Compound-Poisson-process method for the multiple scattering of charged particles

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The theory of multiple scattering for electrons and other changed particles is presented here within a mathematically unifying compound-Poisson-process framework. The compound Poisson model of scattering phenomena allows an arbitrary differential cross section for single scattering, is not restricted to any particular range for the number of collisions experienced by the particle, and is applicable to both the planar coordinate description of scattering (small angle approximation) as well as the spherical coordinate description (exact angle description). An efficient method for computing the angular probability density function after a large number of collisions is derived and then applied in a few example computations. This method is based on the decomposition of the compound Poisson process into hard and soft scattering.

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I. INTRODUCTION

Multiple scattering of charged particles in dense media has received the attention of physicists for almost a century. Classical analysis of the multiple scattering problem by Goudsmit and Saunderson [1,2] and Moliere [3,4] resulted in a solution to the governing Boltzmann transport equation for the angular distribution function when scattering is described on the surface of a unit sphere or on a plane when small angle scattering is assumed, respectively. These classical solutions have found widespread use and, in particular, are incorporated into condensed history Monte Carlo simulation codes [5–11].

Ubiquitous use of the Goudsmit-Saunderson and Moliere theories indicates that the results they provide are often sufficiently accurate. However, this is not uniformly so. The small angle scattering approximation invoked by Moliere [3] underestimates the magnitude of *large* angle scattering, thus presenting significant errors for low-energy electrons undergoing *backscattering*. In addition, Moliere's solution for the angular distribution function [3] is specific to the use of the screened Rutherford cross section and is therefore not applicable for other single scattering cross sections such as those derived from partial wave analysis [12,13], which are generally considered to be more accurate. This limitation of Moliere's solution can lead to significant underestimation of *small* angle scattering for charged particles, especially at low energies. The Goudsmit-Saunderson [1,2] approach does not suffer any of the above limitations of Moliere's theory [10], since their expression for the angular distribution function is exact and any reasonable single scattering cross section may be invoked. However, Goudsmit and Saunderson [1,2] express the angular distribution function as an infinite series of Legendre polynomials and thus there is no effective means of computing the series except by direct summation. Strictly speaking, this sum diverges, and even if it is renormalized it still requires the evaluation of many hundreds or even thousands of terms and hence is computationally inefficient [10].

This paper shows that the mechanism underlying both the Goudsmit-Saunderson and Moliere theories of multiple scattering is that of a compound Poisson process. A method is presented that allows the *direct* calculation of the angular scattering distribution that is practical up to a few hundred collisions. For a greater number of collisions an indirect method is presented that decomposes the compound Poisson process into soft and hard collisions. This indirect method is both accurate and computationally efficient. It is also independent of the single scattering cross section employed. Thus all the limitations of the Goudsmit-Saunderson and Moliere approaches to multiple scattering noted above are avoided.

In Sec. II of this paper we introduce our notation, discuss the parametrization and the geometry for particle scattering, and recall the classical solutions of the problem. We analyze the theories of Moliere and Goudsmit-Saunderson from a different perspective so that in a later part of this article they may be viewed as different manifestations of one unified model of multiple scattering theory. In Sec. III we introduce the compound Poisson process formulation and in Sec. IV show how the classical theories are related to this model. Section V is devoted to the description of methods and ideas that allow us to effectively calculate the multiple scattering cross sections. Finally, in Sec. VI we present a few examples of our calculations and compare them to previously known results.

II. GEOMETRY FOR ANGULAR SCATTERING AND CLASSICAL FORMULATIONS OF THE MULTIPLE SCATTERING PROBLEM

Throughout the paper the instantaneous direction of particle motion, as well as the angular change in direction after single or multiple angular scattering, are represented by points on the surface of a unit sphere S. These directions can also be conveniently interpreted as

arcs on the surface of the unit sphere related to one fixed system of Cartesian coordinates (tangent to the sphere S), especially in the context of the definition of the addition of directions during the multiple scattering of charged particles.

To discuss in more detail how the addition of directions is described in this work we first introduce the following notation (Fig. 1). Throughout the paper we shall customarily denote by Ω the final direction, by Ω' the initial direction, and by Ω'' the change of direction for the scattering particle. Points Ω, Ω', and Ω'' are also designated by their standard angular coordinates for the spherical coordinate system, i.e., we denote $\Omega=(\theta,\varphi)$, $\Omega'=(\theta',\varphi')$, and $\Omega''=(\theta'',\varphi'')$ (Fig. 1). Let Ω_0 denote a "south pole" on the unit sphere, i.e., a point that can be identified with the direction of a particle's motion along the z axis. Let us also denote arcs on the surface of the unit sphere connecting the south pole Ω_0 with points Ω, Ω', and Ω'' by $\Omega_0\Omega$, $\Omega_0\Omega'$, and $\Omega_0\Omega''$, respectively. The summation of the initial direction of the particle's motion with the change of direction during the particle's scattering, resulting in the final direction of the particle's motion after collision(s), is defined as follows. The arc $\Omega_0\Omega''$, which expresses the change of the particle's direction with respect to the local system of Cartesian coordinates tangent to the sphere at Ω_0, is transported along the arc $\Omega_0\Omega'$ together with the local system of coordinates so that the origin Ω_0 coincides with the initial direction of the particle Ω' (Fig. 2). The angles between arc $\Omega_0\Omega'$ and the axes of the local Cartesian system of coordinates remain invariant during their motion along the great circle defined by the arc $\Omega_0\Omega'$. This means, in particular, that the angle between the arc $\Omega_0\Omega'$ and the arc $\Omega_0\Omega''$ also remains invariant during this transport. This transport along the arc $\Omega_0\Omega'$ is therefore equivalent to keeping the reference for the change of direction in the coordinate system related to the scattering particle. Physical interpretation of this transport requires that the end of the arc $\Omega_0\Omega''$, after the transport is performed according to the above description, indicates the final direction Ω of motion for the particle. In other words, the triangle $\Omega_0\Omega'\Omega$ on the sphere (Fig. 3) completely describes the scattering event, with the point Ω' indicating the original and the point Ω indicating the final direction of the particle's motion.

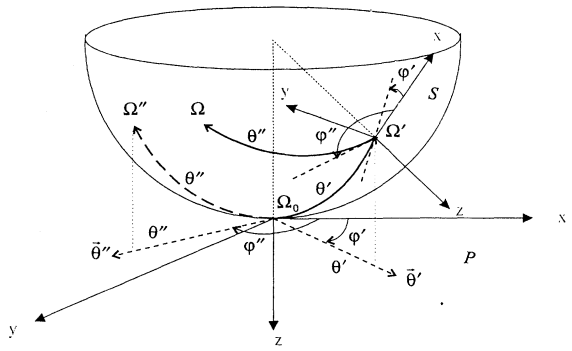

FIG. 2. Addition of the directions for the scattered particle on the sphere S and the plane P.

Using formulas of spherical trigonometry [14], the angular parameters (θ'',φ'') for the change of direction Ω'' may be written in terms of the angular parameters (θ',φ') for the original direction Ω' and the angular parameters (θ,φ) for the final direction Ω. In particular, the parameter θ'', the only active parameter for computations involving rotationally invariant scattering, is related to φ, φ', θ, and θ' by

$$\cos\theta''=\cos\theta\cos\theta'+\sin\theta\sin\theta'\cos(\varphi-\varphi') \ . \tag{1}$$

In the small angle approximation the directions for scattering particles are represented by vectors $\vec{\theta}$ on the plane P tangent to sphere S at Ω_0. The polar coordinates of the vector $\vec{\theta}$, which is equivalent to a direction specified by point $\Omega=(\theta,\varphi)$ on the sphere S, are denoted by (θ,φ), i.e., $\vec{\theta}=(\theta,\varphi)$. The vector $\vec{\theta}$ can also be described by its Cartesian coordinates θ_x and θ_y, i.e., $\vec{\theta}=(\theta_x,\theta_y)$. Thus the coordinates (θ,φ) and (θ_x,θ_y) of the vector $\vec{\theta}$ on the plane P are related as

$$\theta_x=\theta\cos\varphi, \quad \theta_y=\theta\sin\varphi \ , \tag{2}$$

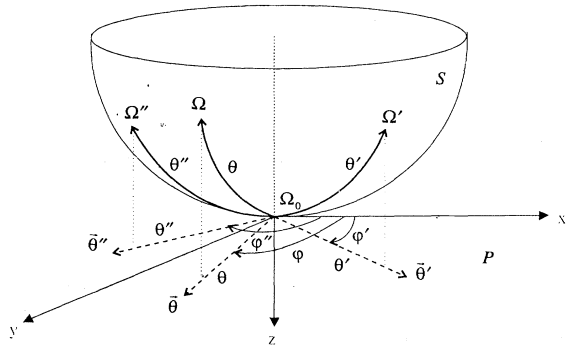

FIG. 1. Directions of motion for the scattered particle represented as (i) points on the surface of the unit sphere S and (ii) vectors on the plane P (in the small angle approximation).

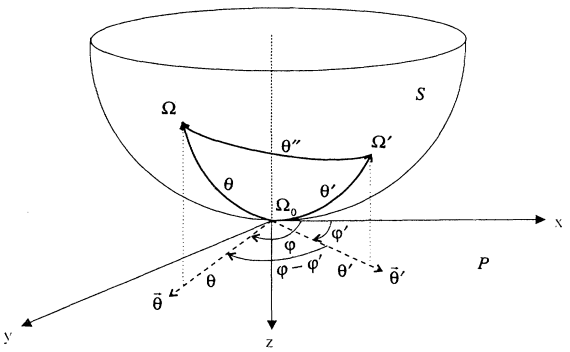

FIG. 3. Spherical triangle $\Omega_0\Omega'\Omega$ describing the addition of the directions of the scattered particle on sphere S.

i.e.,

$$\theta=\sqrt{\theta_x^2+\theta_y^2},\quad \varphi=\arctan\frac{\theta_y}{\theta_x}\ . \tag{3}$$

The addition of directions in the small angle approximation is defined simply as an addition of vectors on the plane P, i.e., if $\vec{\theta}'=\vec{\theta}-\vec{\theta}''=(\theta_x',\theta_y')$ is the initial direction and $\vec{\theta}=(\theta_x,\theta_y)$ is the final direction of the moving particle, then Cartesian coordinates (θ_x'',θ_y'') of the vector $\vec{\theta}''$ describing the change of directions are given by

$$\theta_x''=\theta_x-\theta_x',\quad \theta_y''=\theta_y-\theta_y'\ . \tag{4}$$

Describing this addition of directions in polar coordinates leads to the planar version of formula (1)

$$\theta''=\sqrt{\theta^2+\theta'^2-\theta\theta'\cos(\varphi-\varphi')}\ . \tag{5}$$

The comparison of formulas (5) and (1) shows that the addition of directions under the small angle approximation inherently introduces a distortion in the final direction. In other words, vectorial sum of directions on the plane P, which is equivalent to the exact directions on the unit sphere S, gives a direction on P that is not equivalent to the direction found by addition of exact directions on the sphere S.

In this paper we deal only with rotationally invariant scattering of particles. Therefore many distributions defined over the set of directions Ω (or $\vec{\theta}$), which we consider in this work, exhibit rotational symmetry invariance. This means that functions defined on the unit sphere S, or on the plane P, and expressed in spherical or planar coordinates, respectively, are dependent only on the parameter θ. The notation $\bar{g}(\Omega)$ or $\bar{g}(\vec{\theta})$ is used when the function $\bar{g}$ is a function of the point $\Omega\in S$ or vector $\vec{\theta}\in P$. The notation $g(\theta)$ is used when functions $\bar{g}(\Omega)$ or $\bar{g}(\vec{\theta})$ are seen as dependent only on one argument θ ($\theta\in[0,\pi)$ or $\theta\in[0,\infty)$). Thus we identify the quantities

$$\bar{g}(\Omega)=\bar{g}(\theta,\varphi)=g(\theta),\quad \Omega\in S,\ \theta\in[0,\pi) \tag{6}$$

$$\bar{g}(\vec{\theta})=\bar{g}(\theta,\varphi)=g(\theta),\quad \vec{\theta}\in P,\ \theta\in[0,\infty)\ . \tag{7}$$

If the function $\bar{g}$ is interpreted as the probability density distribution over the sphere S or the plane P, then the following normalization is used:

$$\int_S\bar{g}(\Omega)d\Omega=\int_0^{2\pi}\int_0^{\pi}\bar{g}(\theta,\varphi)\sin\theta\,d\theta\,d\varphi=2\pi\int_0^{\pi}g(\theta)\sin\theta\,d\theta=1 \tag{8}$$

and

$$\int_P\bar{g}(\vec{\theta})d\vec{\theta}=\int_0^{2\pi}\int_0^{\infty}\bar{g}(\theta,\varphi)\theta\,d\theta\,d\varphi=2\pi\int_0^{\infty}g(\theta)\theta\,d\theta=1\ . \tag{9}$$

A. Moliere's theory

Moliere's theory [3] assumes that the evolution of the angular probability density distribution $\bar{f}(\vec{\theta},t)$ on the plane P with path length t satisfies the Boltzmann integro-differential equation given by

$$\frac{\partial\bar{f}(\vec{\theta},t)}{\partial t}=n_a\int_P[\bar{f}(\vec{\theta}-\vec{\theta}'',t)-\bar{f}(\vec{\theta},t)]\frac{d\bar{\sigma}(\vec{\theta}'')}{d\Omega}d\vec{\theta}''\ , \tag{10}$$

where $d\bar{\sigma}(\vec{\theta}'')/d\Omega$ and n_a denote the single scattering cross section of a charged particle and the number of scattering centers per unit volume, respectively. Equation (10), with a Dirac δ-function initial condition $\bar{f}(\vec{\theta},0)=\delta(\vec{\theta})$, can be formally solved [3] by the Fourier transform method. Applying a two-dimensional Fourier transform (with respect to variables θ_x and θ_y) to Eq. (10), solving the transformed equation in the variable t, and then performing the inverse Fourier transform lead to

$$\bar{f}(\vec{\theta},t)=\frac{1}{(2\pi)^2}\int_{P_{\vec{u}}}e^{-n_at\sigma[1-\bar{\varphi}(\vec{u})]}e^{i(\vec{\theta},\vec{u})}d\vec{u}\ , \tag{11}$$

where $\int_{P_{\vec{u}}}e^{-n_at\sigma[1-\bar{\varphi}(\vec{u})]}e^{i(\vec{\theta},\vec{u})}d\vec{u}$ denotes the integration over plane $P_{\vec{u}}$ and σ is the total angular scattering cross section for single scattering given by

$$\sigma=\int_P\frac{d\bar{\sigma}(\vec{\theta})}{d\Omega}d\vec{\theta}\ . \tag{12}$$

In (11), $\bar{\varphi}(\vec{u})$ is a Fourier transform of the normalized single scattering cross section and is given by

$$\bar{\varphi}(\vec{u})=\int_P\frac{1}{\sigma}\frac{d\bar{\sigma}(\vec{\theta})}{d\Omega}e^{-i(\vec{\theta},\vec{u})}d\vec{\theta}\ . \tag{13}$$

At this point we note that the single scattering cross sections, which are used in any theory of multiple scattering of charged particles, are assumed to be rotationally invariant. This means that $d\bar{\sigma}(\vec{\theta})/d\Omega$ is only a function of the radial length θ of the vector $\vec{\theta}$ and, further, it also leads $\bar{\varphi}(\vec{u})$ to exhibit the property of rotational symmetry. Thus $\bar{\varphi}(\vec{u})$ is only a function of radial length u of the vector $\vec{u}$ ($u=|\vec{u}|=\sqrt{u_x^2+u_y^2}$) on the plane $P_{\vec{u}}$. Specifically, after the change from Cartesian coordinates (θ_x,θ_y) to polar coordinates (θ,φ) is done and integration over variable φ is performed, formula (13) can be expressed as the one-dimensional integral

$$\bar{\varphi}(\vec{u})=\varphi(u)=\frac{2\pi}{\sigma}\int_0^{\infty}\frac{d\sigma(\theta)}{d\Omega}J_0(\theta u)\theta\,d\theta\ , \tag{14}$$

where J_0 denotes the Bessel function of order zero. Substituting Eq. (14) for $\bar{\varphi}(\vec{u})$ in (11) shows that $\bar{f}(\vec{\theta},t)$ is also a rotationally invariant function (i.e., a function of the radial length θ only), which can be written as

$$f(\theta,t)=\frac{1}{2\pi}\int_0^{\infty}J_0(\theta u)\exp\left[-n_at\sigma\left[1-\frac{2\pi}{\sigma}\int_0^{\infty}\frac{d\sigma(\theta')}{d\Omega}J_0(\theta' u)\theta' d\theta'\right]\right]u\,du\ . \tag{15}$$

Moliere's theory of multiple scattering evaluates $f(\theta,t)$ from the expression (15) by assuming the screened Rutherford cross section for the single scattering cross section [3]. For this particular cross section, and under some additional assumptions about the parameters that characterize the scattering process [3], the angular probability density $f(\theta,t)$ is expressed approximately as

$$f(\theta,t)=\frac{1}{2\pi}\frac{1}{\chi_c^2 B}\left[f_0(\vartheta)+\frac{1}{B}f_1(\vartheta)+\frac{1}{B^2}f_2(\vartheta)+\cdots\right], \tag{16}$$

where $\vartheta=\theta/\chi_c\sqrt{B}$ and

$$f_n(\vartheta)=\frac{1}{n!}\int_0^\infty J_0(\vartheta)e^{-(1/4)y^2}[\tfrac{1}{4}y^2\ln(\tfrac{1}{4}y^2)]^n y\,dy\ . \tag{17}$$

In particular,

$$f_0(\vartheta)=2e^{-\vartheta^2}\ . \tag{18}$$

The parameter B is defined through the relation $B-\ln B=b$ $(B\geq 1)$ [3], where

$$b=\ln\left[\frac{\chi_c}{\chi_a}\right]^2, \tag{19}$$

$$\chi_c^2=\pi k t\ , \tag{20}$$

$$\chi_a^2=\left[\frac{\lambda\!\!\!^{-}Z^{1/3}}{0.885a_0}\right]^2(1.13+3.76\tilde{\alpha}^2)\ , \tag{21}$$

with $k=n_a[2\sqrt{Z(Z+1)}e^2/pv]^2$ and $\tilde{\alpha}=Z\alpha/\beta$. In the formulas above, Z is the atomic number for the scattering medium, $\lambda\!\!\!^{-}$ is the de Broglie wavelength of incident electron, a_0 is the Bohr radius, n_a is the number of scattering atoms per unit volume, e is the electronic charge, p and v are the momentum and velocity of the electron, α is the fine-structure constant, and β is the ratio of the speed of the electron to the speed of light.

Formulas (16) and (17) provide an efficient, and in the region of their applicability [8,15], an accurate method for the calculation of $f(\theta,t)$, the angular probability density distribution for multiple scattering. However, several shortcomings of Moliere's theory may be identified.

(i) For any reasonable angular scattering cross section which has an integrable derivative, the expression which defines Eq. (15) is divergent. The divergent character of the expression is obvious if we recall that the asymptotic dependence of $J_0(x)$ for large x is $1/\sqrt{x}$. The reason this divergence appears is that, in order to properly accommodate the Dirac δ-function initial conditions, the mathematical model of multiple scattering phenomena should have been investigated in the space of generalized functions whereas it was investigated in the set of standard, pointwise functions.

(ii) The *ad hoc* methods used to deal with this divergence distort the multiple scattering distributions near their initial (Dirac δ-function-like) conditions, i.e., they disturb the expressions that are valid for "no-scattering" or few scattering cases. Thus Moliere's theory is applicable only if the average number of collisions is larger than about 20 [3,8].

(iii) Due to its reliance on the small angle scattering approximation, the results, provided by formulas (16) and (17), are not accurate for large angles.

(iv) The theory is limited to the screened Rutherford single scattering cross section since the derivation of the specific form of the final expressions (16) and (17) is based on this cross section.

(v) The terms f_n given by Eq. (17), for all n except $n=0$, do not have a probabilistic interpretation as they are not positively defined functions.

B. Goudsmit-Saunderson theory

The main feature of Goudsmit and Saunderson's theory [1,2] is the derivation of a formula equivalent to Eq. (14) without the small angle scattering restriction. The angular distribution of multiple scattering $\bar{f}(\Omega,t)=f(\theta,t)$ is again a rotationally invariant function, but in this case it is defined on the surface of the unit sphere S (Fig. 1). As such it can be expressed in the form of a series of Legendre polynomials $P_l(\cos\theta)$ as

$$\bar{f}(\Omega,t)=f(\theta,t)=\sum_{l=0}^{\infty}c_l(t)P_l(\cos\theta)\ , \tag{22}$$

where the coefficients $c_l(t)$ are related to the statistical averages $E\{P_l(\cos\theta)\}$ of the polynomials $P_l(\cos\theta)$ with respect to the probability density distribution $f(\theta,t)$ as

$$E\{P_l(\cos\theta)\}=2\pi\int_0^\pi P_l(\cos\theta)f(\theta,t)\sin\theta\,d\theta=\frac{4\pi}{2l+1}C_l(t)\ ,\qquad l=0,1,2,\ldots\ . \tag{23}$$

The coefficients $c_l(t)$ can be calculated by the substitution of the form (22) of $\bar{f}(\Omega,t)$ into the Boltzmann equation, which describes the angular scattering on the sphere S without the small angle approximation. This equation is, in analogy to Eq. (10), given by

$$\frac{\partial\bar{f}(\Omega,t)}{\partial t}=n_a\int_S[\bar{f}(\Omega-\Omega'',t)-\bar{f}(\Omega,t)]\frac{d\bar{\sigma}(\Omega'')}{d\Omega}d\Omega''\ , \tag{24}$$

where $\Omega-\Omega''$ is a symbolic notation for initial direction Ω' and Ω'' is the change for the particle's direction from Ω' to Ω. $d\bar{\sigma}(\Omega'')/d\Omega$ is the single angular scattering cross section of the particle expressed as a function of direction $\Omega''\in S$. Substituting Eq. (22) into Eq. (24) and applying the addition theorem [14]

$$P_l(\cos\theta)=P_l(\cos\theta_1)P_l(\cos\theta_2)+2\sum_{m=1}^{\infty}P_l^m(\cos\theta_1)P_l^m(\cos\theta_2)\cos m(\varphi_2-\varphi_1)\ ,$$

we obtain a series expansion on both sides of the equation. Grouping terms with the same order of Legendre polynomial, we find that

$$c_l(t)=c_l(0)e^{-n_a t\sigma[1-\langle P_l(\cos\theta_1)\rangle]}\ , \tag{25}$$

where $\langle P_l(\cos\theta_l)\rangle$ denotes the statistical average of the Legendre polynomial of order l with respect to the normalized angular probability density distribution $(1/\sigma)d\bar{\sigma}(\Omega)/d\Omega$. Explicitly, $\langle P_l(\cos\theta_1)\rangle$ is given by

$$\langle P_l(\cos\theta_1)\rangle = 2\pi \int_0^{\pi} \frac{1}{\sigma}\frac{d\sigma(\theta)}{d\Omega} P_l(\cos\theta)\sin\theta\, d\theta \ . \tag{26}$$

Finally, substituting Eq. (25) into Eq. (22) and setting $c_l(0)=2l+1/4\pi$ leads to the expression for $f(\theta,t)$

$$f(\theta,t)=\frac{1}{4\pi}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)e^{-n_a t\sigma[1-\langle P_1(\cos\theta_1)\rangle]} \ . \tag{27}$$

[Note that setting $c_l(0)=2l+1/4\pi$ is equivalent to choosing the two-dimensional Dirac δ-function initial condition $\bar{f}(\Omega,0)=\delta(\Omega-\Omega_0)$ for the density distribution $\bar{f}(\Omega,t)=f(\theta,t)$.] In the limit of small angle scattering the exact spherical formula (27) may be approximated by formula (15).

The main weakness of the Goudsmit-Saunderson theory is the fact that it does not provide any effective means of evaluating formula (27) short of a direct summation of the series. This procedure is computationally inefficient especially when these series are applied to a small number of scatterings [9,10].

III. COMPOUND POISSON PROCESS FORMULATION FOR ANGULAR SCATTERING OF CHARGED PARTICLES

The cumulative angle for the charged particle that has experienced multiple scattering over the path length t is a random variable $\Omega(t)$, which can be represented by a sum of random angular steps Ω_i on the sphere S

$$\Omega(t)=\sum_{i=0}^{N(t)}\Omega_i \ . \tag{28}$$

The random variable $\Omega(t)$ for the case of $N(t)=0$ describes the no-scattering change of direction and its probability density distribution $p^{(0)}(\Omega)$ is given by a Dirac δ function

$$p^{(0)}(\Omega)=\delta(\Omega-\Omega_0) \ . \tag{29}$$

Thus Eqs. (28) and (29) represent the direction $\Omega(t)$ of motion for the particle at path length t provided the initial direction of the particle (at $t=0$) coincides with the z axis, i.e., $\Omega(0)=\Omega_0$. The generalization to the case when $\Omega(0)$ is an arbitrary random variable is straightforward, so we can continue our investigations assuming $\Omega(0)=\Omega_0$ in order to be consistent with the initial conditions used in the classical theories of Moliere and Goudsmit-Saunderson. The symbol Ω_i is used in (28) to denote the change of direction at the ith collision and $N(t)$ is used to denote the number of independent scatterings experienced by the particle on the path length t. For a fixed t, $N(t)$ is a Poisson random variable that is characterized by the probability distribution $\text{Prob}\{N(t)=n\}$ given by

$$\text{Prob}\{N(t)=n\}=e^{-\lambda t}\frac{(\lambda t)^n}{n!}, \quad n=0,1,2,\ldots \ , \tag{30}$$

where $\lambda=n_a\sigma$ (n_a is the number of scattering atoms per unit volume and σ the total angular scattering cross section for the particle per atom). λ is a parameter that is interpreted as the average number of collisions per unit path length. The probability distribution (30) is called a Poisson distribution and $\{N(t),\ t>0\}$ is called a Poisson process [16]. The random variables Ω_i, $i=1,2,\ldots$, are assumed to be independent and identically distributed. We denote the probability density distribution of Ω_i by $\bar{p}(\Omega)$, $i=1,2,\ldots$, and notice that this quantity is synonymous with the normalized angular scattering cross section for single interaction $(1/\sigma)d\bar{\sigma}(\Omega)/d\Omega$. Since $\bar{p}(\Omega)$ is always assumed to be a rotationally invariant function, then in agreement with our previous notation we can write

$$\bar{p}(\Omega)=\frac{1}{\sigma}\frac{d\bar{\sigma}(\Omega)}{d\Omega}=\frac{1}{\sigma}\frac{d\bar{\sigma}(\theta,\varphi)}{d\Omega}=\frac{1}{\sigma}\frac{d\sigma(\theta)}{d\Omega}=p(\theta) \ . \tag{31}$$

The process $\{\Omega(t),\ t\geq 0\}$ defined above is a two-dimensional compound Poisson process [17] and its transition probability density distribution from the direction $\Omega=\Omega_0$ (at $t=0$) to an arbitrary direction Ω at path length t is given by

$$\bar{f}(\Omega,t)=e^{-\lambda t}\sum_{n=0}^{\infty}\frac{(\lambda t)^n}{n!}\bar{p}^{(n)}(\Omega) \ , \tag{32}$$

where $\bar{p}^{(n)}(\Omega)$ denotes the normalized angular distribution of the charged particle that has experienced *exactly* n collisions [16,17]. Since the angular distribution $\bar{p}(\Omega)$ of the single scattering is rotationally symmetric, it can be shown that the same property will be valid for the multiple scattering distribution. Hence we can write

$$\bar{p}^{(n)}(\Omega)=p^{(n)}(\theta), \quad n=0,1,2,\ldots \ . \tag{33}$$

As a result, Eq. (32) can be rewritten as

$$\bar{f}(\Omega,t)=f(\theta,t)=e^{-\lambda t}\sum_{n=0}^{\infty}\frac{(\lambda t)^n}{n!}p^{(n)}(\theta) \ . \tag{34}$$

The explicit recursive formulas for $p^{(n)}(\theta)$ in terms of single scattering angular density distribution $p(\theta)$ are found as follows. (i) For $n=0$, $\bar{p}^{(0)}(\vec{\theta})=\delta(\vec{\theta})$. (ii) For $n=1$, $p^{(1)}(\theta)=p(\theta)$, i.e., $p^{(1)}(\theta)$ is just the probability density distribution (normalized cross section) for single angular scattering. (iii) For $n\geq 2$, $p^{(n)}(\theta)$ is given by the recursive relation

$$p^{(n)}(\theta)=\int_0^{\infty}p^{(n-1)}(\theta')q(\theta,\theta')\theta' d\theta' \tag{35}$$

for the planar coordinate system, where $q(\theta,\theta')$ is calculated as $q(\theta,\theta')=\int_0^{2\pi}p(\theta'')d\varphi'$ and the angle θ'' is given by formula (5), or

$$p^{(n)}(\theta)=\int_0^{\pi}p^{(n-1)}(\theta')q(\theta,\theta')\sin\theta' d\theta' \tag{36}$$

for the spherical coordinate system, where $q(\theta,\theta')$ is calculated as $q(\theta,\theta')=\int_0^{2\pi}p(\theta'')d\varphi'$ and the angle θ'' is given by formula (1). The explicit formulas for $q(\theta,\theta')$ in all cases considered in this work are provided in Appendix B.

The direct calculation of the transition density distribution $\bar{f}(\Omega,t)$ from Eq. (34) is possible if the average number of collisions experienced by the particle is small. When the average number of collisions is large a special method has to be developed for the calculation. The description of this method will be presented in Sec. V. First, however, let us demonstrate that the compound Poisson process model for multiple angular scattering of charged particles is in fact equivalent to the Goudsmit-Saunderson model and that it also underlies Moliere's calculations if the small angle scattering restriction is imposed.

IV. GOUDSMIT-SAUNDERSON AND MOLIERE THEORIES AS SPECIAL CASES OF THE COMPOUND POISSON PROCESS

The Poisson process $\{N(t),\ t>0\}$ that governs the distribution of scattering events along a charged particle's path t is characterized by the following properties of its probability distribution on an infinitesimal path length dt [16]:

$$\text{Prob}\{N(dt)=0\}=1-\lambda dt+o(dt)\ , \tag{37}$$

$$\text{Prob}\{N(dt)=1\}=\lambda dt+o(dt)\ , \tag{38}$$

$$\text{Prob}\{N(dt)\geq 2\}=o(dt)\ , \tag{39}$$

where $\text{Prob}\{N(dt)=k\}$, $k=0,1,2,\ldots$, denotes the probability that exactly k scattering events took place on the interval dt; $o(dt)$ denotes a function that decreases to zero faster than dt and λ is the parameter interpreted as the average number of collisions per unit path length. Formulas (37)–(39) imply that for the compound Poisson process (28) the transition probability density $\bar{p}_{dt}(\Omega|\Omega')$ for the particle to change direction from Ω' to Ω on the infinitesimal path length dt equals

$$\bar{p}_{dt}(\Omega|\Omega-\Omega'')=\delta(\Omega'')(1-\lambda dt)+\bar{p}(\Omega'')\lambda dt+o(dt)\ , \tag{40}$$

where $\delta(\Omega'')$ is a Dirac delta function and $\bar{p}(\Omega'')$ is the probability density distribution for the change of direction in each collision from $\Omega-\Omega''$ to Ω. Thus the angular density distribution $\bar{f}(\Omega,t+dt)$ for a multiple scattered particle at path length $t+dt$ is related to the angular density distribution $\bar{f}(\Omega,t)$ at path length t by

$$\bar{f}(\Omega,t+dt)=\int_S\bar{f}(\Omega-\Omega'',t)\times[\delta(\Omega'')(1-\lambda\,dt)+\bar{p}(\Omega'')\lambda\,dt]d\Omega''+o(dt)\ . \tag{41}$$

Equation (41) may be transformed into a Boltzmann equation by integrating the Dirac δ-function term in (41), then moving the term $\bar{f}(\Omega,t)$ to the left-hand side of (41), dividing both sides by dt, followed by taking a limit $dt\to 0$,

$$\frac{\partial\bar{f}(\Omega,t)}{\partial t}=\lambda\int_S[\bar{f}(\Omega-\Omega'',t)-\bar{f}(\Omega,t)]\bar{p}(\Omega'')d\Omega''\ . \tag{42}$$

Notice that Eq. (42) is identical to (24) because $\bar{p}(\Omega)=(1/\sigma)d\bar{\sigma}(\Omega)/d\Omega$ and $\lambda=n_a\sigma$. In the small angle approximation Eq. (42) is reduced to a Boltzmann equation on the plane P given by

$$\frac{\partial\bar{f}(\vec{\theta},t)}{\partial t}=\lambda\int_P[\bar{f}(\vec{\theta}-\vec{\theta}'',t)-\bar{f}(\vec{\theta},t)]\bar{p}(\vec{\theta}'')d\vec{\theta}''\ , \tag{43}$$

which is equivalent to Eq. (10) used in Moliere's theory. The identity of Eqs. (42) and (24) and Eqs. (43) and (10) means that the Goudsmit-Saunderson and Moliere theories are based on the compound Poisson process description of multiple angular scattering, which was described in Sec. III.

V. CALCULATIONS BASED ON THE DECOMPOSITION OF COMPOUND POISSON PROCESS

The method of calculating transition density $\bar{f}(\Omega,t)=f(\theta,t)$ directly from formulas (34)–(36) is practical when the average number of collisions is less than a few hundred. For problems with a larger average number of collisions, the method of direct calculation from the formulas breaks down since it requires computational operations with extremely small and extremely large numbers. Moreover, the time of calculations grows prohibitively long when the average number of collisions is large. Thus, in such cases, it is necessary to apply an indirect method for evaluation of the transition density $f(\theta,t)$. A very efficient strategy for these computations can be based on the theorem that states that any compound Poisson process can be decomposed into the sum of independent compound Poisson processes [17]. For our purposes, the decomposition of $\Omega(t)$ into just two independent processes is satisfactory. Let us formulate therefore the special case of this theorem, pertinent to our calculations (for a proof of the general case of this theorem see [17]).

Theorem. Let $S_{\theta_{\text{sep}}},\bar{S}_{\theta_{\text{sep}}}$ denote two sets that define a partition of the sphere S (or the plane P when the small angle scattering approximation is used) by a circle $\theta=\theta_{\text{sep}}$ such that

$$\Omega\in S_{\theta_{\text{sep}}}\quad\text{if } \Omega=(\theta,\varphi),\ \theta<\theta_{\text{sep}}$$

or

$$\Omega\in\bar{S}_{\theta_{\text{sep}}}\quad\text{if } \Omega=(\theta,\varphi),\ \theta\geq\theta_{\text{sep}}\ .$$

Let $I_A(\Omega)$ denote the characteristic (indicator) function of the set A. Then the processes $\Omega^{\text{soft}}(t)$ and $\Omega^{\text{hard}}(t)$ defined by

$$\Omega^{\text{soft}}(t)=\sum_{k=0}^{N(t)}\Omega_k I_{S_{\theta_{\text{sep}}}}(\Omega_k) \tag{44}$$

and

$$\Omega^{\text{hard}}(t)=\sum_{k=0}^{N(t)}\Omega_k I_{\bar{S}_{\theta_{\text{sep}}}}(\Omega_k) \tag{45}$$

are mutually independent compound Poisson processes (CPPs) and their sum is equal to $\Omega(t)$. This also means that the probability density distribution $\bar{f}(\Omega,t)$ for variable $\Omega(t)$ can be written as

$$\bar{f}(\Omega,t)=\int_S \bar{f}^{\text{soft}}(\Omega-\Omega'',t)\bar{f}^{\text{hard}}(\Omega'',t)d\Omega'' , \tag{46}$$

where $\bar{f}^{\text{soft}}(\Omega,t)$ and $\bar{f}^{\text{hard}}(\Omega,t)$ denote the probability densities for the random variables $\Omega^{\text{soft}}(t)$ and $\Omega^{\text{hard}}(t)$, respectively.

Notice that the process $\Omega^{\text{soft}}(t)$ consists of "small angle" scattering only [i.e., that for which each individual change of direction $\Omega_k=(\theta_k,\varphi_k)$ satisfies $\theta_k<\theta_{\text{sep}}$, $k=0,1,\ldots,N(t)$] and the process $\Omega^{\text{hard}}(t)$ consists of "large angle" scattering only [i.e., that for which each individual change of direction $\Omega_i=(\theta_i,\varphi_i)$ satisfies $\theta_i\geq\theta_{\text{sep}}$, $i=1,2,\ldots,N(t)$]. Hence we may call the process $\Omega^{\text{soft}}(t)$ the soft collision process and the process $\Omega^{\text{hard}}(t)$ the hard collision process. If the overall average number of collisions λt is small (e.g., <500), then the distribution for both processes $\Omega^{\text{soft}}(t)$ and $\Omega^{\text{hard}}(t)$ can be found directly. If, however, the overall average number of collisions λt is large (from a few hundred to a few thousand), such calculations are impractical or even impossible. In this case at least one group of collisions (hard or soft) has to contain a large number of scattering events. How many scattering events are classified as hard and how many as soft depends on the choice of the parameter θ_{sep}. For a typical (strongly peaked at $\Omega=\Omega_0$) normalized angular scattering cross section $\bar{p}(\Omega)$, even relatively small values of the parameter θ_{sep} (e.g., $\theta_{\text{sep}}\approx 1°$) lead to a small average number of hard collisions $\lambda^{\text{hard}}t$. (Notice that Moliere's definition of the angle χ_c is equivalent to setting $\chi_c=\theta_{\text{sep}}$, where θ_{sep} defines the average number of hard collisions as equal to 1, i.e., $\lambda^{\text{hard}}t=1$). This means that the average number of soft collisions $\lambda^{\text{soft}}t$ is large because $\lambda^{\text{soft}}t$ is equal to $\lambda t-\lambda^{\text{hard}}t$. Since all these soft scatterings are characterized by small angular changes, the process $\Omega^{\text{soft}}(t)$ has all the characteristics of a diffusion process [17,18].

The relatively large average number of soft collisions allows us to closely approximate the density distribution $\bar{f}^{\text{soft}}(\Omega,t)$ for the soft collision process $\Omega^{\text{soft}}(t)$ by the density distribution $\bar{f}^{\text{diff}}(\Omega,t)$ for the diffusion process $\Omega^{\text{diff}}(t)$ [18]

$$\bar{f}^{\text{diff}}(\Omega,t)=\lim_{\substack{\theta_{\text{sep}}\to 0\\ n_{\text{soft}}\to\infty}}\bar{f}^{\text{soft}}(\Omega,t) , \tag{47}$$

where n_{soft} denotes the average number of soft collisions $\lambda^{\text{soft}}t$. On the other hand, the relatively small average number of hard collisions allows us to calculate the distribution $\bar{f}^{\text{hard}}(\Omega,t)$ for the hard collision process $\Omega^{\text{hard}}(t)$ directly from formulas (34)–(36). [Notice that the density distributions $\bar{f}^{\text{hard}}(\Omega,t)$ and $\bar{f}^{\text{diff}}(\Omega,t)$ are both rotationally invariant due to the rotational symmetry of single angular scattering. We therefore will use the notations $f^{\text{hard}}(\theta,t)$, $f^{\text{diff}}(\theta,t)$, and $f(\theta,t)$ in place of $\bar{f}^{\text{hard}}(\Omega,t)$, $\bar{f}^{\text{diff}}(\Omega,t)$, and $\bar{f}(\Omega,t)$, respectively.] Analogous to (34), the explicit formula for the density distribution $f^{\text{hard}}(\theta,t)$ can be written as

$$f^{\text{hard}}(\theta,t)=e^{-\lambda^{\text{hard}}t}\sum_{n=0}^{\infty}\frac{(\lambda^{\text{hard}}t)^n}{n!}p^{\text{hard}(n)}(\theta) , \tag{48}$$

where $p^{\text{hard}(n)}(\theta)$ denotes the normalized angular density distribution of the charged particle that has experienced exactly n collisions, each changing the particle's direction by an angle larger than θ_{sep}. The explicit recursive formulas for $p^{\text{hard}(n)}(\theta)$, in terms of various single "hard" scattering angular density distributions $p^{\text{hard}}(\theta)$, are given in Appendix B. In fact, we only perform summation over a finite number n_{hard} of terms in (48), where n_{hard} is appropriately larger than the average number of hard collisions $\lambda^{\text{hard}}t$. This is justified since the total contribution from all terms with indices larger than n_{hard} is negligible.

The explicit formula for the density distribution $f^{\text{diff}}(\theta,t)$ is given by [17,19]

$$f^{\text{diff}}(\theta,t)=\frac{1}{4\pi}\sum_{n=0}^{\infty}e^{-(1/2)n(n+1)Dt}(2n+1)P_n(\cos\theta) \tag{49}$$

for the calculations in the spherical coordinate system and by

$$f^{\text{diff}}(\theta,t)=\frac{1}{2\pi Dt}e^{-\theta^2/2Dt} \tag{50}$$

for the calculations in the planar coordinate system. In (49) and (50) D denotes the diffusion constant for the process $\Omega^{\text{diff}}(t)$. The diffusion constant D is a local characteristic of the process $\Omega^{\text{diff}}(t)$ and thus it has the same value in both the spherical coordinate system and the planar coordinate system (i.e., when the small angle approximation is imposed). Thus we can write

$$D=D_{\text{sphere}}=D_{\text{plane}}=\lambda\sigma^2 , \tag{51}$$

where λ is the average number of soft scattering per unit path length and σ^2 the angular scattering variance of the electron for a single soft collision. Substituting (49) into (46) leads to the following representation of $f(\theta,t)$ in the spherical coordinate system:

$$f_{\text{sphere}}(\theta,t)=\frac{1}{4\pi}\sum_{n=0}^{\infty}(2n+1)e^{-(1/2)n(n+1)Dt}\times\int_0^{2\pi}\int_0^{\pi}P_n(\cos\theta')f^{\text{hard}}_{\text{sphere}}(\theta'',t)\times\sin\theta' d\theta' d\varphi' , \tag{52}$$

where $\cos\theta''=\cos\theta\cos\theta'+\sin\theta\sin\theta'\cos\varphi'$. Similarly, substituting (50) into (46) leads to the following representation of $f(\theta,t)$ in the planar coordinate system:

$$f_{\text{plane}}(\theta,t)=\frac{1}{2\pi Dt}\int_0^{2\pi}\int_0^{\pi}e^{-\theta'^2/2Dt}f^{\text{hard}}_{\text{plane}}(\theta'',t)\theta' d\theta' d\varphi' , \tag{53}$$

where $\theta''=\sqrt{\theta^2+\theta'^2-\theta\theta'\cos\varphi'}$. For both formulas

$f^{\text{hard}}(\theta,t)$ is calculated according to the direct method represented by (34).

To verify when the diffusion limit for soft collisions holds [i.e., how large n_{soft} and how small θ_{sep} should be so that $f^{\text{soft}}(\theta,t)$ is closely approximated by Eq. (49) or (50)], the following two tests were performed.

(i) For as large a number of average collisions as possible (λt of the order of a few hundreds, $f(\theta,t)$ was calculated directly from formulas (34)–(36). Then the calculations for $f(\theta,t)$ were also performed using the indirect decomposition method. One can observe in Fig. 4 that for decreasing values of θ_{sep}, the function $f_{\theta_{\text{sep}}}(\theta,t)$, calculated by the decomposition method, converged to the exact function $f(\theta,t)$, calculated by the direct method using formulas (34)–(36). This convergence indicates that, for multiple scattering with an average number of collisions λt of the order of 100, the process $\Omega^{\text{soft}}(t)$ already exhibits the character of a diffusion process $\Omega^{\text{diff}}(t)$. This means that in the case under consideration, $f^{\text{soft}}(\theta,t)$ can be set equal to $f^{\text{diff}}(\theta,t)$ with a high degree of accuracy, i.e., that the limit condition specified in (47) applies here.

(ii) For an average total number of collisions too large for direct calculations (λt is larger than a few thousand), calculations of $f(\theta,t)$ were performed using the indirect decomposition method for various values of parameter θ_{sep}. We know from test (i) that the number of collisions in this new case is large enough that $\Omega^{\text{soft}}(t)$ will exhibit a convergence to the diffusion $\Omega^{\text{diff}}(t)$ with decreasing θ_{sep}. Therefore it was expected that $f^{\text{soft}}(\theta,t)$ will converge to $f^{\text{diff}}(\theta,t)$ and that $f(\theta,t)$, calculated according to formulas (52) and (53), will converge to the exact angular probability density distribution function $f(\theta,t)$ given by (46). This convergence is exactly what we observed when the calculations were performed for a few chosen cases (see, e.g., Fig. 7). Thus we were able to identify the function obtained in this limit with the exact angular density distribution function $f(\theta,t)$.

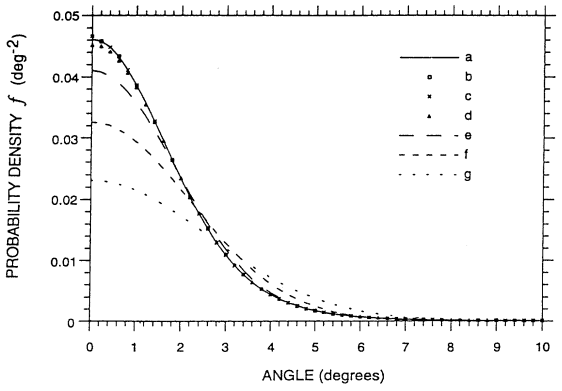

FIG. 4. Angular distributions of a 15.7-MeV electron after penetrating a 0.001-cm gold foil, calculated by the CPP method in the spherical coordinate system using the screened Rutherford cross sections. (a) $r=100\%$ (direct), $\theta_{\text{sep}}=0°$; (b) $r=20\%$, $\theta_{\text{sep}}=0.2°$; (c) $r=10\%$, $\theta_{\text{sep}}=0.3°$; (d) $r=1\%$, $\theta_{\text{sep}}=1.0°$; (e) $r=0.1\%$, $\theta_{\text{sep}}=3.1°$; (f) $r=0.01\%$, $\theta_{\text{sep}}=9.8°$; (g) $r=0.000\,25\%$, $\theta_{\text{sep}}=57.1°$.

VI. CALCULATIONS

Figure 4 illustrates the convergence of the decomposition method calculations for decreasing values of θ_{sep}. All curves presented in this graph are calculated according to the compound Poisson process method on the sphere for a 15.7-MeV electron penetrating a 0.001-cm gold foil. They are calculated using the screened Rutherford single scattering cross section and assuming a standard normalization of the density function $f(\theta,t)$ [see formula (8)]. Different curves are obtained by assuming different values of θ_{sep} in the decomposition method. The values of θ_{sep} may change from zero to π. For $\theta_{\text{sep}}=0$ all collisions are classified as hard and the density function $f(\theta,t)$ is calculated based on formulas (34)–(36), i.e., direct calculation. For $\theta_{\text{sep}}=\pi$ all collisions are classified as soft and the density $f(\theta,t)$ is calculated based on formula (49). The value of θ_{sep} determines uniquely the ratio r of the average hard collision number to the average total collision number. Therefore the ratio r equals 100% (direct) if $\theta_{\text{sep}}=0$ and it is 0% if $\theta_{\text{sep}}=\pi$. The r values for different θ_{sep} are listed in Table I.

Figure 5 presents graphs of the angular probability density distributions calculated by the indirect CPP method in the planar coordinate system by setting θ_{sep} equal to 1° and 57.1°, respectively. The results are compared with that calculated by Fermi-Eyges (FE) theory and Moliere theory. As may be expected, the graph from CPP calculations with $\theta_{\text{sep}}=57.1°$ ($\approx$ rad) and $r=0.0025\%$ is almost identical to the graph from the Fermi model [15]. This is so because (i) Fermi model calculations are identical to CPP calculations, which include soft collisions only and for which θ_{sep} is being set equal to a cutoff angle that is not larger than 1 rad, and (ii) the effect of a small average number of hard collisions (which are included in the graph of CPP calculation in the figure with $\theta_{\text{sep}}=57.1°$ and $r=0.0025\%$) on the final distribution function $f(\theta,t)$ is negligible. On the other hand, the graph based on Moliere theory agrees very well with the graph of a function parametrized by $\theta_{\text{sep}}=1°$ ($r=1\%$). Both these latter graphs should give an accurate description of the angular scattering process according to the discussion provided in Sec. V. This prediction is convincingly confirmed by comparing our results to the experi-

TABLE I. $r=\lambda^{\text{hard}}_{\text{sphere}}t/\lambda_{\text{sphere}}t$ and θ_{sep} for the graphs in Fig. 2.

r (%)	θ_{sep} (deg)
100 (direct)	0
20	0.2
10	0.3
1	1.0
0.1	3.1
0.01	9.8
0.000 25	57.1
FE theory	$\theta_m=57.3$
Moliere theory	$\chi_c=1.1$

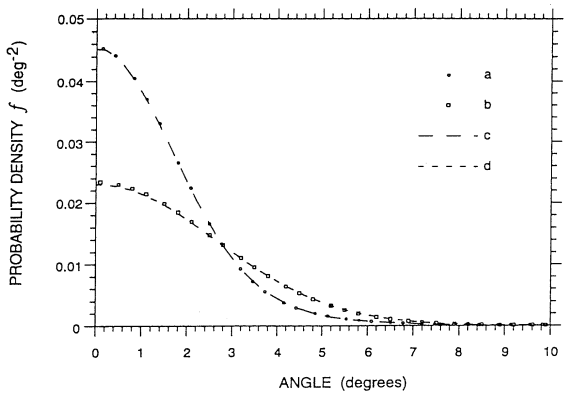

FIG. 5. Angular distributions of a 15.7-MeV electron after penetrating a 0.001-cm gold foil. (a) Moliere's theory; (b) Fermi's theory; (c) the CPP method, $r=1\%$, $\theta_{sep}=1.0°$; (d) the CPP method, $r=0.000\,25\%$, $\theta_{sep}=57.1°$. Both (c) and (d) are calculated in a planar coordinate system using the screened Rutherford cross sections.

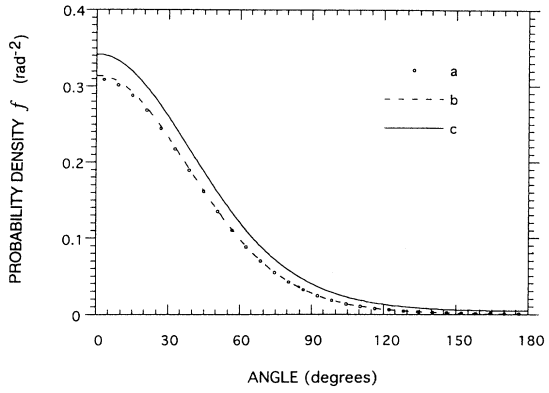

FIG. 7. Angular distribution of a 1-MeV electron after penetrating a 701-μm aluminum foil. (a) Moliere's theory; (b) $r=1\%$, $\theta_{sep}=4.3°$, planar coordinates; (c) $r=1\%$, $\theta_{sep}=4.3°$, spherical coordinates. Both (b) and (c) are calculated using the screened Rutherford cross sections.

mental data of Hanson *et al.* [20]. Thus Fig. 5 may be seen as clarifying the relationship between the Fermi and Moliere models of multiple angular scattering. They are both manifestations of approximate evaluations of a compound Poisson process model of angular scattering in the planar coordinate system.

Figures 6 and 7 show a few graphs of $f(\theta,t)$ calculated by the method described in this paper. The graphs are compared with that obtained by Moliere theory. They show that, for the particular cases considered, our approach is advantageous. In particular, Fig. 6 illustrates how Moliere theory breaks down for a few collisions (and even gives negative probability densities) while the CPP method leads to the correct result. Figure 7 shows how the small angle approximation in Moliere theory can substantially distort the distribution for low-energy electrons. Finally, Fig. 8 illustrates how the unavoidable reliance on the screened Rutherford cross section can be responsible for overestimation of the small angle and underestimation of the large angle contributions to the angular spectrum of low-energy electrons.

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APPENDIX A: INSTRUCTION FOR CALCULATIONS USING THE CPP METHOD

Utilizing the method of compound Poisson processes described in this work, a sequence of calculations was performed for the angular scattering probability density function $f(\theta,t)$. The calculations were performed in both the spherical coordinate system and in the planar coordinate system (when the small angle approximation was imposed). The single scattering angular cross section

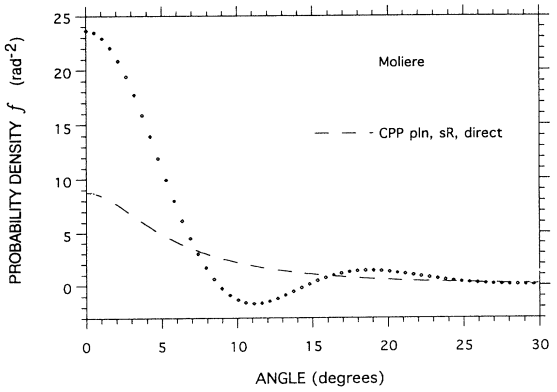

FIG. 6. Angular distributions of a 0.128-MeV electron after penetrating a 0.1770-μm gold foil.

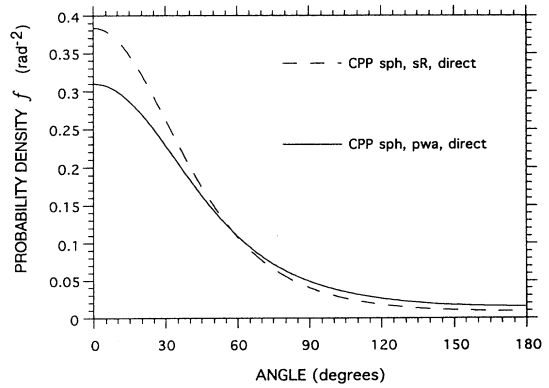

FIG. 8. Angular distributions of a 0.128-MeV electron after penetrating 1.33-μm gold foil, calculated directly in the spherical coordinate system using the screened Rutherford cross section and the partial wave analysis cross section.

TABLE II. Categories of the calculations performed.

	Spherical coordinate system			Planar coordinate system		
		Indirect			Indirect	
Method	Direct	Soft	Hard	Direct	Soft	Hard
Screened Rutherford	A	B	C	D	E	F
Partial wave	G	H	I			

used was either the screened Rutherford cross section or the more accurate partial wave analysis cross section. Moreover, the calculations were performed using both the direct and indirect approaches. To illustrate concisely all the categories for which the calculations were performed we present Table II.

Each one of the nine letters (from A to I) labeled in Table II indicates a category for which the calculation of $f(\theta,t)$ was performed. For each direct calculation method we have to know only the formulas for $p^{(n)}(\theta)$ and λ [Eq. (34)]. We may compute $p^{(n)}(\theta)$ for all $n=2,3,4,\ldots$ according to the recursive relation of formula (36) only if expressions for $p(\theta)$ and $q(\theta,\theta')$ are known. Therefore, in the Appendix we list the basic formulas for λ, $p(\theta)$, and $q(\theta,\theta')$ for each category of direct calculation of $f(\theta,t)$ [14]. To avoid confusion, in each category under consideration, the quantities λ, $p(\theta)$, and $q(\theta,\theta')$ will be equipped with appropriate subscripts and superscripts to indicate the kind of calculations to which they pertain. For example, the categories D, E, and F involve computations with the screened Rutherford single scattering cross section and small angle approximation (planar coordinates), subsequently the quantities λ, $p(\theta)$, and $q(\theta,\theta')$ are denoted by $\lambda_{\text{plane,SR}}$, $p_{\text{plane,SR}}(\theta)$, and $q_{\text{plane,SR}}(\theta,\theta')$, respectively. Similarly for the categories C, F, and I of the hard component of indirect calculations, the basic quantities λ, $p(\theta)$, and $q(\theta,\theta')$ are denoted by λ^{hard}, $p^{\text{hard}}(\theta)$, and $q^{\text{hard}}(\theta,\theta')$. Thus for category F the quantities λ, $p(\theta)$, and $q(\theta,\theta')$ are denoted by $\lambda^{\text{hard}}_{\text{plane,SR}}$, $p^{\text{hard}}_{\text{plane,SR}}(\theta)$, and $q^{\text{hard}}_{\text{plane,SR}}(\theta,\theta')$, respectively. Finally, for the soft component of the indirect calculations the basic quantities, as seen from Eq. (51), are λ^{soft} and the scattering variance $(\sigma^2)^{\text{soft}}$. They determine uniquely the diffusion constant D and also the diffusion component $f^{\text{diff}}(\theta,t)$ of the angular probability density distribution $f(\theta,t)$. Therefore the quantities λ and σ^2 with appropriate subscripts and superscripts [e.g., $\lambda^{\text{soft}}_{\text{plane,SR}}$ and $(\sigma^2)^{\text{soft}}_{\text{plane,SR}}$] are also listed in Appendix B.

APPENDIX B: BASIC FORMULAS FOR λ, $p(\theta)$, AND $q(\theta,\theta')$

For category A,

$$\lambda_{\text{sphere,SR}}=\frac{4\pi k}{\theta^2_{\min}(4+\theta^2_{\min})},$$

$$p_{\text{sphere,SR}}(\theta)=\frac{\theta^2_{\min}(4+\theta^2_{\min})}{16\pi(1+\frac{1}{2}\theta^2_{\min}-\cos\theta)^2},$$

$$q_{\text{sphere,SR}}(\theta,\theta')=\frac{\theta^2_{\min}(4+\theta^2_{\min})(1+\frac{1}{2}\theta^2_{\min}-\cos\theta\cos\theta')}{8[(1+\frac{1}{2}\theta^2_{\min}-\cos\theta\cos\theta')^2-(\sin\theta\sin\theta')^2]^{3/2}};$$

for category B,

$$\lambda^{\text{soft}}_{\text{sphere,SR}}=\frac{\pi k(1-\cos\theta_{\text{sep}})}{\theta^2_{\min}(1+\frac{1}{2}\theta^2_{\min}-\cos\theta_{\text{sep}})},$$

$$(\sigma^2)^{\text{soft}}_{\text{sphere,SR}}=(\sigma^2)^{\text{soft}}_{\text{plane,SR}}\frac{\Delta^{\text{soft}}_{\text{plane,SR}}}{\lambda^{\text{soft}}_{\text{sphere,SR}}}$$

[see category E for $(\sigma^2)^{\text{soft}}_{\text{plane,SR}}$ and $\lambda^{\text{soft}}_{\text{plane,SR}}$] and for category C,

$$\lambda^{\text{hard}}_{\text{sphere,SR}}=\frac{\pi k(1+\cos\theta_{\text{sep}})}{(4+\theta^2_{\min})(1+\frac{1}{2}\theta^2_{\min}-\cos\theta_{\text{sep}})},$$

$$p^{\text{hard}}_{\text{sphere,SR}}(\theta)=\begin{cases}0, & 0\le\theta<\theta_{\text{sep}}\\ \dfrac{(4+\theta^2_{\min})(1+\frac{1}{2}\theta^2_{\min}-\cos\theta_{\text{sep}})}{4\pi(1+\cos\theta_{\text{sep}})(1+\frac{1}{2}\theta^2_{\min}-\cos\theta)^2}, & \theta_{\text{sep}}\le\theta\le\pi.\end{cases}$$

TABLE III. Conditional formulas for $q^{\text{hard}}_{\text{sphere,SR}}(\theta,\theta')$.

Condition on θ and θ'	$q^{\text{hard}}_{\text{sphere,SR}}(\theta,\theta')$
$\theta+\theta' \le \theta_{\text{sep}}$ or $2\pi-(\theta+\theta') < \theta_{\text{sep}}$	0
$\lvert\theta-\theta'\rvert > \theta_{\text{sep}}$	$\dfrac{(4+\theta^2_{\text{min}})(1+\frac{1}{2}\theta^2_{\text{min}}-\cos\theta_{\text{sep}})(1+\frac{1}{2}\theta^2_{\text{min}}-\cos\theta\cos\theta')}{2(1+\cos\theta_{\text{sep}})[(1+\frac{1}{2}\theta^2_{\text{min}}-\cos\theta\cos\theta')^2-(\sin\theta\sin\theta')^2]^{3/2}}$
$\theta=0,\ \theta_{\text{sep}} < \theta' \le \pi$	$\dfrac{(4+\theta^2_{\text{min}})(1+\frac{1}{2}\theta^2_{\text{min}}-\cos\theta_{\text{sep}})}{2(1+\cos\theta_{\text{sep}})(1+\frac{1}{2}\theta^2_{\text{min}}-\cos\theta')^2}$
$\theta_{\text{sep}} < \theta \le \pi,\ \theta'=0$	$\dfrac{(4+\theta^2_{\text{min}})(1+\frac{1}{2}\theta^2_{\text{min}}-\cos\theta_{\text{sep}})}{2(1+\cos\theta_{\text{sep}})(1+\frac{1}{2}\theta^2_{\text{min}}-\cos\theta)^2}$
$\lvert\theta-\theta'\rvert < \theta_{\text{sep}}$ and $\theta+\theta' > \theta_{\text{sep}}$	$\dfrac{(4+\theta^2_{\text{min}})(1+\frac{1}{2}\theta^2_{\text{min}}-\cos\theta_{\text{sep}})}{2\pi(1+\cos\theta_{\text{sep}})}\left\{\dfrac{\pi a}{(a^2-b^2)^{3/2}}+\dfrac{b\sin\varphi'_1}{(a^2-b^2)(a+b\cos\varphi'_1)}-\dfrac{2a}{(a^2-b^2)^{3/2}}\arctan\left[\dfrac{\sqrt{a^2-b^2}\tan(\frac{1}{2}\varphi'_1)}{a+b}\right]\right\}$

The conditional formulas for $q^{\text{hard}}_{\text{sphere,SR}}(\theta,\theta')$ are given in Table III, where $a=1+\frac{1}{2}\theta^2_{\text{min}}-\cos\theta\cos\theta'$, $b=-\sin\theta\sin\theta'$, and $\varphi'_1=\arccos[(\cos\theta_{\text{sep}}-\cos\theta\cos\theta')/\sin\theta\sin\theta']$.

For category D,

$$\lambda_{\text{plane,SR}}=\frac{\pi k}{\theta^2_{\text{min}}}\ ,$$

$$p_{\text{plane,SR}}(\theta)=\frac{\theta^2_{\text{min}}}{\pi(\theta^2+\theta^2_{\text{min}})^2}\ ,$$

$$q_{\text{plane,SR}}(\theta,\theta')=\frac{2\theta^2_{\text{min}}(\theta^2+\theta'^2+\theta^2_{\text{min}})}{[(\theta^2+\theta'^2+\theta^2_{\text{min}})^2-4\theta^2\theta'^2]^{3/2}}\ ;$$

for category E,

$$\lambda^{\text{soft}}_{\text{plane,SR}}=\frac{\pi k\theta^2_{\text{sep}}}{\theta^2_{\text{min}}(\theta^2_{\text{min}}+\theta^2_{\text{sep}})}\ ,$$

$$(\sigma^2)^{\text{soft}}_{\text{plane,SR}}=\frac{1}{2}\theta^2_{\text{min}}\left[\frac{\theta^2_{\text{min}}+\theta^2_{\text{sep}}}{\theta^2_{\text{sep}}}\ln\left[\frac{\theta^2_{\text{min}}+\theta^2_{\text{sep}}}{\theta^2_{\text{min}}}\right]-1\right]\ ;$$

and for category F,

$$\lambda^{\text{hard}}_{\text{plane,SR}}=\frac{\pi k}{\theta^2_{\text{min}}+\theta^2_{\text{sep}}}\ ,$$

$$p^{\text{hard}}_{\text{plane,SR}}(\theta)=\begin{cases}0, & 0\le\theta<\theta_{\text{sep}}\\ \dfrac{\theta^2_{\text{min}}+\theta^2_{\text{sep}}}{\pi(\theta^2+\theta^2_{\text{min}})^2}, & \theta_{\text{sep}}\le\theta<\infty\ .\end{cases}$$

The conditional formulas for $q^{\text{hard}}_{\text{plane,SR}}(\theta,\theta')$ are given in Table IV, where $a=\theta^2+\theta'^2+\theta^2_{\text{min}}$, $b=-2\theta\theta'$, and $\varphi'_1=\arccos[(\theta^2+\theta'^2-\theta^2_{\text{sep}})/2\theta\theta']$.

TABLE IV. Conditional formulas for $q^{\text{hard}}_{\text{plane,SR}}(\theta,\theta')$.

Condition on θ and θ'	$q^{\text{hard}}_{\text{plane,SR}}(\theta,\theta')$
$\theta+\theta' \le \theta_{\text{sep}}$	0
$\lvert\theta-\theta'\rvert \ge \theta_{\text{sep}}$	$\dfrac{2(\theta^2_{\text{min}}+\theta^2_{\text{sep}})(\theta^2+\theta'^2+\theta^2_{\text{min}})}{[(\theta^2+\theta'^2+\theta^2_{\text{min}})^2-4\theta^2\theta'^2]^{3/2}}$
$\lvert\theta-\theta'\rvert < \theta_{\text{sep}}$	$\dfrac{\theta^2_{\text{min}}+\theta^2_{\text{sep}}}{\pi}\left\{\dfrac{2\pi a}{(a^2-b^2)^{3/2}}+\dfrac{2b\sin\varphi'_1}{(a^2-b^2)(a+b\cos\varphi'_1)}-\dfrac{4a}{(a^2-b^2)^{3/2}}\arctan\left[\dfrac{\sqrt{a^2-b^2}\tan(\frac{1}{2}\varphi'_1)}{a+b}\right]\right\}$

For category G,

$$\lambda_{\text{sphere,PWA}}=\frac{N_0\rho}{A}\sigma_{\text{sphere,PWA}}\ ,$$

$$p_{\text{sphere,PWA}}(\theta)=\frac{R}{\sigma_{\text{sphere,PWA}}}\left[\sum_{m=1}^{4}\frac{A_m}{(1-\cos\theta+2B)^m}+\sum_{n=0}^{6}C_nP_n(\cos\theta)\right],$$

$$q_{\text{sphere,PWA}}(\theta,\theta')=\frac{2\pi R}{\sigma_{\text{sphere,PWA}}}\left\{\sum_{m=1}^{4}\frac{A_m}{(a^2-b^2)^{m/2}}P_{m-1}\left[\frac{a}{\sqrt{a^2-b^2}}\right]+\sum_{n=0}^{6}C_nP_n(\cos\theta)P_n(\cos\theta')\right\},$$

$$\sigma_{\text{sphere,PWA}}=2\pi R\left\{A_1\ln\left[\frac{1+B}{B}\right]+\sum_{m=2}^{4}\frac{A_m}{(m-1)2^{m-1}}\left[\frac{1}{B^{m-1}}-\frac{1}{(1+B)^{m-1}}\right]+2C_0\right\};$$

for category H,

$$\lambda^{\text{soft}}_{\text{sphere,PWA}}=\frac{N_0\rho}{A}\sigma^{\text{soft}}_{\text{sphere,PWA}}\ ,$$

$$(\sigma^2)^{\text{soft}}_{\text{sphere,PWA}}=\frac{\pi R^2}{\sigma^{\text{soft}}_{\text{sphere,PWA}}}\int_0^{\theta_{\text{sep}}}\left[\sum_{m=1}^{4}\frac{A_m}{(\frac{1}{2}\theta^2+2B)^m}+\sum_{n=0}^{6}C_nP_n(1-\tfrac{1}{2}\theta^2)\right]\theta^3d\theta\ ,$$

$$\sigma^{\text{soft}}_{\text{sphere,PWA}}=2\pi R\left\{A_1\ln\left[\frac{1+2B-\cos\theta_{\text{sep}}}{2B}\right]+\sum_{m=2}^{4}\frac{A_m}{m-1}\left[\frac{1}{(2B)^{m-1}}-\frac{1}{(1+2B-\cos\theta_{\text{sep}})^{m-1}}\right]\right.$$
$$\left.+C_0(1-\cos\theta_{\text{sep}})-\sin\theta_{\text{sep}}\sum_{n=1}^{6}\frac{C_n}{n(n+1)}P_n^1(\cos\theta_{\text{sep}})\right\};$$

TABLE V. Conditional formulas for $q^{\text{hard}}_{\text{sphere,PWA}}(\theta,\theta')$.

Condition on θ and θ'	$q^{\text{hard}}_{\text{sphere,PWA}}(\theta,\theta')$
$\theta+\theta'<\theta_{\text{sep}}$	0
$\theta=0$ and $\theta_{\text{sep}}\le\theta'\le\pi$	$\frac{2\pi R}{\sigma^{\text{hard}}_{\text{sphere,PWA}}}\left\{\sum_{m=1}^{4}\frac{A_m}{(1-\cos\theta'+2B)^m}+\sum_{n=0}^{6}C_nP_n(\cos\theta')\right\}$
$\theta_{\text{sep}}\le\theta\le\pi$ and $\theta'=0$	$\frac{2\pi R}{\sigma^{\text{hard}}_{\text{sphere,PWA}}}\left\{\sum_{m=1}^{4}\frac{A_m}{(1-\cos\theta+2B)^m}+\sum_{n=0}^{6}C_nP_n(\cos\theta)\right\}$
$\theta,\theta'\neq0$ and $\lvert\theta-\theta'\rvert\ge\theta_{\text{sep}}$	$\frac{2\pi R}{\sigma^{\text{hard}}_{\text{sphere,PWA}}}\left\{\sum_{m=1}^{4}\frac{A_m}{(a^2-b^2)^{m/2}}P_{m-1}\left[\frac{a}{\sqrt{a^2-b^2}}\right]+\sum_{n=0}^{6}C_nP_n(\cos\theta)P_n(\cos\theta')\right.$
$\theta,\theta'\neq0$ and $\lvert\theta-\theta'\rvert<\theta_{\text{sep}}$	$\left.\frac{R}{\sigma^{\text{hard}}_{\text{sphere,PWA}}}\left\{\sum_{m=1}^{4}A_mI_{A_m}+\sum_{n=0}^{6}C_nI_{C_n}\right\}\right.$

where $I_{A_1}=\frac{2}{\sqrt{a^2-b^2}}\left[\pi-2\arctan\left[\frac{\sqrt{a^2-b^2}\tan(\frac{1}{2}\varphi_1')}{a+b}\right]\right]$

$$I_{A_2}=\frac{2b\sin\varphi_1'}{(a^2-b^2)(a+b\cos\varphi_1')}+\frac{a}{a^2-b^2}I_{A_1}$$

$$I_{A_3}=\frac{1}{a^2-b^2}\left\{\frac{b\sin\varphi_1'}{a+b\cos\varphi_1'}\left[\frac{1}{a+b\cos\varphi_1'}+\frac{3a}{a^2-b^2}\right]+\frac{2a^2+b^2}{2(a^2-b^2)}I_{A_1}\right\}$$

$$I_{A_4}=\frac{1}{3(a^2-b^2)}\left\{\frac{b\sin\varphi_1'}{a+b\cos\varphi_1'}\left[\frac{2}{(a+b\cos\varphi_1')^2}+\frac{5a}{(a^2-b^2)(a+b\cos\varphi_1')}+\frac{11a^2+4b^2}{(a^2-b^2)^2}\right]+\frac{6a^3+9ab^2}{2(a^2-b^2)^2}I_{A_1}\right\}$$

$$I_{C_n}=2(\pi-\varphi_1')P_n(\cos\theta)P_n(\cos\theta)-4\sum_{m=0}^{n}\frac{(n-m)!}{(n+m)!}P_n^m(\cos\theta)P_n^m(\cos\theta')\frac{\sin m\varphi_1'}{m}$$

and for category I,

$$\lambda^{\text{hard}}_{\text{sphere,PWA}}=\frac{N_0\rho}{A}2\pi R\left\{A_1\ln\left[\frac{2(1+B)}{1+2B-\cos\theta_{\text{sep}}}\right]+\sum_{m=2}^{4}\frac{A_m}{m-1}\left[\frac{1}{(1+2B-\cos\theta_{\text{sep}})^{m-1}}-\frac{1}{(2+2B)^{m-1}}\right]\right.$$
$$\left.+C_0(1+\cos\theta_{\text{sep}})+\sin\theta_{\text{sep}}\sum_{n=1}^{6}\frac{C_n}{n(n+1)}P_n^1(\cos\theta_{\text{sep}})\right\},$$

$$p^{\text{hard}}_{\text{sphere,PWA}}=\begin{cases}0, & 0\le\theta<\theta_{\text{sep}}\\ \dfrac{\pi R}{\sigma^{\text{hard}}_{\text{sphere,PWA}}}\left[\displaystyle\sum_{m=1}^{4}\frac{A_m}{(1-\cos\theta+2B)^m}+\sum_{n=0}^{6}C_nP_n(\cos\theta)\right], & \theta_{\text{sep}}\le\theta\le\pi.\end{cases}$$

The conditional formulas for $q^{\text{hard}}_{\text{sphere,PWA}}(\theta,\theta')$ are given in Table V, where $a=1+\frac{1}{2}\theta^2_{\min}-\cos\theta\cos\theta'$, $b=-\sin\theta\sin\theta'$ and $\varphi_1'=\arccos[(\cos\theta_{\text{sep}}-\cos\theta\cos\theta')/\sin\theta\sin\theta']$.

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