. The integrand is rationalized [using y_1 given by (30)] giving

$$\frac{\frac{(4t+\alpha_2)^{\frac{1}{2}}\left[(t\alpha_1\alpha_2)^{\frac{1}{2}}(2\alpha_2+5t)-4\alpha_2t(4t+\alpha_2)^{\frac{1}{2}}\right]e^{st}}{t\left[\alpha_1(2\alpha_2+5t)^2-16\alpha_2t(4t+\alpha_2)\right]}}{f_1(0,s)=\frac{1}{2\pi i}\left(\frac{2A}{15}\right)\int_C\frac{15(t+2)\left[45t(t+\alpha_2)\right]}{t\left[\frac{1}{2\pi i}\left(\frac{2A}{15}\right)\right]}dt}$$

with the contour as shown in Fig. 2. The second term contributes nothing so we can write

$$f_{1}(0, s) = \frac{2A(15)^{\frac{1}{2}}}{2\pi i} \int_{C} \times \frac{(t+2)[(t+1)(t+3)(t+5/3)]^{\frac{1}{2}}}{t^{\frac{1}{2}}(t-t_{1})(t-t_{2})(t-t_{3})} e^{st} dt. \quad (35)$$

Integrating along the cuts gives

$$f_1(0,s) = \frac{2A(15)^{\frac{1}{2}}}{\pi} [P(s) + Q(s)], \qquad (36)$$

where

$$\begin{split} P(s) &= -i \int_{0}^{-1} \frac{(t+2) [(t+1)(t+3)(t+5/3)]^{\frac{1}{2}}}{t^{\frac{1}{2}}(t-t_{1})(t-t_{2})(t-t_{3})} e^{st} dt, \\ Q(s) &= -i \int_{-5/3}^{-3} \frac{(t+2) [(t+1)(t+3)(t+5/3)]^{\frac{1}{2}}}{t^{\frac{1}{2}}(t-t_{1})(t-t_{2})(t-t_{3})} e^{st} dt. \end{split}$$

These are evaluated in the appendix and plotted in Fig. 1.

Figure 1 illustrates the behaviour of the convergence of the polynomial expansion. For large s the main contribution in the t integral comes from the singularities near the origin and, as was seen above, this brings the higher approximation into agreement with the lower one. However for s small the singularities away from the origin contribute. These arise in the higher approximation because more terms α_l are involved in the roots of D(y). This is to be expected since the P_1 ap-



FIG. 2. Contour in t-plane for P_2 approximation.

The denominator can be rewritten, expanding the α_l and collecting terms in t, to give

$$15t(-3t^3+t^2+120t+180)$$

The roots of this polynomial are

$$t_1 = -1.6305, t_2 = -5.1633, t_3 = 7.1271.$$
 (34)

All of these as well as t=0 are roots of the numerator, therefore there are no poles. Expanding the numerator, we get

$$\frac{15(t+2)[45t(t+1)(t+3)(3t+5)]^{\frac{1}{2}}-60t(t+3)(3t+5)}{t(t-t_1)(t-t_2)(t-t_3)}e^{st}dt,$$

proximation gives the diffusion approximation (see next section) and therefore should give good results when s is sufficiently far from the source. The next approximation, involving the next spherical harmonic, is then the improvement on this and one should expect P_2 to deviate most from P_1 for small s, that is before the diffusion region is reached.

From an elementary calculation (see appendix) it can be shown that f_1 should approach the value $\frac{1}{4}A$ as s approaches zero. It can be seen from Fig. 1 that P_2 improves on P_1 in this respect deviating from the correct end point by only about 3 percent.

V. ENERGY DEPENDENCE

The *s* dependence of the distribution function can be related to the energy through the empirical rangeenergy relation and thus the energy dependence may be obtained. However our treatment of the Boltzmann equation did not include the energy dependence of the cross section and therefore of the variation in the mean free path. No satisfactory way was found to take account of this in the solution of the Boltzmann equation. However a rough estimate of this effect on the spectrum at the surface may be obtained by use of the age equation employed in neutron diffusion.⁹ Solutions for this for constant and for variable cross section are compared with the previous solution and an estimate is then made of the necessary correction.

We now consider the cross section as a function of s. Starting with the system of Eqs. (19) of the P_1 approximation the additional approximation is made that $\partial f_1/\partial s$ is small (that is, that the fractional change of f_1

⁹ See R. E. Marshak, Revs. Modern Phys. 19, 212 (1947).

along s in a transport mean free path is small). This is a good approximation when far enough away from the source, as will be seen. In fact, since f_2 has already been neglected, for large s this may be more consistent than the previous procedure near discontinuities in x since the variation in s might be less than the neglected higher harmonics. The system then becomes

$$\frac{\partial f_0}{\partial s} + \frac{\partial f_1}{\partial x} = 0,$$

$$3\kappa_1(s)f_1 + \frac{\partial f_0}{\partial x} = 0.$$
(37)

Eliminating f_1 and defining the age variable

$$\tau(s) = \int_0^s ds / \kappa_1(s),$$

we get the age diffusion equation

$$\partial f_0 / \partial \tau = \frac{1}{3} \partial^2 f_0 / \partial x^2. \tag{38}$$

The boundary condition can be obtained by utilizing the relation existing between f_0 and f_1 in the P_1 approximation as a condition for no returning current, that is

$$f_0 = -2f_1.$$

Combining with the second of (37) gives

$$\partial f_0/\partial x = -\frac{3}{2}\kappa_1(s)f_0$$
, at $x=0$. (39)

The initial condition is given by

$$f_0=A$$
, at $\tau=0$.

To solve this problem with this boundary condition is difficult. However, since $\kappa_1(s)$ is slowly varying in s under certain conditions (e.g., large Z of the scatterer, not too large s) we make the approximation that in the boundary condition κ_1 is constant, that is $\kappa_1 = \kappa_1(0)$. This then is the heat problem of a constant initial temperature and radiation at the surface into zero temperature.¹⁰ The solution is

$$f_{0} = A \left\{ \operatorname{erf} \left[x \left(\frac{3}{4\tau} \right)^{\frac{1}{2}} \right] + e^{\frac{3}{2}x + \frac{3}{4}\tau} \operatorname{erfc} \left[x \left(\frac{3}{4\tau} \right)^{\frac{1}{2}} + \left(\frac{3\tau}{4} \right)^{\frac{1}{2}} \right] \right\}. \quad (40)$$

The current at x=0 is given by

$$f_1 = -\frac{1}{3\kappa_1(s)} \left(\frac{\partial f_0}{\partial x}\right)_{x=0} = -\frac{A}{2\kappa_1(s)} e^{\frac{3}{4}\tau(s)} \operatorname{erfc}(\frac{3}{4}\tau(s)). \quad (41)$$

VI. COMPARISON WITH EXPERIMENT

The experimental situation with which the above results could best be compared would be the energy spectrum of an internal conversion line produced in a thick layer of fairly heavy material and measured with an instrument of known resolving power. Such data were not found. We shall, therefore, compare results with the data of Hornyak, Lauritsen, and Rasmussen¹¹ on the photoelectron spectrum of the 411-kev gamma-radiation of Au^{198} converted in thorium (301.3-kev maximum electron energy).

To make the comparison for this case it is first necessary to estimate the energy-dependence correction to the derived spectrum as discussed in section V above. Then the corrected spectrum in s must be transformed to a function of energy. The resulting spectrum is then integrated with the known window curve of the spectrometer to get the spectrum as it appears experimentally.

A. Correction for Energy Dependence

We now evaluate $f_1(0, s)$ in Eq. (41). Over the range of s considered here the transport mean free path $1/\kappa_1(s) = \lambda(s)$ does not vary much in s so we can write

$$\lambda(s) = \lambda(0) \left[1 + \frac{1}{\lambda(0)} \left(\frac{d\lambda}{dE} \frac{dE}{ds} \right)_{E = E_{\max}} s \right].$$
(42)

For $d\lambda/dE$ we use the relativistic form of (4)

$$\kappa_1 = \frac{2\pi N Z^2 e^4}{(mc^2)^2 (\gamma - \gamma^{-1})^2} \left[\ln \frac{1}{\psi} - 1 \right],$$

where

$$\psi = \hbar^2 / [4a^2m^2c^2(\gamma^2 - 1)], \quad \gamma = (1 - v^2/c^2)^{-\frac{1}{2}}$$

For this case, the kinetic energy is 301.3 kev, A = 232, and Z = 90. Then $\lambda(0) = 11.63 \text{ mg/cm}^2$ and $d\lambda/dE = 0.0602 \text{ mg/cm}^2$ kev). For the factor dE/ds we will use the energy loss relation:

$$\frac{dE}{dx} = \frac{2\pi NZe^4}{mc^2(\gamma - \gamma^{-1})}$$

$$\times \left[\ln \frac{(mc^2)^2}{2I^2} + \ln(\gamma^2 - 1)(\gamma - 1) - \left(\frac{2}{\gamma} - \frac{1}{\gamma^2}\right) \ln 2 + \frac{1}{\gamma^2} \right]$$

FIG. 3. Theoretical primary spectrum $f_1(0, s)$ corrected for energy dependence for case of 301.3-kev photoelectrons produced in thorium.

¹¹ Hornyak, Lauritsen, and Rasmussen, Phys. Rev. 76, 731 (1949).

¹⁰ See Carslaw and Jaeger, *Conduction of Heat in Solids*, (Oxford University Press, London, 1946), p. 51.

For the average ionization potential I/Z we will use the value of 9.6 ev determined for uranium by Segrè and Bakker.¹² This gives, at 301.3 kev

$$dE/dx = -1.145 \text{ kev}/(\text{mg/cm}^2).$$
 (43)

Since s is measured in units of $\lambda(0)$, Eq. (42) becomes

$$\lambda(s)/\lambda(0) = 1 - 0.0688s.$$
 (44)

Using this, the age solution (41) is calculated and plotted in Fig. 3. From this solution the correction to the P_2 solution is then extrapolated to the correct end point.

B. Integration over Window Curve

In order to obtain the resultant spectrum we integrate the primary spectrum over the window curve which we take to be gaussian. The resulting distribution is

$$N(E) = \int_{0}^{E_{m}} f(E_{m} - E') \\ \times \exp[-(E' - E)^{2}/(aE')^{2}]dE', \quad (45)$$

where f is the primary spectrum with maximum energy E_m and a is determined by the resolution of the spectrometer. In this calculation we use for the resolution a width of 1.5 percent at half-maximum.¹³ This gives $a=9.0\times10^{-3}$.

To facilitate the integration we notice that the main contribution comes from the region E'=E to E'-E=aE' and since a is small, we have

$$(E'-E)/E\ll 1$$
.

The denominator in the exponential can then be written

$$(aE')^{-2} = (aE)^{-2} [1 - 2(E' - E)/E].$$

Placing this into (45) and expanding the exponential due to the last term we get

$$N(E) = \int_{0}^{E_{m}} f(E_{m} - E) \exp[-(E' - E)^{2}/(aE)^{2}] \times [1 + 2(E' - E)^{3}/a^{2}E^{3}]dE'.$$
(46)

Over the range of integration a linear approximation for the primary spectrum can be used, so that

$$f(E_m-E)=f(E_m)-(df/dE)E_m(E_m-E).$$

In terms of *s* we have

$$\frac{df}{dE} = \frac{df}{ds} \frac{ds}{dE} = \frac{1}{\lambda(0)} \frac{df}{ds} \frac{dx}{dE'},$$

¹² E. Segrè and C. J. Bakker, Phys. Rev. 81, 489 (1951).



FIG. 4. Theoretical spectrum of 411-kev radiation from Au¹⁹⁸ converted in thick Th foil (301.3-kev maximum energy of photoelectron). 1.5 percent resolution of spectrometer.

where df/ds is determined by the extrapolated curve in Fig. 3, and dE/dx is given by (43). Thus we can write (taking df/ds = 0.0470)

$$f(E_m - E) = A - B(E_m - E) \tag{47}$$

with A = 0.250 and B = 0.00353. Integrating (46) gives

$$N(E) = aE\{\frac{1}{2}(A - By)\pi^{\frac{1}{2}}[1 + erf(y/aE)] - a[(A - By)(1 + [y/aE]^{2}) + \frac{1}{2}EB]\exp[-(y/aE)^{2}]\}, \quad (48)$$

where $y = E_m - E$. This is plotted in Fig. 4.

C. Discussion of Results

Perhaps the most interesting result of the calculations in the previous section is the peak shift, that is the shift in the maximum of the spectrum from that of the primary spectrum. The above theoretical calculation gives a value of about 4.3 kev. Hornyak, *et al.* give, for a converter thickness of 0.0005 inch (16 mg/cm²), a value of 3.2 kev. For thicker converters their data indicates the results in Table I. The value for 0.001 inches is taken from a plotted spectrum in their article and has the most uncertainty. They also make a theoretical estimation of the upper limit, i.e., for an infinitely thick converter.

One of the largest sources of error in our calculations is the estimation for the energy dependence correction. An error in the slope df/ds of 10 percent results in an error in the peak shift of about 5 percent. Another source of difference is that the photoelectrons are not produced isotropically, although there will be some averaging out due to the angular distribution of the incident gamma-rays. With this in mind, we see that the peak shift comparison, although not conclusive, seems to give fairly good agreement.

TABLE I. Experimental and theoretical peak shifts for spectra of

301.3-kev photoelectrons produced in thorium.

	Converter thickness	Peak shift
Exp.	0.0005 in. (16 mg/cm ²) 0.001 in. (25 mg/cm ²) 0.003 in. (78 mg/cm ²)	3.2 kev 3.5 kev 3.8 kev
Theor.	upper limit, Hornyak <i>et al</i> . infinite, our calculation	4.3 kev 4.3 kev

One interesting point is that Hornyak *et al.* perform an "unfolding" of their experimental spectrum to obtain the primary spectrum. They obtain a curve with a marked peak at the maximum energy in sharp contrast to our results. They remark that the unfolding operation is quite sensitive to the experimental position of the maximum energy and that a shift of the order of the probable error results in a much smoother curve—a curve which would be in much better agreement with our results.

One more remark can be made and that concerns the effect of a finite width source. It was noticed in the solutions in Secs. III and IV that, for a given depth x, the initial solution is undisturbed until $s = \sqrt{3}x$. (As was pointed out in Sec. III this is only true in the P_1 and P_2 approximations and is an oversimplification.) Therefore, for a finite thickness, the spectrum will be unaltered until $s = \sqrt{3}l$, where l is the width of the slab.¹⁴ To estimate the value of l below which the peak will be changed from its limiting position, we note that the window curve has a half-width of about 4.5 kev. Adding this to the limiting peak shift, we get 8.8 kev. If the primary spectrum is altered below this value then the peak will be changed. This corresponds to a value of l of about 4.4 mg/cm². Hornyak, et al., note that the peak position is changed most when going from a converter of 7 mg/cm² to one of 16 mg/cm² and thereafter the change is small. Thus our results give a value of the right order of magnitude.

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TABLE II. Coordinates and weights for Gauss quadrature of the integral $\int_{-1}^{1} (1-x^2)^{-\frac{1}{2}} P(x) dx$ for n=3 and m=5.

0.0660	
$x_1 = -0.8000$ $a_1 = 1.$	0472
$x_2 = 0$ $a_2 = 1.$	0472
$x_3 = +0.8660$ $a_3 = 1.$	0472

¹⁴ The solution of the problem for a finite slab in the P_1 approximation can be obtained as a series containing the semiinfinite solution plus integrals that are nonvanishing when $s > \sqrt{3}l$, $s > 2\sqrt{3}l$, $s > 3\sqrt{3}l$, etc.

VII. APPENDIX

A. Evaluation of $f_1(0,s)$ in P_1 Approximation

From Eq. (27) we had

$$f_1(0, s) = -\frac{A}{\pi} \int_0^1 \left[\frac{3(1-t)}{t} \right] \frac{e^{-st}}{(t+3)} dt$$

For large s the main contribution comes from near t=0 so the coefficient of e^{-st} in the integrand can be expanded in powers of t and the integral evaluated term by term. This gives

$$f_1(0,s) = -\frac{A}{\pi\sqrt{3}} \left(\frac{1}{s^4} \gamma(\frac{1}{2},s) - \frac{5}{6} \frac{1}{s^4} \gamma(\frac{3}{2},s) + \frac{11}{72} \frac{1}{s^{5/2}} \gamma(5/2,s) \right), \quad (A1)$$

where $\gamma(n, s)$ is the incomplete gamma-function.

For small s the integrand is rewritten by the substitution t=(1+u)/2

$$f_1(0,s) = -\frac{A\sqrt{3}e^{-s/2}}{\pi} \int_{-1}^1 \frac{(1-u)e^{-su/2}}{(1-u^2)^{\frac{1}{2}}(u+7)} du.$$
(A2)

The integral is written in this form in order to facilitate numerical integration by Gauss' method.¹⁵

We will briefly examine the Gauss method. For an integral of the form

$$\int_{a}^{b} P(x)w(x)dx \tag{A3}$$

where w(x) is some known function and P(x) is a polynomial of degree *m* in *x*, it is possible to construct a quadrature formula using *n* values of P(x) at points x_i with weights a_i so that the integral is given exactly by

$$\int_{a}^{b} P(x)w(x)dx = \sum_{i=1}^{n} a_{i}P(x_{i})$$
(A4)

with $n = \frac{1}{2}(m+1)$. For the integral (A2) it is convenient to take

$$w(u) = (1 - u^2)^{-\frac{1}{2}}.$$

If the a_i and the x_i are determined for n=3, the error involved can be estimated by examining the expansion of $e^{-(s_{10})/2}$ up to and including (s_{10}) .⁵ The error at the extremes of the interval will be small if $s^6/6! < 1$ or $s \sim 3$. Thus the error of the quadrature will be small for values of s somewhat over s=3. We therefore take n=3and m=5. The points and weights determined for this case are given in Table II. Using these values the integral (A2) is evaluated and plotted in Fig. 1.

B. Evaluation of $f_1(0,s)$ in P_2 Approximation

For the evaluation of the integrals (36) we will use the same procedure as before for small s. For the integral P(s) we make the transformation t = (u-1)/2. Then

$$P(s) = e^{-s/2} \int_{-1}^{1} \frac{(u+3)(u+1)[(u+5)(u+7/3)]^{\frac{1}{2}}e^{us/2}}{(1-u^2)^{\frac{1}{2}}(u-u_1)(u-u_2)(u-u_3)} du,$$

where $u_1 = -2.2610$, $u_2 = -9.3266$, $u_3 = 15.2542$. This method, with weights and divisions for a polynomial of fifth degree, still gives good results for this integral. The worst factor in the integrand, $(u+2.2610)^{-1}$, approximated by a polynomial of second degree only has an error of 8.5 percent at the end points $u = \pm 1$. For the evaluation of Q(s) let t = (2v-7)/3. Then

$$Q(s) = \frac{e^{-7s/3}}{\sqrt{2}} \int_{-1}^{1} \frac{(2v-1)(1-v^2)(2-v)^{\frac{1}{2}}e^{2vs/3}}{(1-v^2)^{\frac{1}{2}}(7-2v)^{\frac{1}{2}}(v-v_1)(v-v_2)(v-v_3)} dv,$$

where $v_1 = 1.0542$, $v_2 = -4.2449$, $v_3 = 14.191$. To assume that the coefficient of $(1-v^2)^{-\frac{1}{2}}$ in this case approximates a fifth-order polynomial seems questionable because of the factor $(v-1.0542)^{-1}$ near the limits $v = \pm 1$. However, (a) the main contribution to the

¹⁵ See S. Chandrasekhar, *Radiative Transfer* (Oxford University Press, London, 1950), p. 57.

integral comes from the central part of the interval because of the factor $(1-v^2)$, (b) the factor $e^{-(7e)/3}$ rapidly reduces the contribution of Q to f_1 for larger s, and (c) even for s=0 the contribution of Q to f_1 is only about 4 percent. Therefore it seems justified to use this more convenient method in this case also. Integral (36) is plotted in Fig. 1.

C. End-Point Calculation

In this section we calculate the value of $f_1(s, x)$ at the boundary x=0 when $s \rightarrow 0$ by simply considering the distribution f(s, x, u)before many collisions have occurred. The density and the current for a given distance s, integrated over unit volume, are given by

> $D = \int f(s, x, u) d\Omega = 2\pi \int_{-1}^{1} f du$ $J = \int u f d\Omega = 2\pi \int_{-1}^{1} u f du.$

PHYSICAL REVIEW

Since

we have

$$f_l = \frac{1}{2} \int_{-1}^{1} P_l f du$$

 $D = 4\pi f_0, J = 4\pi f_1.$

The number of particles that go a distance s without a collision is given by the kernel $e^{-s}/(4\pi s^2)$. If we consider a distance s sufficiently small so that the initial, spherically symmetric distribution with density $D=4\pi A$ is undisturbed, then the current is given by

$$J = -\int \frac{e^{-\bullet}}{4\pi s^2} 4\pi A \, \cos\theta s^2 d\Omega$$

(negative since current is out). At x=0 this is

 $J = -2\pi A e^{-s} \int_{0}^{1} u du = -\pi A e^{-s}.$

In the limit as $s \rightarrow 0$, $J = -A\pi$ and therefore $f_1 = -\frac{1}{4}A$.

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Total Cross Section of Nitrogen for Fast Neutrons*

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The total neutron cross section of nitrogen has been measured for neutron energies from 0.15 to 1.45 Mev. Resonances in the total cross section are observed at 0.433, 0.640, 1.00, 1.12, 1.35, and 1.45 Mev. The second, third, and last of these resonances correspond in energy to resonances observed in the disintegration of nitrogen. Application of the nuclear dispersion theory indicates that the resonances at 0.64 and 1.00 Mev are caused by neutrons of zero orbital angular momentum forming compound states of spin $\frac{1}{2}$ and $\frac{3}{2}$, respectively. An experiment is proposed which would, in conjunction with these measurements, determine the relative parity of C14 and N14.

I. PROCEDURE AND RESULTS

FOR the interpretation of previously published results on the disintegration of nitrogen by fast neutrons,¹ a knowledge of the total neutron cross section of nitrogen is desirable. A preliminary measurement² of this cross section in which NaN₃ was used as the scattering material showed a resonance at 440 kev, the same energy at which a prominent resonance occurs in oxygen. It was, therefore, suspected that the NaN3 might have contained some water. Furthermore, it was desirable to use nitrogen combined with elements having no resonances in the range of neutron energies considered.

In the present measurements aminotetrazole $(N_5 CH_3)$ was used. It had been purified by recrystallization, and the water of crystallization was driven off quantitatively by heating.3 Sufficient carbon was added to give a mixture with the empirical formula $N_{10}(CH_2)_3$. The

effect of the nitrogen was observed by comparing the neutron attenuation produced by the mixture with that of a polythene sample having the same number of carbon and hydrogen atoms as the mixture. The cross section of nitrogen was determined in a simple transmission experiment,⁴ assuming exponential attenuation of the neutron flux by nitrogen. Corrections were applied for the background of neutrons scattered from the walls and the floor and for scattering by nitrogen into the detector.

In the lower portion of Fig. 1 the observed total cross section of nitrogen is shown as a function of neutron energy. Points were taken at intervals less than the neutron energy spread except in the energy range from 0.7 to 0.9 Mev where the NaN_3 data had shown no resonances. Cross sections given in Fig. 1 agree with those previously obtained using NaN₃. The results also agree with the observations of Frisch⁵ for neutron energies below 0.4 Mev, but not for neutron energies from 0.5 to 0.8 Mev.

In the upper part of Fig. 1 is plotted the sum of the N(n, p) and $N(n, \alpha)$ cross sections previously reported.¹

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