Multiple Scattering in an Infinite Medium

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The integro-differential diffusion equation of the multiple scattering problem in an infinite, homogeneous, medium, is studied without the usual small-angle approximation. An expansion in spherical harmonics is carried out which is rapidly convergent in the case of large-angle scattering, whose coefficients can be exactly determined, and which leads to expressions for the various moments of the spatial and angular distributions. The latter alone has previously been obtained by Goudsmit and Saunderson, and, in the small-angle approximation, by Snyder and Scott. Our results are shown to include these.

I. INTRODUCTION

It is the purpose of this paper to describe a direct method of obtaining exact results from the diffusion equation of the multiple scattering problem, without the usual small-angle approximation. The main limitation of the method lies in the fact that we are restricted to an infinite and uniform medium, which precludes the treatment of problems involving plates or foils, or of the reflection problem at boundaries between different media. We will take into account energy loss, simply by regarding the energy of the particle as a function of its residual range, which is permissible as long as the straggling in energy loss is small, and we do not concern ourselves with the question of the individual scattering cross section at a single atom. The former condition limits us to energies below the critical energy of shower theory in the medium in question, which is (except in the heaviest elements) the only region in which the small-angle approximation may not be adequate.

The question of the angular distribution in large-angle multiple scattering has been studied by Goudsmit and Saunderson,[1] who exploited a persistence property of the Legendre polynomials. Their method leads in the most direct way to Eq. (7) below, which we take the liberty of re-deriving, but does not seem to be easily extensible to the study of spatial distributions.

Bethe, Rose, and Smith[2] have considered the penetration of electrons through thick plates, neglecting energy loss, using the Fokker-Planck differential equation of the problem. The major disadvantage of the Fokker-Planck approximation stems from the well-known fact[3] that in the small-angle approximation it leads to a Gaussian solution, hence omits the tail of the angular distribution. Snyder and Scott[4] have recently studied the diffusion equation in its integral form, and in the small-angle approximation, and have derived exact solutions for this case, which show clearly the transition from the Gaussian-like inner region of the curve to the long single-scattering tail. We will show later that, in the small-angle case, our solution passes exactly into theirs.

II. BASIC EQUATION

If the direction of motion of the charged particle is given by the unit vector $\mathbf{v}$, the cross section for scattering, per unit solid angle, by σ, the position by $\mathbf{x}$, and the distribution function by $f(\mathbf{x}, \mathbf{v}, s)$, then the diffusion equation for the problem is

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

where s is the arc length traversed by the particle, N the number of atoms per unit volume, and the integration is over the solid angle. We will want to solve this equation under the boundary conditions $f(\mathbf{x}, \mathbf{v}, 0) = \delta(\mathbf{x})\delta(\mathbf{v})$, corresponding to a single particle, incident at the origin, and moving in the z direction. To put the equation in a more tractable form, we expand the solution in normalized surface harmonies in $\mathbf{v}$, so that

$$f=\sum_{lm} f_{lm}(\mathbf{x}, s)Y_{lm}(\mathbf{v}) \quad (2)$$

and obtain from (1) and (2)

$$(\partial f_{lm}/\partial s)+\sum_{\lambda\mu} \nabla f_{\lambda\mu}\cdot \mathbf{Q}_{lm}{}^{\lambda\mu} = N\sum_{\lambda\mu} f_{\lambda\mu}\int\int Y_{lm}{}^*(\mathbf{v})[Y_{\lambda\mu}(\mathbf{v}')-Y_{\lambda\mu}(\mathbf{v}) \times\sigma(\mathbf{v}-\mathbf{v}')d\mathbf{v}d\mathbf{v}', \quad (3)$$

where

$$\mathbf{Q}_{lm}{}^{\lambda\mu}=\int Y_{lm}{}^*\mathbf{v}Y_{\lambda\mu}d\mathbf{v}$$

is a constant vector, which is zero if $|\lambda-l|$ or $|\mu-m|$ is greater than unity. The last integral in (3) can be carried out most easily by expanding σ in Legendre polynomials, using the addition theorem for the spherical harmonics, and finally the orthogonality and normalization. The result is

$$(\partial f_{lm}/\partial s)+\kappa_l f_{lm}=-\sum_{\lambda\mu} \nabla f_{\lambda\mu}\cdot \mathbf{Q}_{lm}{}^{\lambda\mu}, \quad (4)$$

[1] S. Goudsmit and J. L. Saunderson, Phys. Rev. 57, 24 (1940) and 58, 36 (1940).
[2] Bethe, Rose, and Smith, Proc. Am. Phil. Soc. 78, 573 (1938).
[3] B. Rossi and K. Greisen, Rev. Mod. Phys. 13, 240 (1941).
[4] H. Snyder and W. T. Scott, Phys. Rev. 76, 220 (1949).

where

$$\kappa_l = 2\pi N \int_0^\pi \sigma(\vartheta)[1-P_l(\cos\vartheta)]\sin\vartheta d\vartheta, \qquad (5)$$

and the $P_l(\cos\vartheta)$ here are the usual (unnormalized) Legendre polynomials. The Fokker-Planck approximation can be obtained by expanding the Legendre polynomial in powers of ϑ^2, and keeping only the first two terms, one of which will cancel the unity in the square bracket.

The boundary conditions to be satisfied by the f_{lm} are

$$f_{lm}(\mathbf{x}, 0) = \delta_{m0}\delta(\mathbf{x})Y_{l0}(0) = [(2l+1)/4\pi]^{\frac{1}{2}}\delta_{m0}\delta(\mathbf{x}). \qquad (4')$$

III. THE ANGULAR DISTRIBUTION

To obtain the angular distribution alone, we integrate (4) over all space, thus losing the last term, and find

$$(\partial F_l/\partial s) + \kappa_l F_l = 0, \qquad (6)$$

where $F_l(s) = \int f_{l0}(\mathbf{x}, s)d\mathbf{x}$. The terms with $m \neq 0$ vanish because of the cylindrical symmetry of the problem. The solution to (6) is, of course,

$$F_l(s) = [(2l+1)/4\pi]^{\frac{1}{2}} \exp\left(-\int_0^s \kappa_l ds\right),$$

which satisfies the boundary conditions, so that

$$F(\mathbf{v}, s) = \int f(\mathbf{x}, \mathbf{v}, s)d\mathbf{x}$$

$$= (1/4\pi)\sum_{l=0}^{\infty}(2l+1)P_l(\cos\vartheta)\exp\left(-\int_0^s \kappa_l ds\right), \qquad (7)$$

where we have inserted the unnormalized polynomials, and regard κ_l as a function of s because of the energy dependence of the scattering cross section. This result has been obtained by Goudsmit and Saunderson[1] by a different method, and they have carried out a number of numerical examples. They have also described the approximation in which this distribution becomes Gaussian.

It is clear from (7) that the convergence of this expression depends upon the magnitudes of the expressions $\int \kappa_l ds$. These are, in turn, related to the mean scattering angles, as can be seen, for example, from the fact that

$$\langle\cos\vartheta\rangle_{\text{Av}} = \exp\left(-\int_0^s \kappa_1 ds\right),$$

or more generally,

$$\langle P_l(\cos\vartheta)\rangle_{\text{Av}} = \exp\left(-\int_0^s \kappa_l ds\right).$$

Thus, in the small-angle case, we can take

$$P_l(\cos\vartheta) \approx 1 - \tfrac{1}{4}l(l+1)\vartheta^2$$

so that

$$\int \kappa_l ds \approx \tfrac{1}{4}l(l+1)\langle\vartheta^2\rangle_{\text{Av}},$$

and, in this case, convergence will set in at around $l \sim 2(\langle\vartheta^2\rangle_{\text{Av}})^{-\frac{1}{2}}$. This makes it possible (in fact mandatory) in the latter case, to replace the sum in (7) by an integral, which will turn out to be just the Snyder-Scott integral, after the appropriate transformations.

IV. EVALUATION OF THE κ_l FOR A PARTICULAR CASE

If we now use the simplified potential $V = (Ze/r)e^{-r/a}$, the exponential factor schematizing the effect of screening, and calculate the scattering cross section by the Born approximation, we find, for a singly charged particle

$$\sigma(\vartheta) = \frac{Z^2e^4}{p^2v^2(1-\cos\vartheta+2\beta)^2}, \qquad (8)$$

where $\beta = \hbar^2/4a^2p^2$, and p and v are the momentum and velocity, respectively, of the scattered particle. Thus

$$\kappa_l = A\int_{-1}^{1}\frac{[1-P_l(\mu)d\mu]}{(1-\mu+2\beta)^2} = A(I_l - J_l), \qquad (9)$$

where $A = (2\pi NZ^2e^4)/(p^2v^2)$, and I_l and J_l are the integrals involving the two terms in the square bracket, respectively. The first is elementary and yields

$$I_l = 1/[2\beta(1+\beta)]. \qquad (10)$$

The second can be simplified by inserting Rodrigues' formula for the Legendre polynomial, integrating by parts l times, and making the substitution $1-\mu = 2\lambda$. One obtains

$$J_l = \tfrac{1}{2}(l+1)\int_0^1 \frac{\lambda^l(1-\lambda)^l d\lambda}{(\lambda+\beta)^{l+2}}. \qquad (11)$$

This is recognizable as a hypergeometric function,[5] and is

$$J_l = \tfrac{1}{2}\beta^{-l-2}\frac{\Gamma(l+1)\Gamma(l+2)}{\Gamma(2l+2)}F(l+1, l+2; 2l+2; -\beta^{-1}). \qquad (12)$$

Since β is small, in general, it is convenient to make the hypergeometric transformation to the reciprocal argument (WW289); the formula given there does not apply when the first two parameters of the function differ by an integer, as in our case, so that it is necessary to take the given transformation and carry out a limiting process to obtain a useful result. In addition,

[5] Whittaker and Watson, *Modern Analysis* (Oxford University Press, New York, 1946), American edtion, p. 293. We will have a number of references to this book, and in the future, will simply insert them into the body of the text, as, for example (WW293), for the above.

the formula given has a number of incorrect signs, and must be modified accordingly. After the transformation one has

$$2J_l=\frac{1}{\beta}+\sum_{\nu=0}^{l-1}\frac{\beta^\nu}{\nu!(\nu+1)!}\frac{(l+\nu+1)!}{(l-\nu-1)!}[\ln\beta-\psi(\nu+1)$$
$$-\psi(\nu+2)+\psi(l-\nu)+\psi(l+\nu+2)]-M_l(\beta), \quad (13)$$

where $\psi(z)=(d/dz)\ln\Gamma(z)$ and

$$M_l(\beta)=(-)^l\sum_{\nu=l}^{\infty}\frac{(-\beta)^\nu}{\nu!}\frac{(l+\nu+1)!(\nu-l)!}{(\nu+1)!}. \quad (13')$$

Since β is small in all physical cases, M_l can be neglected, for all l. This is not true of the first sum in (13), since the coefficient of β^ν is of the order of $l^{2\nu+2}$, which may be large.

One can now use the recursion formula for the ψ-functions to write the expression in the square bracket as

$$-G_{l\nu}=-\left[\ln(1/\beta)+\sum_1^\nu m^{-1}+\sum_1^{\nu+1}m^{-1}\right.$$
$$\left.-\sum_1^{l-\nu-1}m^{-1}-\sum_1^{l+\nu+1}m^{-1}\right]. \quad (14)$$

Here it is to be understood that sums in which the upper limit is less than unity are to be omitted. Thus, from (9), (10), (13), and (14), neglecting $M_l(\beta)$ and replacing $1/(1+\beta)$ by $1-\beta$, we have

$$\kappa_l=\tfrac{1}{2}A\left[-1+\sum_{\nu=0}^{l-1}\frac{\beta^\nu}{\nu!(\nu+1)!}\frac{(l+\nu+1)!}{(l-\nu-1)!}G_{l\nu}\right]. \quad (15)$$

All this applies only for $l\neq 0$; for $l=0$, $\kappa_l\equiv 0$, from its definition. For moderate values of l, it is sufficient to use

$$\kappa_l\approx\tfrac{1}{2}Al(l+1)\left[\ln\frac{1}{\beta}+1-2\sum_1^l m^{-1}\right]. \quad (15')$$

V. TRANSITION TO SMALL ANGLES

To carry out the transition to the case in which only small-angle scattering is important, we need only notice, as mentioned in Section III, that in this case the major contributions to the sum in (7) come from large values of l. Accordingly, we replace the sum in (7) by an integral, and consider the expressions (14) and (15) in the limit of large l.

In (14) we use the fact that the sum of the partial harmonic series is given by

$$\sum_1^A m^{-1}=\ln(A+\tfrac{1}{2})+C+O(A^{-2}), \quad (16)$$

where C is Euler's constant, and is equal to 0.5772. Using this fact in the sums in (15) that involve l in the upper limit, we find

$$G_{l\nu}\approx\ln(1/l^2\beta)-2C+\sum_1^\nu m^{-1}+\sum_1^{\nu+1}m^{-1} \quad (17)$$

for $\nu\ll l$. We also replace $(l+\nu+1)!$ in (15) by $l^{\nu+1}l!$ and similarly in the denominator, which approximation is valid for $\nu^2\ll l$, obtaining

$$\kappa_l\approx\tfrac{1}{2}Al^2\sum_{\nu=0}^{\infty}[(l^2\beta)^\nu/\nu!(\nu+1)!]G_{l\nu}$$
$$\approx lA\beta^{-\frac{1}{2}}[K_1(2l\beta^{\frac{1}{2}})]+\tfrac{1}{2}l\beta^{\frac{1}{2}}], \quad (18)$$

where $K_1(z)$ is the modified Bessel function of the second kind (WW374). We must now approximate the Legendre polynomials in (7) for small angles, and then project them on a plane, in order to make our result comparable with that of Snyder and Scott. The former is achieved by

$$P_l(\cos\vartheta)\approx J_0(l\vartheta) \quad (19)$$

(WW 367) where J_0 is the Bessel function of zero order, the latter by writing $\vartheta=(\varphi^2+\chi^2)^{\frac{1}{2}}$ with φ and χ the projections of ϑ on two mutually perpendicular planes through the polar axis, and integrating with respect to χ. Thus (WW 357, 377)

$$\int_{-\infty}^{\infty}J_0[l(\varphi^2+\chi^2)^{\frac{1}{2}}]d\chi=2l^{-1}\cos l\varphi, \quad (20)$$

if we take into account the fact that

$$\int_0^\infty J_n(z)dz=1,$$

for all n. Thus, finally, the distribution in φ becomes (if we neglect energy loss),

$$F(\varphi)\approx\frac{1}{\pi}\int_0^\infty\cos l\varphi\exp(-\kappa_l s)dl \quad (21)$$

with κ_l given by (18). This is just the result given by Snyder and Scott, since our β is equal to their $\frac{1}{4}\eta_0^2$.

VI. SPATIAL DISTRIBUTIONS

A. Longitudinal Distribution

In order to find the spatial distribution of the scattered particle, we would like to solve Eq. (4) for f_{00}. However, because the differential equations for the various f_{lm} are coupled equations, this turns out to be impracticable, and one must resort to a somewhat less satisfying procedure involving the evaluation of the moments of the spatial distributions (and correlation functions with the angles). This is, in principle, completely equivalent to the evaluation of the function, though somewhat less useful. We illustrate the procedure on the longitudinal distribution.

First we integrate (4) with respect to x and y, and define

$$g_{lm}(z,s)=\int\int f_{lm}(\mathbf{x},s)dxdy.$$

Then

$$\left(\frac{\partial}{\partial s}+\kappa_l\right)g_{lm}+\sum_{\lambda\mu}\frac{\partial g_{\lambda\mu}}{\partial z}(Q_{lm}{}^{\lambda\mu})_z=0. \tag{22}$$

The boundary conditions for the g_{lm} are

$$g_{lm}(z,0)=[(2l+1)/4\pi]^{\frac{1}{2}}\delta_{m0}\delta(z).$$

From these, and from the fact that Q_z is zero unless $\mu=m$, we conclude that $g_{lm}=0$ for $m\neq 0$. We will simply use the notation $g_l(z,s)$ for $g_{l0}(z,s)$. Now we use the well-known expression[6] for Q_z, namely,

$$\begin{aligned}(Q_{l0}{}^{\lambda 0})_z&=\frac{l\delta_{l-1,\lambda}}{(4l^2-1)^{\frac{1}{2}}}+\frac{(l+1)\delta_{l+1,\lambda}}{[4(l+1)^2-1]^{\frac{1}{2}}}\\&=\alpha_l\delta_{l-1,\lambda}+\alpha_{l+1}\delta_{l+1,\lambda}\end{aligned} \tag{23}$$

in which we give the coefficients a name. Thus,

$$\left(\frac{\partial}{\partial s}+\kappa_l\right)g_l+\frac{\partial}{\partial z}[\alpha_l g_{l-1}+\alpha_{l+1}g_{l+1}]=0. \tag{24}$$

For $l=0$, the first term in the square brackets of course does not appear. Now define

$$H_{ln}=\int_{-\infty}^{\infty}g_l(z,s)z^n dz,$$

so that, if we multiply (24) by z^n, and integrate, one integration by parts yields

$$\left(\frac{\partial}{\partial s}+\kappa_l\right)H_{ln}-n[\alpha_l H_{l-1,n-1}+\alpha_{l+1}H_{l+1,n-1}]=0 \tag{25}$$

which is a set of differential equations for the H_{ln}, which can be solved in ascending order in n. For example, if we call

$$\exp\left(-\int_0^s\kappa_l ds\right)=k_l(s),$$

since the k_l will appear frequently,

$$H_{l0}=[(2l+1)/4\pi]^{\frac{1}{2}}k_l(s) \tag{26}$$

and

$$H_{l1}=\left(\frac{2l+1}{4\pi}\right)^{\frac{1}{2}}k_l(s)\int_0^s\frac{d\sigma}{k_l(\sigma)}[lk_{l-1}(\sigma)+(l+1)k_{l+1}(\sigma)],$$

where we have inserted the explicit values of the α_l. This process can be continued.

It follows from (26) that the mean value of z is given by $(4\pi)^{\frac{1}{2}}H_{01}$, so that, since $\kappa_0=0$, and $k_0(s)=1$,

$$\langle z\rangle_{\text{Av}}=\int_0^s k_1(\sigma)d\sigma. \tag{27}$$

We can also calculate correlation functions of z with various functions of ϑ, by considering H_{l1} for $l\neq 0$. For example,

$$\begin{aligned}\langle z\cos\vartheta\rangle_{\text{Av}}&=(4\pi/3)^{\frac{1}{2}}H_{11}(s)\\&=k_1(s)\int_0^s[1+2k_2(\sigma)][k_1(\sigma)]^{-1}d\sigma.\end{aligned} \tag{28}$$

We can also find $\langle z^2\rangle_{\text{Av}}$, for example, by calculating the H_{l2}.

In order to obtain numerical results for a particular case, one must express the various κ_l as functions of energy [according to (15) or (15′), if one wishes to use the cross section (8)], and combine these results with the range-energy curves in the medium in question, to find the $k_l(s)$, where the integral involved can be done numerically if need be. The $k_l(s)$ then appear in all the physically interesting expressions.

B. Transverse Distribution

In order to calculate the moments of the transverse distribution, we follow the same pattern as in the preceding section; namely, to integrate (4) with respect now to (say) y and z, write in the value of $(Q_{lm}{}^{\lambda\mu})_x$, then multiply by x^n, integrate, and solve the resulting differential equations for the moments. The latter turn out to be, for the x direction,

$$\begin{aligned}\left(\frac{\partial}{\partial s}+\kappa_l\right)h_{lm}{}^{(n)}(s)=\frac{n}{2}\bigg\{&A_m{}^l h_{l-1,m-1}^{(n-1)}+A_{m+1}^{l+1}h_{l+1,m+1}^{(n-1)}\\&-A_{-m}{}^l h_{l-1,m+1}^{(n-1)}-A_{-m+1}^{l+1}h_{l+1,m+1}^{(n-1)}\bigg\},\end{aligned} \tag{29}$$

where we have defined

$$A_m{}^l=\left[\frac{(l+m)(l+m-1)}{4l^2-1}\right]^{\frac{1}{2}}$$

and

$$h_{lm}{}^{(n)}(s)=\int_{-\infty}^{\infty}x^n f_{lm}(\mathbf{x},s)d\mathbf{x}. \tag{30}$$

The boundary conditions are $h_{lm}{}^{(n)}(0)=0$ for $n\neq 0$, and

$$h_{lm}{}^{(0)}(s)=[(2l+1)/4\pi]^{\frac{1}{2}}\delta_{m0}k_l(s). \tag{30'}$$

These equations yield, for example $h_{lm}{}^{(1)}(s)=0$ for $m^2\neq 1$, and

$$\begin{aligned}h_{l1}{}^{(1)}=-h_{l,-1}{}^{(1)}=\frac{k_l(s)}{4}\left[\frac{l(l+1)}{\pi(2l+1)}\right]^{\frac{1}{2}}\int_0^s\frac{d\sigma}{k_l(\sigma)}\\\times[k_{l-1}(\sigma)-k_{l+1}(\sigma)].\end{aligned} \tag{31}$$

By going to $n=2$, one also finds, for example,

$$\langle x^2+y^2\rangle_{\text{Av}}=\frac{4}{3}\int_0^s d\sigma k_1(\sigma)\int_0^\sigma d\tau[1-k_2(\tau)]/k_1(\tau) \tag{32}$$

which can easily be shown to reduce to the correct result when the scattering is small.

[6] H. Bethe, *Handbuch der Physik* (1933), Vol. 24/1, p. 551. (*Anhang uber Kugelfunktionen.*)