Theory of the Deep Penetration of Electrons and Charged Particles

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Charged particle penetration is amenable to elementary analysis if the continuous-slowing-down, small-angle, and diffusion-in-angle approximations are made. Such calculations are carried out in this paper, partly for their own interest and partly to demonstrate procedures of use in more realistic calculations. The present calculations can be considered an extension of Yang's work to problems including energy loss. One section of the paper goes beyond the approximation of diffusion in angle to derive results for a scattering function with a large-angle tail.

I. INTRODUCTION

THE theory of the interplay of deflection and slowing down of fast charged particles, and its effect on penetration, has never been well mastered. Such effects are dominant for electron penetration and important for the straggling aspect of heavy particle penetration. Most of the work on multiple scattering and penetration of electrons has been directed instead to the investigation of deflection, straggling, and slowing down, considered as separate effects. Studies have been made of energy loss spectra,[1] penetration without energy loss,[2] energy loss straggling,[3] angular distributions integrated over all space, and thin foil angular distributions.[4,5] Only a few papers from the extensive literature are mentioned here; a more complete summary of work on these problems is given by Birkhoff.[6]

In this paper we calculate electron penetration taking into account both energy loss and deflections. Three approximations are used in the main series of calculations: (1) continuous slowing down (i.e., neglect of straggling effects); (2) small-angle approximations; (3) diffusion in angle. The results are also applicable to the study of the penetration of protons and other charged particles.

The material in this paper relates to other calculations as follows: In an earlier paper by one of us[7] (to be referred to as I), electron spatial distributions were calculated using spatial moments and a knowledge of the trend of the distribution when the penetration nearly equals the range. The derivation of the deep penetration trend given in that paper is suggestive of some of the calculations of this paper, which are more complete. (See also the paper on neutron penetration by Wick.)[8]

Yang made calculations some years ago of the path length distribution of electrons passing through thin foils.[9] The procedures of the present paper represent an extension of that work to large-energy-loss problems. Yang's results follow from a limiting case of the results given here, and his series expressions can be summed or rewritten as integrals by these methods.

Recently, we have been programming electron penetration calculations of several types using FORTRAN; and we have been able to calculate the spatial moments of the flux of slowed-down electrons, taking into account the energy straggling as well as the deflections. In these numerical calculations, straggling must dominate the large-penetration tail. The calculations reported in this paper are intended as support for this numerical work, partly through more complete domination of the non-straggling problem, and partly as a first step towards a deep penetration theory which includes the straggling.

The remarkable feature about the present calculations is the fact that elementary methods suffice to obtain spectra and angular distributions in the form of quadratures. We take advantage of this simplicity to exhibit and interrelate several methods which might be applied in further, more realistic, studies in which the three main approximations of this paper are not made.

II. THE TRANSPORT EQUATION

We start by writing down the appropriate transport equation[10] for a plane source in an infinite medium, using the notation of I:

$$[\partial I(t,\theta,x)/\partial t]+\cos\theta[\partial I(t,\theta,x)/\partial x]$$
$$=\int d\Omega'\, S(t,\Theta)[I(t,\theta',x)-I(t,\theta,x)] +(2\pi)^{-1}\delta(x)\delta(t-1)\delta(\cos\theta-1). \quad (1)$$

If T is the kinetic energy of the electrons, (dT/dr) the average energy loss per unit *decrease* in the path length

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[9] C. N. Yang, Phys. Rev. **84**, 599 (1951).
[10] For a general reference on penetration theory, see U. Fano, L. V. Spencer, and M. J. Berger, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1959), Vol. 38, p. 660.

remaining to be traveled, and if

$$r=\int_0^T dT\,(dT/dr)^{-1} \tag{2}$$

is this residual path length, then $t=(r/r_0)$, r_0 being the residual path length of source electrons of energy T_0. Further, if z is the actual separation distance of the electrons from a plane on which all were generated, then $x=(z/r_0)$. The scattering function $S(t,\Theta)$ is given by

$$S(t,\Theta)=r_0N\sigma(r,\Theta), \tag{3}$$

where Θ is the angle between directions before and after scattering, N is the number of atoms per gram of material, and σ is the scattering cross section per atom. $I(t,\theta,x)$ is defined as $I(r,\theta,z)dr/dt$, where $I(r,\theta,z)dr \times d\cos\theta d\varphi$ is the number of electrons per second with residual ranges between r and $r+dr$ striking a small detector, per unit cross-sectional area of the detector, while traveling in directions contained in a small cone of solid angle $d\cos\theta d\varphi$, which is inclined at an obliquity angle θ to the normal to the source plane. Note that t varies between 0 and 1, and that x varies between -1 and $+1$.

The source term in Eq. (1) expresses the generation of electrons of residual range $t=1$, at the plane $x=0$, and at an initial obliquity $\cos\theta=1$.

As in I, we expand in spherical harmonics of the electron direction of travel. However, instead of integrating to obtain spatial moments, we make a Laplace transformation in the space variable x. Thus, if

$$\Phi_l(t,p)=\int_{4\pi} d\Omega\, P_l(\cos\theta)\int_{-\infty}^{1-t} dx \times\exp\{-p[(1-t)-x]\}I(t,\theta,x), \tag{4}$$

and

$$S_l(t)=\int_{4\pi} d\Omega\,[1-P_l(\cos\Theta)]S(t,\Theta), \tag{5}$$

Eq. (1) yields a linked system of differential equations for the transform coefficients $\Phi_l(t,p)$, namely,

$$-(\partial\Phi_l/\partial t)-\tfrac{1}{2}p\Delta_l\Phi_l+S_l(t)\Phi_l=\delta(t-1), \tag{6}$$

where

$$\Delta_l\Phi_l=[\Phi_{l+1}-2\Phi_l+\Phi_{l-1}+\tfrac{1}{2}(\Phi_{l+1}-\Phi_{l-1})/(l+\tfrac{1}{2})]. \tag{7}$$

Of greatest interest is the behavior of Eq. (6) for large, real, positive values of p. We see from Eq. (4) that values of x near $(1-t)$ make the main contribution to Φ_l when p is large. Since the electrons which reach the largest x values are those which have traveled most directly away from the source plane, we expect their obliquity distribution to be peaked around $\theta=0$. The coefficients $\Phi_l(t,p)$ should then decrease comparatively slowly with increasing l, so that large l values are required in the representation of these angular distributions. Under such circumstances, l (or rather $l+\frac{1}{2}$) can be considered a continuous variable, which we designate σ, and

$$\Delta_l\Phi_l(t,p)=\left(\frac{\partial^2}{\partial\sigma^2}+\frac{1}{\sigma}\frac{\partial}{\partial\sigma}\right)\Phi(t,\sigma,p)=\Delta_\sigma\Phi(t,\sigma,p). \tag{8}$$

This is the small-angle approximation, and is equivalent to replacing $\cos\theta$ by $1-\frac{1}{2}\theta^2$.

As was discussed in I, the scattering coefficients $S_l(t)$ can be quite accurately written in the form

$$S_l(t)\approx\alpha d_l/t(t+\alpha), \tag{9}$$

where α and d_l are nearly energy independent and can be treated as constants. At low source energies, values for α become large, so that a simpler form may be used, namely,

$$S_l(t)\approx d_l/t. \tag{10}$$

Under most circumstances, the dominant part of the scattering is due to the Coulomb field of the nucleus; and a screened Rutherford cross section can be used to exhibit the main penetration phenomena. The constants d_l are then calculated by recursion from the system given by Eq. (10) of I. Goudsmit and Saunderson[5] have given an approximate solution of high accuracy to this recursion system. (See the Appendix for an alternative derivation. Lewis[7] and Bethe[11] also give derivations.) Using this result, the d_l can be approximated by

$$d_l=\frac{l(l+1)}{2}\frac{(Z+1)}{4B}\ln\frac{1}{\eta(\gamma l+1)e}, \tag{11}$$

$\gamma=1.781\cdots$, $e=2.718\cdots$, and B is the stopping number which depends logarithmically on the energy. The screening parameter η is usually a very small number. The logarithmic factors in Eq. (11) may be written in the form

$$\{\ln[\eta(\gamma+1)e]^{-1}/B\}+(1/B)\ln[(\gamma+1)/(\gamma l+1)],$$

in which the first term is much larger than the second except for large l, and is only weakly energy dependent. Note that there is a partial cancellation of logarithmic energy variations of numerator and denominator in the first term. If the second term is omitted entirely, the resulting approximation is the one we are referring to as diffusion in angle. In addition, we assume the first term to be completely energy independent. In small-angle approximation, Eq. (11) takes the form

$$d(\sigma)=\sigma^2S_1, \tag{11'}$$

$$S_1=[(Z+1)/8B]\ln[1/\eta(\gamma+1)e]. \tag{12}$$

If this expression and Eqs. (8) and (6) are combined, we arrive at the partial differential equation whose solution will occupy most of the remainder of this

[11] H. A. Bethe, Phys. Rev. **89**, 1256 (1953).

paper, namely,

$$-[\partial\Phi(t,\sigma,p)/\partial t]-\tfrac{1}{2}p\Delta_\sigma\Phi(t,\sigma,p)+S(t)\sigma^2\Phi(t,\sigma,p)=\delta(t-1). \quad (13)$$

where

$$S(t)=\alpha S_1/t(t+\alpha). \quad (14)$$

III. FORMAL SOLUTION OF THE DIFFUSION EQUATION

Equation (13) has the form of a two-dimensional Schrödinger oscillator equation with time-variable elastic constant. It is not immediately apparent that the equation is separable, but such is the case. The reason is that in each small t interval the angular changes are due to a diffusion process which produces a characteristic Gaussian broadening. Combination of effects due to different small t intervals is accomplished by convolution, which transforms Gaussians into Gaussians. We are, therefore, led to the Ansatz

$$\Phi(t,\sigma,p)=a(t,p)\exp[-b(t,p)\sigma^2], \quad (15)$$

with the initial condition $b(t,p)\to 0$ as $t\to 1$, but with $a(t,p)$ and $b(t,p)$ otherwise undetermined. Inserting Eq. (15) into Eq. (13) we obtain the two equations

$$-(da/dt)+2pba=\delta(1-t), \quad (16)$$

and

$$(db/dt)-2pb^2+S(t)=0. \quad (17)$$

These equations, together with the initial condition for b, reduce the solution of Eq. (13) to quadrature. The numerical solution of Eqs. (16) and (17) is elementary, and some computational results will be presented in a later section. The major remaining difficulty lies in the inversion of the transformation.

Though the results most useful to us can be derived from Eqs. (16) and (17) by expansion procedures, we first continue the exact analysis to obtain a few expressions having formal interest. Three cases occur, namely $S(t)\approx\alpha S_1/t(t+\alpha)$, $S(t)\approx t^{-1}S_1$, and $S(t)=S_1$. If the first, and more general, expression for $S(t)$ is inserted in Eq. (17), and if the usual transformation from a Riccati equation to a second-order linear differential equation is made, i.e., $b(t,p)=-S(t)y/y'$, the equation for y turns out to be

$$t(t+\alpha)y''+(2t+\alpha)y'-2\alpha pS_1y=0. \quad (18)$$

This is a form of Legendre's equation, and has, as a general solution, a combination of the functions $P_\nu(\lambda)$, $Q_\nu(\lambda)$, where $\lambda=(1+2t/\alpha)$ and $(\nu+\frac{1}{2})=(2\alpha pS_1+\frac{1}{4})^{1/2}$. The initial conditions are satisfied if we take

$$y(t,p)=k[P_\nu(\lambda)Q_\nu(\lambda_0)-Q_\nu(\lambda)P_\nu(\lambda_0)], \quad (19)$$

where $\lambda_0=(1+2/\alpha)$ and k is an arbitrary constant. The variables $a(t,p)$ and $b(t,p)$ are given by

$$b(t,p)=-S(t)y(t,p)/y'(t,p),$$
$$a(t,p)=\frac{S(t)}{S(1)}\frac{y'(1,p)}{y'(t,p)}, \quad (20)$$

regardless of the analytic expression for y. Inserting these equations into Eq. (15) and writing $\Delta=(1-t)-x$, and

$$I(t,\theta,x)=\frac{1}{2\pi i}\int dp\, e^{\Delta p}\int_0^\infty \sigma d\sigma\, J_0(\sigma\theta)\Phi(t,\sigma,p), \quad (21)$$

we may evaluate the σ integral to obtain $I(t,\theta,x)$ as a Laplace integral, namely,

$$I(t,\theta,x)=\frac{1}{2\pi i}\int dp\, e^{\Delta p}\left(-\frac{y'(1,p)}{2S(1)y(t,p)}\right)\times\exp\left(\frac{\theta^2}{4S(t)}\frac{d}{dt}\ln y(t,p)\right), \quad (22)$$

where $y(t,p)$ is given by (19).

The simpler form $S(t)=t^{-1}S_1$ corresponds in Eq. (18) to the limit as $\alpha\to\infty$. The resulting Bessel equation has for its solution

$$y(t,p)=k\{I_0[(8pS_1t)^{1/2}]K_0[(8pS_1)^{1/2}]-K_0[(8pS_1t)^{1/2}]I_0[(8pS_1)^{1/2}]\}. \quad (23)$$

Finally, if $S(t)=S_1$, we obtain

$$y(t,p)=k\{\exp[(2pS_1)^{1/2}t-(2pS_1)^{1/2}]-\exp[-(2pS_1)^{1/2}t+(2pS_1)^{1/2}]\} \quad (24)$$
$$=-2k\sinh[(2pS_1)^{1/2}(1-t)].$$

In this last case, Eq. (22) takes the simple form

$$I(t,\theta,x)=(2\pi i)^{-1}\int dp\, e^{\Delta p}(p/2S_1)^{1/2}\times\operatorname{csch}[(1-t)(2pS_1)^{1/2}]\exp\{-\tfrac{1}{4}\theta^2(2p/S_1)^{1/2}\times\coth[(1-t)(2pS_1)^{1/2}]\}. \quad (25)$$

Equation (25) is closely analogous to the series given by Yang in his Eq. (8). By integrating over θ (case I) or by setting $\theta=0$ (case II), and then expanding the integrand into a geometric series of exponentials, his functions B_{I} and B_{II} can be obtained. If his Eq. (7) is treated in a manner similar to our Eq. (13), an expression like (25) for his function Ψ is obtainable.

IV. SOLUTIONS BY EXPANSION

Evaluation of the integral, Eq. (22), by means of Eqs. (19), (23), or (24), would require expansions of the integrand. It is more instructive to obtain the expansions directly from Eqs. (16) and (17). First, we dis-

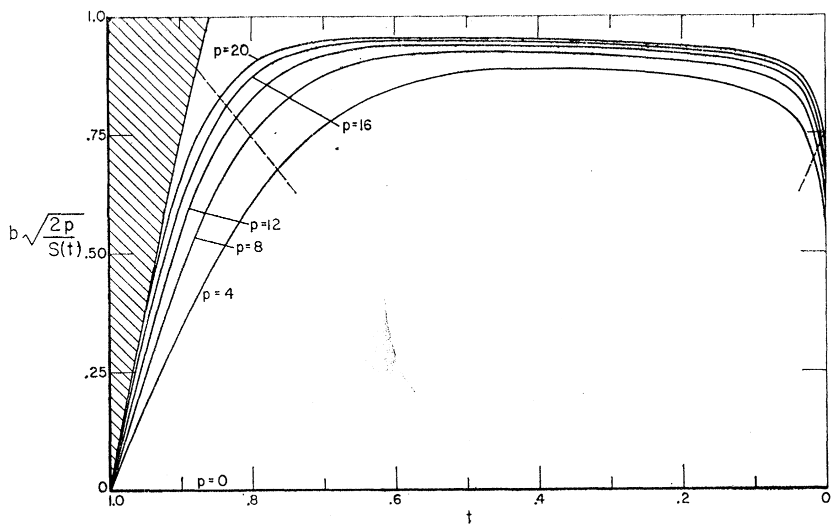

FIG. 1. Numerical calculations of $b(t,p)$ for 1-MeV electrons in aluminum. The curves have been divided by the values expected for the asymptotic trend, so that unity on the vertical axis corresponds to complete asymptoticity. The close approach to unity, even for relatively small values of p, indicates that the asymptotic form describes the actual trend fairly well over a rather wide range of penetrations when t is well below unity.

tinguish between three regions of t, namely, $t\approx 1$, $t\approx 0$, and the region intermediate between these two.

In the first region, corresponding to small energy loss we can expand both $b(t)$ and $S(t)$ in rising powers of $(1-t)$. The solution to Eq. (17) is easily obtained as a power series:

$$b=S(1)(1-t)-\tfrac{1}{2}S'(1)(1-t)^2 +[\tfrac{1}{6}S''(1)-\tfrac{2}{3}pS^2(1)](1-t)^3+\cdots. \quad (26)$$

From this we see that near $t=1$, b is independent of p; but it is clear that this region becomes progressively narrower as p increases in size and the third term in the series becomes correspondingly more important.

If t is fixed, while p is made to increase, there will be a region of p such that high-order terms are important in the series, Eq. (26). We then need another expression valid for large p, corresponding to penetrations, x, nearly as large as the path length, $(1-t)$. This is obtained by expansion of Eq. (17) in inverse powers of $\sqrt{p}$;

$$b\approx\left(\frac{S(t)}{2p}\right)^{1/2}+\frac{S'(t)}{8S(t)p}+\frac{1}{64\sqrt{2}}\left[\frac{4S''}{S^{3/2}}-\frac{5S'^2}{S^{5/2}}\right]\frac{1}{p^{3/2}}+\cdots. \quad (27)$$

Since $S'(t)$ is negative, b is always a little less than $[S(t)/2p]^{1/2}$ at large p.

If we now consider the $t\approx 0$ region (i.e., the low-energy case), we see from Eq. (27) that for fixed and very large p, a decrease in t eventually results in the increasing importance of the higher terms of Eq. (27). Referring back to Eq. (14), we note that as $t\to 0$, $S\to S_1t^{-1}$, so that the last term in Eq. (17) becomes dominant over the middle term in this limit. The parameter b is then seen to have the variation

$$b\approx S_1\ln(t_0/t)+b(t_0), \quad (28)$$

where t_0 is an upper bound to this region.

The three regions are indicated in Fig. 1, which shows the results of numerical integrations of Eq. (17). The quantity graphed is $[2p/S(t)]^{1/2}b(t,p)$. Dashed lines are used to indicate roughly the boundaries between t regions. We see that for t near unity and near zero the dependent variable tends to vanish, while at intermediate values it tends to unity. For increasing p, regions I and III shrink, while in region II the curve everywhere approaches unity.

To obtain the trend of the flux in space and angle, we must evaluate the integrals

$$I_0(t,x)=(2\pi i)^{-1}\int dp\, e^{\Delta p}\exp\left(-\int_t^1 dt'2pb\right), \quad \text{(total flux)} \quad (29)$$

and

$$I(t,\theta,x)=-\left(\frac{1}{\theta}\frac{\partial}{\partial\theta}\right)(2\pi i)^{-1}\int dp\, e^{\Delta p} \times\exp\left(-\int_t^1 dt'2pb-\frac{\theta^2}{4b}\right). \quad (30)$$

Our primary interest is in the trend when $\Delta=(1-t)-x$ is small, i.e., when the electrons almost achieve the limiting depth of penetration for a given t. In this case it is possible to use expressions for b which are valid at large p only, e.g., expressions derived from Eq. (27).

To obtain a suitable large-p expression for the exponent, we first write

$$b\approx[(S/2p)^{1/2}+S'/8pS](1-T), \quad (31)$$

where T is unity at $t=1$, and drops rapidly to near zero for lower energies. Inserting this into (17) and cancelling all terms except those of lowest order in p^{-1}, we obtain the equation

$$-\frac{1}{(2pS)^{1/2}}\frac{dT}{dt}+2T-T^2=0,$$

TABLE I. This table gives the ratio of the exact values of $a(t,p)$ to the values of $a_{\rm approx}$, where $a_{\rm approx}$ is given by Eq. (35), and the values of the constants used are listed at the bottom of the table. The distributions corresponding to $a_{\rm approx}$ can be obtained from Eq. (36). These distributions will be valid for large x, but not for small or negative x. To obtain more accurate distributions, it would be necessary to obtain a better fit for $a(t,p)$ for small and even negative p, or to invert $a(t,p)$ by some other means.

$p \backslash t$	0.98	0.75	0.50	0.25	0.02
0	0.99991	0.76133	0.79476	0.89375	1.29208
4	0.99993	0.91829	0.98979	1.00210	1.02251
8	0.99994	0.96352	0.99837	1.00093	1.00825
12	0.99996	0.98225	0.99966	1.00044	1.00382
16	0.99998	0.99114	0.99993	1.00022	1.00190
20	0.99999	0.99566	0.99999	1.00011	1.00095
24	0.99999	0.99801	1.00000	1.00005	1.00044
28	1.00000	0.99922	1.00000	1.00002	1.00018
32	1.00000	0.99979	1.00000	1.00001	1.00005
36	1.00000	1.00000	1.00000	1.00000	1.00000
40	1.00000	1.00000	1.00000	1.00000	1.00000
$\sqrt{2}A(t)$	0.035609	0.48198	1.0734	1.8729	3.3131
$c(t)$	2.7084	2.2114	2.4588	2.9777	5.6491
$K(t)$	782.74	1.1682	0.38958	0.27315	0.35996

which has as a solution

$$T=2\bigg/\left(1+\exp\left\{2\int_t^1 dt'\,[2pS(t')]^{1/2}\right\}\right).$$

Inserting this expression for T into (31), we obtain

$$\int_t^1 2pb(t')dt'\approx A(t)(2p)^{1/2}+\tfrac{1}{4}\ln\frac{S(1)}{S(t)}-\ln 2, \quad (32)$$

where $A(t)=\int_t^1 [S(t')]^{1/2}dt'$. If these are inserted into Eqs. (29) and (30), and if we use the approximation $b^{-1}\approx[2p/S(t)]^{1/2}-S'/(4S^2)$, we may evaluate the inversion integrals to obtain

$$I_0(t,x)\approx\frac{2}{(2\pi)^{1/2}}\left[\frac{S(t)}{S(1)}\right]^{1/4}A(t)\Delta^{-3/2}\exp\left[-\frac{A^2(t)}{2\Delta}\right], \quad (33)$$

$$I(t,\theta,x)\approx\left(-\frac{1}{\theta}\frac{\partial}{\partial\theta}\right)\frac{2}{(2\pi)^{1/2}}\left[\frac{S(t)}{S(1)}\right]^{1/4}B\Delta^{-3/2}\times\exp\left\{-\frac{B^2}{2\Delta}+\frac{\theta^2}{16}\frac{S'(t)}{S^2(t)}\right\}, \quad (34)$$

where $B=A(t)+\theta^2/\{4[S(t)]^{1/2}\}$.

To get better results, it is probably desirable to utilize numerical solutions, but a complete numerical inversion of the transformation requires a large computational effort. However, the results given by Eqs. (33) and (34) can be substantially improved in the following simple way. We note that the factor 2 comes from the approximate evaluation of an integral. Also, we observe that higher terms in the expansion, Eq. (27), have the effect of translating the value of p, i.e., replacing it by, say $p+K(t)$. We, therefore, determine values of two parameters $c(t)$ and $K(t)$ so that the numerical solutions of Eqs. (16) and (17) are well represented by the expression

$$a(t,p)\approx c(t)\exp\{-(2)^{1/2}A(t)[p+K(t)]^{1/2}\}. \quad (35)$$

Inversion of Eq. (35) then gives

$$I_0(t,x)\approx\frac{c(t)}{(2\pi)^{1/2}}\frac{A(t)}{\Delta^{3/2}}\exp\left\{-K(t)\Delta-\frac{A^2(t)}{2\Delta}\right\}. \quad (36)$$

Figure 1 and Table I give the results of sample numerical calculations of $b(t,p)$ and $a(t,p)$ for a 1-MeV source in Al. These were obtained by direct integration of Eqs. (16) and (17), using $\alpha=2.965$ and $S_1=2.093$.

V. SOLUTION BY AN EIGENFUNCTION EXPANSION

The analysis just completed depends for its success on the special properties of Eq. (13); and it cannot easily be applied to more realistic treatments of electron penetration which involve equations analogous to Eq. (13). Examples are: (a) equations with more realistic scattering functions; (b) the difference equations, Eq. (6); (c) perhaps even the integral equations which apply to discrete rather than continuous energy losses. An eigenfunction approach similar to that of Wick[8] seems to have greater flexibility. We, therefore, consider expansions of Eq. (13) in well-chosen eigenfunctions.

The same reasoning that suggested the Gaussian Ansatz used previously suggests an expansion in eigenfunctions of the Gaussian type. The width of the distribution in σ is not known *a priori*. Therefore, we consider an expansion in eigenfunctions of the equation

$$-\tfrac{1}{2}p\Delta_\sigma\Psi(t,\sigma,p)+R(t,p)\sigma^2\Psi(t,\sigma,p)=\lambda\Psi(t,\sigma,p). \quad (37)$$

This equation is constructed from the second and third terms on the left side of Eq. (13) by replacing the unknown function $\Phi(t,\sigma,p)$ with Ψ, and the known function $S(t)$ with an arbitrary function $R(t,p)$ which is not as yet specified, but which determines the width of the distribution. The resulting equation has the same form as the Schrödinger equation for a two-dimensional oscillator and we consider only solutions which have cylindrical symmetry. The equation can be solved to give a complete set of eigenfunctions $\Psi_k(t,\sigma,p)$ which depend on the arbitrary function R. If we define s^2 by the equation

$$s^2=\sigma^2(2R/p)^{1/2}, \quad (38)$$

the (normalized) eigenfunctions are the Laguerre polynomials in s^2,

$$\Psi_k(t,\sigma,p)=(8R/p)^{1/4}\exp(-s^2/2)L_k(s^2); \quad (39)$$

the eigenvalues are

$$\lambda_k(t,p)=(2k+1)(2Rp)^{1/2},\quad k=0,1,2,\cdots. \quad (40)$$

To utilize the eigenfunctions to solve Eq. (13), we shall

need the matrix elements for σ^2 and $\partial/\partial t$, which are

$$\int_0^\infty \sigma d\sigma\, \Psi_n \sigma^2 \Psi_m = \left(\frac{p}{2R}\right)^{1/2} \times[(2n+1)\delta_{n,m} - n\delta_{n,m+1} - (n+1)\delta_{n,m-1}], \quad (41)$$

$$\int_0^\infty \sigma d\sigma\, \Psi_n \frac{\partial \Psi_m}{\partial t} = -\frac{1}{4}\frac{d}{dt}(\ln R)[n\delta_{n,m+1} - (n+1)\delta_{n,m-1}].$$

Using the representation

$$\Phi(t,\sigma,p) = \sum_{n=0}^{\infty} \varphi_n(t,p)\Psi_n(t,\sigma,p), \quad (42)$$

we expand each term in Eq. (13) into these eigenfunctions. Equation (13) then takes the form

$$\sum_{n=0}^{\infty} \Psi_n \left\{ -\frac{\partial \varphi_n}{\partial t} + \varphi_n(2n+1)\left[1+\frac{S(t)}{R}\right]\left(\frac{Rp}{2}\right)^{1/2} + \varphi_{n-1} n\left[R - S(t) - \frac{1}{4}\left(\frac{2}{Rp}\right)^{1/2}\frac{dR}{dt}\right]\left(\frac{p}{2R}\right)^{1/2} + \varphi_{n+1}(n+1)\left[R - S(t) + \frac{1}{4}\left(\frac{2}{Rp}\right)^{1/2}\frac{dR}{dt}\right]\left(\frac{p}{2R}\right)^{1/2}\right\} = \delta(1-t). \quad (43)$$

The function R is still at our disposal and should clearly be chosen to minimize the linkage terms in Eq. (43). If we choose R to be a solution of the equation

$$R - S(t) - \tfrac{1}{4}(2/Rp)^{1/2}(dR/dt) = 0, \quad (44)$$

then the terms of Eq. (43) may be grouped as follows:

$$\Psi_0\left\{-\frac{\partial \varphi_0}{\partial t} + \varphi_0\left[1+\frac{S(t)}{R}\right](Rp/2)^{1/2}\right\} - \delta(1-t) + \left\{\frac{\varphi_1}{2R}\frac{dR}{dt}\Psi_0 + \sum_{n=1}^{\infty}\Psi_n\left[-\frac{d\varphi_n}{dt} + \varphi_n(2n+1) \times(1+S/R)(Rp/2)^{1/2} + \varphi_{n+1}(n+1)\frac{1}{2R}\frac{dR}{dt}\right]\right\} = 0. \quad (45)$$

The noteworthy thing about Eq. (45) is the nonappearance of φ_0 in the last curly bracket term on the left. If, therefore, φ_0 satisfies the equation

$$\Psi_0(t,\sigma,p)\left\{-\frac{d\varphi_0}{dt} + \varphi_0\left[1+\frac{S(t)}{R}\right](Rp/2)^{1/2}\right\} - \delta(1-t) = 0, \quad (46)$$

the solution to Eq. (45) is obtained by setting $\varphi_n = 0$, $n > 0$. The solution exists, however, only if $\Psi_0(t,\sigma,p)$ does not depend on σ in the limit $t \to 1$; and this requires that $R \to 0$ as $t \to 1$, thus completing the specification of R. Equations (44) and (46) reduce to Eqs. (17) and (16), if we make the substitutions $R = 2b^2 p$ and $\varphi_0 = a(p/8R)^{1/4}$.

It is instructive to see what we would have obtained by making a different choice of R which would correspond to the expansion of Yang as well as that used in (I), namely, the choice $R = S(t)$. In this case the $\Psi_n(t,\sigma,p)$ are well behaved at $t=1$. We multiply the delta function on the right side of Eq. (43) by $1 = \sum_{n=0}^{\infty}(-1)^n \Psi_n[2p/S(t)]^{1/4}$, and then equate the coefficients of the $\Psi_n(t,\sigma,p)$ to zero

$$-\frac{d\varphi_n}{dt} + \varphi_n(2n+1)(2pS)^{1/2} + [(n+1)\varphi_{n+1} - n\varphi_{n-1}]\frac{1}{4}\frac{d}{dt}\ln S(t) = (-1)^n(2p/S)^{1/4}\delta(1-t). \quad (47)$$

If $S(t)$ is, in fact, constant, the linkage terms in Eq. (47) all vanish and integration of the resulting equations yields a series analogous to Yang's. If $S(t)$ is not constant, the linkage terms must be considered. Equation (47) may be written in integral form

$$\varphi_n = (-1)^n[2p/S]^{1/4} \times \exp\left\{-(2n+1)\int_t^1 dt'\,[2pS(t')]^{1/2}\right\} + \int_t^1 dt'\,\{n\varphi_{n-1} - (n+1)\varphi_{n+1}\}\left\{\frac{1}{4}\frac{\partial}{\partial t'}\ln S(t')\right\} \times \exp\left\{-(2n+1)\int_t^{t'} dt''\,[2pS(t'')]^{1/2}\right\}. \quad (48)$$

For large p, the integrand on the right drops very rapidly as $(t'-t)$ increases, because of the exponential factor. A rough estimate of the integral may be made by assigning the more slowly varying factors their value at $t' = t$

$$\varphi_n \approx (-1)^n[2p/S(t)]^{1/4} \times \exp\left\{-(2n+1)\int_t^1 dt'\,[2pS(t')]^{1/2}\right\} + \left[\frac{n}{2n+1}\varphi_{n-1} - \frac{(n+1)}{2n+1}\varphi_{n+1}\right] \times \frac{[2pS(t)]^{-1/2}}{4}\frac{\partial}{\partial t}\ln S(t). \quad (49)$$

From (49) it is clear that when the linkage terms dominate, one may have for large p the relations $\varphi_n \propto (p)^{-1/2}\varphi_{n-1}$ and therefore $\varphi_n \propto p^{-n/2}\varphi_0$. But the linkage terms in no case upset the dominance of the φ_0 term as given by the first term of (48), in the large-p limit.

VI. EXTENSION TO MORE REALISTIC SCATTERING FUNCTIONS

Finally, we present calculations for a more realistic scattering law, namely, the small-angle approximation to Eqs. (9) and (11),

$$S(t,\sigma)=S(t)s(\sigma) \approx S(t)\sigma^2(1-\epsilon\ln\sigma), \quad \sigma \text{ not extremely large.} \tag{50}$$

The function $s(\sigma)$ tends toward a very large constant as $\sigma\to\infty$. We could specify $S(t)$ and $s(\sigma)$ more completely, but it is not necessary to do so. The parameter ϵ is small, and in the limit $\epsilon\to 0$ the case under discussion approaches the diffusion-in-angle approximation already treated.

In this calculation we take advantage of the fact that the flux angular distributions are nearly Gaussian detpite the changes which result from (50). In line with she approach of Sec. V, we construct an eigenfunction equation involving arbitrary but unspecified functions in place of the scattering function. Thus, the equation for Φ is

$$-(\partial\Phi/\partial t)-\tfrac{1}{2}p\Delta_\sigma\Phi(t,\sigma,p) +S(t)s(\sigma)\Phi(t,\sigma,p)=\delta(1-t), \tag{51}$$

and the eigenfunctions to be considered are solutions of

$$-\tfrac{1}{2}p\Delta_\sigma\Psi(t,\sigma,p)+R(t,p)r(\sigma)\Psi(t,\sigma,p) =\lambda(t,p)\Psi(t,\sigma,p). \tag{52}$$

We leave R and r both unspecified, except that $r(\sigma)$ will be so chosen that an infinite set of discrete eigenfunctions will exist. The matrix elements of $s(\sigma)$, $r(\sigma)$, and $\partial/\partial t$ will be designated s_{nm}, r_{nm}, and q_{nm}; and the following relations are easily derived:

$$q_{nm}(\lambda_n-\lambda_m)=-(dR/dt)r_{nm}+(d\lambda_m/dt)\delta_{mn}, \quad q_{nn}=0. \tag{53}$$

Writing $\Phi=\sum_{n=0}^{\infty}\varphi_n\Psi_n$ as previously [Eq. (42)], we obtain an expansion analogous to Eq. (43)

$$\sum_{n=0}^{\infty}\Psi_n\left\{-\frac{d\varphi_n}{dt}+\varphi_n[\lambda_n+S(t)s_{nn}-Rr_{nn}] +\sum_{m=0}^{\infty}{}'\varphi_m\left[S(t)s_{nm}-Rr_{nm} +\left(\frac{r_{nm}}{\lambda_n-\lambda_m}\right)\frac{dR}{dt}\right]\right\}=\delta(1-t), \tag{54}$$

where the $m=n$ term is not included in the $\sum_m{}'$. Equation (54) may be rearranged and written similarly to Eq. (45)

$$\Psi_0\{-(d\varphi_0/dt)+\varphi_0[\lambda_0+S(t)s_{00}-Rr_{00}]\}-\delta(1-t) +\left\{\Psi_0\sum_{m=1}^{\infty}\varphi_m\left[S(t)s_{0m}-Rr_{0m}+\left(\frac{r_{0m}}{\lambda_0-\lambda_m}\right)\frac{dR}{dt}\right]\right\} +\left\{\sum_{n=1}^{\infty}\Psi_n\left[-\frac{d\varphi_n}{dt}+\varphi_n[\lambda_n+S(t)s_{nm}-Rr_{nm}] +\sum_{m=1}^{\infty}{}'\varphi_m\left(S(t)s_{nm}-Rr_{nm}+\frac{r_{nm}}{\lambda_n-\lambda_m}\frac{dR}{dt}\right) +\varphi_0\left(S(t)s_{n0}-Rr_{n0}+\frac{r_{n0}}{\lambda_n-\lambda_0}\frac{dR}{dt}\right)\right]\right\}=0. \tag{55}$$

To obtain a complete solution as before it is necessary to remove φ_0 entirely from the third curly brackets, since φ_0 acts as a source from which the other coefficients are generated. Removal of φ_0 could be accomplished providing $R(t,p)$ and $r(\sigma)$ are such that for all n,

$$S(t)s_{n0}-R(t,p)r_{n0}+[r_{n0}/(\lambda_n-\lambda_0)]dR/dt=0. \tag{56}$$

It may be possible to do this, though it would not be easy. Instead, we choose $r(\sigma)=\sigma^2$ and thus ensure that $r_{0m}=0$ for $m>1$. At the same time the s_{0m} are $\sim\epsilon$ and decreasing for $m>1$:

$$s_{0m}=(p/2R)^{1/2}\{[1+\tfrac{1}{2}\epsilon(-1+C+\ln(2R/p)^{1/2})]\delta_{m0} +[-1-\tfrac{1}{2}\epsilon(-2+C+\ln(2R/p)^{1/2})]\delta_{m1} -\tfrac{1}{2}\epsilon[(-1)^m(2m-1)/m(m-1)]\delta_{mi}\}, \quad i\geq 2, \quad C=0.5772\cdots. \tag{57}$$

To obtain an approximate solution to Eq. (55), we first eliminate the $n=1$ term in the last curly brackets by requiring that

$$S(t)s_{10}-R(t,p)r_{10}+[r_{10}/(\lambda_1-\lambda_0)]dR/dt=0. \tag{58}$$

We next set the coefficients of Ψ_n, $n\geq 1$, in the last curly brackets equal to zero. The resulting linked system of differential equations has source terms of order $[\epsilon S(t)\varphi_0]$, so that the solutions, i.e., the φ_n, $n\geq 1$, are also small of order ϵ. The middle curly bracket term is, therefore, of order ϵ^2. If this term is neglected, and if we require that $R\to 0$ as $t\to 1$, we obtain a second equation, namely,

$$(8R/p)^{1/4}\{-(d\varphi_0/dt) +\varphi_0[\lambda_0+S(t)s_{00}-Rr_{00}]\}=\delta(1-t). \tag{59}$$

For large p and small ϵ, approximate solutions to these equations are

$$R\approx S(t)s_{10}/r_{10}=S(t)\{1+\tfrac{1}{2}\epsilon[\ln(2S/p)^{1/2}-2+C]\},$$

$$\begin{aligned}\varphi_0\Psi_0(t,0,p)&=\left(\frac{S(t)}{S(1)}\right)^{1/4}\\&\quad\times\exp\left\{-\int_t^1 dt'\left[\lambda_0+S(t)\left(s_{00}-\frac{r_{00}s_{10}}{r_{10}}\right)\right]\right\}\\&\approx\left(\frac{S(t)}{S(1)}\right)^{1/4}\exp\left\{-\int_t^1 dt'\,[2pS(t')]^{1/2}\right.\\&\qquad\left.\times\left[1+\frac{\epsilon}{4}\ln\left(\frac{\gamma}{e}\left(\frac{2S}{p}\right)^{1/2}\right)\right]\right\},\end{aligned}\tag{60}$$

where $\gamma=1.78\cdots$, $e=2.718\cdots$. This result neglects the contribution from the nonasymptotic region $t\approx 1$, which, as shown in the arguments leading to (33), gives mainly an additional numerical factor ≈ 2.

A more adequate solution of (58) and (59) would not only give this factor accurately, but would also give details of the distributions in the nonasymptotic region. Equations (58) and (59) can be solved numerically, of course. Further, solutions can, in principle, be put back into (55) to serve as a basis for an iterative solution correct to higher order in powers of ϵ. Note that the assumption that the angular distribution is basically Gaussian in shape, makes it difficult to get information about fine features of the angular distribution by this procedure.

The calculation just outlined is essentially a variational calculation using a Gaussian trial function and varying the width of the distributon. This may be demonstrated in the large-p limit as follows: Choose $r(\sigma)=s(\sigma)$, at least out to large values of σ. Then $r_{nm}=s_{nm}$, $R=S(t)$, and $1=\sum_{n=0}^{\infty}d_n(t,p)\Psi_n$, where

$$d_n(t,p)=\int_0^\infty \sigma d\sigma\,\Psi_n(t,\sigma,p).\tag{61}$$

Using these expressions in Eq. (54), and equating coefficients of Ψ_n to zero, we obtain equations

$$-\frac{\partial\varphi_n}{\partial t}+\lambda_n\varphi_n+\sum_{m=0}^{\infty}\varphi_m\left(\frac{r_{nm}}{\lambda_n-\lambda_m}\right)\frac{dS}{dt}=d_n(1,p)\delta(1-t).\tag{62}$$

The ratios $r_{nm}/(\lambda_n-\lambda_m)$ are not exactly as obtained using Eqs. (40) and (41), but they will be nearly independent of p. Similarly, λ_n will not be precisely $(2n+1)(2Sp)^{1/2}$, but the p dependence will not be much changed. In the limit of large p, therefore, the φ_m terms may be dropped because they are multiplied by factors which decrease in proportion to $p^{-1/2}$ relative to λ_n. The resulting equations give

$$\varphi_n\approx d_n(1,p)\exp\left[-\int_t^1 dt'\,\lambda_n(t',p)\right],\tag{63}$$

and it is clear that the $n=0$ term is dominant. An approximate evaluation of λ_0 is easily made, *using a Gaussian trial function in a Ritz variational calculation, and varying the width of the Gaussian.* The result is

$$\lambda_0=[2pS(t)]^{1/2}\left\{1+\tfrac{1}{4}\epsilon\ln\left[\frac{\gamma}{e}\left(\frac{2S}{p}\right)^{1/2}\right]\right\}.\tag{64}$$

If this value for λ_0 is inserted in Eq. (63) and if values for d_0 and $\Psi_0(t,o,p)$ are obtained from the variational function, the result agrees with Eq. (60), except for the factor of 2 already mentioned.

VII. FINAL COMMENTS

Extension of eigenfunction calculations to accurate scattering cross sections is straightforward, but appears to be relatively unimportant because of the continuous-slowing-down assumption. In actuality, the neglected energy-loss range fluctuations dominate over deflection effects at the large penetrations. Accurate calculations at all penetrations by numerical solution of Eqs. (16) and (17) or by extensive use of expansions like Eqs. (18) and (19) are possible and would yield interesting spectral and angular information. This information would have more qualitative than quantitative significance.

Application of these results to heavy particle penetration is possible; but range straggling due to statistical fluctuations in the succession of (finite) energy losses tends to determine the deep penetration trend rather than the deflection straggling.

APPENDIX

An approximate form for the d_l scattering coefficients can be obtained by noting first that the screened Rutherford cross section leads to Eq. (7) $d_l=DC_l$, $D\approx\frac{1}{4}(Z+1)/B$, where B is the stopping number and

$$\begin{aligned}&C_0=0,\quad C_1=\ln\left(\frac{1+\eta}{\eta}\right)-\frac{1}{1+\eta};\\&C_{l+1}=(2+l^{-1})(1+2\eta)C_l\\&\qquad-(1+l^{-1})C_{l-1}-(2+l^{-1})(1+\eta)^{-1}.\end{aligned}\tag{65}$$

Dropping the terms proportional to the screening constant η out of the recursion equation we obtain the simple form

$$l[C_{l+1}-C_l]-(l+1)[C_l-C_{l-1}]=-(2l+1),\tag{66}$$

and similarly $C_1\approx\ln(1/e\eta)$. It can be seen by substitution that

$$C_l^{(1)}=l(l+1)\tag{67}$$

is a solution of the homogeneous difference Eq. (66), and that

$$C_l^{(2)}=l(l+1)\sum_{i=1}^{l}\frac{1}{i}\approx l(l+1)\ln(\gamma l+1),\tag{68}$$

where $\gamma=1.781\cdots$, is a particular solution of the inhomogeneous difference equation. Taking

$$C_l=AC_l^{(1)}+C_l^{(2)},\tag{69}$$

and determining A to give the correct value of C_1, we obtain the expression for C_l given in Eq. (11).