

Fokker-Planck description of electron and photon transport in homogeneous media

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Starting from a Fokker-Planck description of particle transport, which is valid when the scattering is forwardly peaked and the energy change in scattering is small, we systematically obtain an approximate diffusionlike equation for the particle density by eliminating the direction variable $\hat{\Omega}$ with an elimination scheme based on Zwanzig's projection operator formalism in the interaction representation. The elimination procedure closely follows one described by Grigolini and Marchesoni [in *Memory Function Approaches to Stochastic Problems in Condensed Matter*, edited by Myron W. Evans, Paolo Grigolini, and Guisepe P. Parravicini, *Advances in Physical Chemistry*, Vol. 62 (Wiley-Interscience, New York, 1985), Chap. II, p. 29], but with a different projection operator. The resulting diffusion equation is correct up to the second order in the coupling operator between the particle direction and position variable. The diffusion coefficients and mobility in the resulting diffusion equation depend on the initial distribution of the particles in direction and on the path length traveled by the particles. The full solution is obtained for a monoenergetic and monodirectional pulsed point source of particles in an infinite homogeneous medium. This solution is used to study the penetration and the transverse and longitudinal spread of the particles as they are transported through the medium. Application to diffusive wave spectroscopy in calculating the path-length distribution of photons, as well as application to dose calculations in tissue due to an electron beam are mentioned. [S1063-651X(97)11706-8]

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I. INTRODUCTION

Electron transport in tissue has received increasing attention in recent years because of its importance for determining the dose delivered during the treatment of localized malignancies with well-collimated electron beams. A quantitative knowledge of the spread of the beam before reaching its target tumor, as well as the expected dose delivered by the electrons to both the healthy and malignant tissues, is obviously essential in the planning of an appropriate treatment procedure.

Such dose calculations have been based, until now, on the Fermi-Eyges [1,2] theory of pencil-like electron beams. However, this theory is valid only during the electrons' initial penetration into the tissue, before the beam has undergone appreciable spread transverse to its primary direction of travel. In the Fermi-Eyges theory it is assumed that electrons in the beam lose their energy continuously, suffering a large number of small-angle collisions without changing their initial direction significantly, and the beam, therefore, initially maintains its overall forward direction of travel. But at the later stages of the beam's transport the direction of travel of the electrons becomes randomized, so that their mean velocity approaches zero while their mean position approaches a fixed point. This point defines the penetration distance of the collimated beam from its injection location. During this final stage of transport, the electrons diffuse isotropically about their fixed mean position, and continue losing their kinetic

energy during this random Brownian motion. The Fermi-Eyges theory is, however, not applicable to the description of electron motion in its final diffusive stage, and it is increasingly less applicable during the transition from pencil-beamlike to diffusive behavior. Clearly, a more comprehensive and tractable theory is needed for the more accurate calculation of electron dose rates in tissue.

Some progress has recently been made in this direction by Akcasu and Larsen [3] and by Larsen *et al.* [4] by assuming that the electron flux satisfies a diffusion equation in configuration space with time-dependent transverse and longitudinal diffusion coefficients, and a time-dependent mobility. The diffusion coefficients and the mobility are explicitly obtained [3] by requiring that the proposed diffusion equation exactly reproduce the true first and second spatial moments of the electron distribution function. These moments are calculated starting from the Fokker-Planck description of electron transport in an infinite homogeneous isotropic medium in Ref. [3], and directly from the Boltzmann equation in Ref. [4] by using the so called "transport space-angle moment" method. Numerical comparison with Monte Carlo calculations [4] for electron beams show that the new diffusion equation yields accurate closed-form expressions for depth-doses and radial-dose profiles.

In this paper we first present a systematic derivation of an exact diffusion equation for the scalar electron flux in an homogeneous medium, including the effect of particle absorption. We start from the Fokker-Planck equation for the energy-dependent angular electron flux, and exactly eliminate the effects of absorption and the energy variable for the case of monoenergetic initial data. We next eliminate the direction variable using the Zwanzig [5,6] projection opera-

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tor formalism in the interaction representation, resulting in an exact diffusionlike equation with memory terms. We then show that the diffusion equation form which was assumed in Refs. [3] and [4] actually follows from this exact form by expanding the memory function in the projection operator formalism in powers of the coupling between the angle and position variables. The elimination procedure used in the present derivation is one of the methods often referred to as the ‘‘elimination of fast variables’’ in the literature [7,8]. The particular elimination method employed in this paper is an extension of the elimination method developed in Grigolini and Marchesoni [8].

Photon transport, on the other hand, has become an active field of both theoretical [9] and experimental [10] research over the past decade, especially in connection with diffusive wave spectroscopy. The diffusive character of the light enters in the analysis of the time correlation function of the scattered light, and is crucial in the understanding of the optical experiments designed to study dynamic properties of particles suspended in fluids, such as their diffusion coefficient. The central issue in the theory of diffusive wave spectroscopy is the calculation of the path-length distribution of multiply scattered photons for a given linear displacement from their injection point. The current theoretical modeling [9] of the photon flux in diffusive wave spectroscopy assumes that the beam of light has fully randomized in direction about a fixed penetration depth, so that standard isotropic diffusion theory is applicable; in contrast to the Fermi-Eyges theory which holds during the initial penetration of radiation into the medium, this isotropic diffusion is true only in the final stage of the photon transport process. The modified diffusion equation derived in this paper is applicable to both the initial forward directed photon beam and to the eventual isotropic photon diffusion, and thereby provides the missing connection between these two behaviors.

It should be mentioned at the outset that the Fokker-Planck description of photon transport presented in this paper in terms of a particle transport equation is approximate, and applicable only to the *diffusive* transport of unpolarized photons. It does not take into account the complexities arising from the strong polarization dependence of photon scattering, which would require a transport equation that includes photon polarization as another vector particle property, like direction of motion. However, it describes the gradual transition from the coherent to incoherent (or diffusive) regime more accurately than the usual treatment of wave transport as a superposition of the coherent and diffusive components [9] as demonstrated in this paper.

II. FOKKER-PLANCK DESCRIPTION OF PARTICLE TRANSPORT

We start with the Fokker-Planck description [11,12] of electron transport, which can be obtained from the conventional linear Boltzmann equation by assuming that the scattering is forwardly peaked, and that the energy change in scattering is small [13]. The derivation of the Fokker-Planck equation is conventional and well documented [11–14]; we shall not repeat it here. For the present application, we write the Fokker-Planck equation as

$$\frac{\partial n}{\partial t} = -v \hat{\Omega} \cdot \nabla n - v \Sigma_a n + \frac{\partial}{\partial E} [S v n] - \frac{v \bar{\Sigma}}{2} L^2 n, \quad (1)$$

where $n(\mathbf{x}, E, \hat{\Omega}, t)$ is the position, energy, direction, and time-dependent particle density; $S(E)$ is the energy loss per unit distance, or stopping power; $\Sigma_a(E)$ is the macroscopic absorption cross section; $\bar{\Sigma} = \Sigma_{tr} - \Sigma_a$, where $\Sigma_{tr}(E)$ is the transport cross section; the vector $\hat{\Omega}$ is the unit vector in the direction of particle velocity; $v(E)$ is the particle speed corresponding to the particle energy E ; and L^2 is the angular momentum operator defined by

$$L^2 = - \left[\frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial}{\partial \mu} + \frac{1}{1 - \mu^2} \frac{\partial^2}{\partial \phi^2} \right], \quad (2)$$

where μ is the cosine of the polar angle describing the unit vector $\hat{\Omega}$, and ϕ is the azimuthal angle. The sign of L^2 is chosen such that its eigenfunctions $Y_{lm}(\hat{\Omega})$, i.e., the spherical harmonics, satisfy $L^2 Y_{lm} = l(l+1) Y_{lm}$. The definitions of stopping power, $S(E)$, and penetration cross section, $\bar{\Sigma}(E)$, in terms of the differential cross section Σ_s are

$$S(E) = \int_0^\infty dE' \int_{4\pi} d\hat{\Omega}' (E - E') \Sigma_s(E \rightarrow E', \hat{\Omega}' \cdot \hat{\Omega}) \quad (3)$$

$$\bar{\Sigma}(E) = 2\pi \int_0^\infty dE' \int_{-1}^1 (1 - \mu) \Sigma_s(E \rightarrow E', \mu) \quad (4)$$

III. ELIMINATION OF ABSORPTION AND ENERGY

The energy dependence and absorption effects can be completely eliminated from Eq. (1) in the case of a monoenergetic initial distribution at energy E_0 . To do so, let us first define the nonabsorption probability

$$p(E) = \exp \left[- \int_E^{E_0} \frac{\Sigma_a(E')}{S(E')} dE' \right] \quad (5)$$

and use it to rewrite Eq.(1) as

$$\frac{\partial n}{\partial t} = -v \hat{\Omega} \cdot \nabla n + p \frac{\partial}{\partial E} \left[\frac{S n v}{p} \right] - \frac{v \bar{\Sigma}}{2} L^2 n. \quad (6)$$

Now write

$$n(\mathbf{x}, E, \hat{\Omega}, t) = \delta[E - \mathcal{E}(s(t))] p(E) f(\mathbf{x}, \hat{\Omega}, s(t)), \quad (7)$$

where f will be a function to be determined, and $\mathcal{E}(s)$ is the energy of a particle that has traveled a path length s , which is given by

$$\frac{d\mathcal{E}}{ds} = -S(\mathcal{E}) \quad (8)$$

along with the initial condition $\mathcal{E}(0) = E_0$. Also note that we can write $s(t)$ as the path length traveled in time t by a particle starting at energy E_0 , and that $ds/dt = v(\mathcal{E}(s))$. Now, substituting the form of n from Eq. (7) into Eq. (6) and noting that

$$\begin{aligned} \frac{\partial}{\partial E} [\delta(E - \mathcal{E}(s))v(E)S(E)f] \\ = \delta'(E - \mathcal{E}(s))v(\mathcal{E}(s))S(\mathcal{E}(s))f, \end{aligned} \quad (9)$$

yields the required equation for f

$$\frac{\partial f}{\partial s} = -\hat{\Omega} \cdot \nabla f - \frac{\bar{\Sigma}(\mathcal{E}(s))}{2} L^2 f. \quad (10)$$

Equation (10) is also of Fokker-Planck form but for the reduced function $f(\mathbf{x}, \hat{\Omega}, s)$; it is easier to handle than the Fokker-Planck equation for the full direction-dependant density $n(\mathbf{x}, E, \hat{\Omega}, t)$. It can be interpreted as the one-speed Fokker-Planck equation for the angular particle density in the absence of absorption, and its solution provides us with the solution of Eq. (1) for the case of monoenergetic initial data

$$n(\mathbf{x}, E, \hat{\Omega}, 0) = \delta(E - E_0)f(\mathbf{x}, \hat{\Omega}, 0). \quad (11)$$

Frequently we are not interested in the direction information, but are instead satisfied by a knowledge of the direction-independent density

$$N(\mathbf{x}, E, t) = \int_{4\pi} n(\mathbf{x}, E, \hat{\Omega}, t) d\hat{\Omega}.$$

We will therefore seek an equation for the energy-independent and direction-independent particle density defined by

$$F(\mathbf{x}, s) = \int_{4\pi} f(\mathbf{x}, \hat{\Omega}, s) d\hat{\Omega}, \quad (12)$$

since from this we can compute

$$N(\mathbf{x}, E, t) = \delta[E - \mathcal{E}(s(t))]p(E)F(\mathbf{x}, s(t)). \quad (13)$$

IV. EXACT ELIMINATION OF THE ANGULAR VARIABLE

The objective of this section is to obtain an exact equation for the scalar density $F(\mathbf{x}, s)$ by eliminating the angular dependence in the effective one-speed density $f(\mathbf{x}, \hat{\Omega}, s)$ which satisfies Eq. (10). We do so through an extension of the Zwanzig projection operator method [8]. The extension that we require for our application to Eq. (10) is described in Sec. IV A, and applied in Sec. IV B.

A. Elimination of irrelevant variables

In the mathematical description of many physical systems there is often an interplay of mechanisms involving vastly different relaxation times. By eliminating the irrelevant variables, which are usually responsible for fast variations on a scale of no interest, we can sometimes obtain a tractable approximate description of the slow scale evolution of the system. Numerous elimination methods have been developed for a variety of applications, and many of these were reviewed by van Kampen [7]. One of these methods involves Zwanzig's projection operator technique [5,6] in the interac-

tion representation, and was explained in detail by Grigolini and Marchesoni [8], who also provided several illustrative examples and physical applications. We shall modify this method for application to the problem at hand.

We abstract the problem as follows: assume that the system evolution is described by an equation of the form

$$\frac{df}{ds} = L_a f + L_b(s)f + L_c(s)f, \quad (14)$$

where the operators L_a and $L_b(s)$ act on different sets of independent variables \mathbf{a} and \mathbf{b} , which we shall call the relevant and irrelevant variables, respectively; because they act on different independent variables the operators L_a and $L_b(s)$ commute. We also allow L_b to depend explicitly on "time" s . The operator $L_c(s)$ need not commute with either L_a or $L_b(s)$, and will be called the coupling operator. From Eq. (14) we wish to obtain an equation for the reduced distribution $F(\mathbf{a}, s) = \int f(\mathbf{a}, \mathbf{b}, s) d\mathbf{b}$.

The allowed time dependance of L_b is a slight deviation from Grigolini and Marchesoni's derivation, and is needed in our application to the Fokker-Planck equation. The time dependance of L_c is also an extension of Grigolini and Marchesoni, but is not required for our application; we include it only because it requires no additional work to do so. Note that in the expressions below we shall avoid noting the functional dependance of various quantities on the independent variables, especially \mathbf{a} and \mathbf{b} , except when it seems explicitly useful to do so.

To introduce the interaction representation let $U(s)$ be the solution of

$$\frac{d}{ds} U(s) = [L_a + L_b(s)]U(s), \quad (15)$$

with the initial condition $U(0) = I$ where I is the identity operator. Because L_a and $L_b(s)$ commute, the operator $U(s)$ can be factored as $U(s) = U_a(s)U_b(s) = U_b(s)U_a(s)$, where U_a and U_b describe the decoupled evolution of the \mathbf{a} and \mathbf{b} variables; specifically

$$\frac{dU_a}{ds} = L_a U_a, \quad (16)$$

with $U_a(0) = I$, and

$$\frac{dU_b}{ds} = L_b(s)U_b, \quad (17)$$

again with identity initial data. In the interaction representation we then write $f(s) = U(s)\tilde{f}(s)$, and substituting this into Eq. (14) discover that \tilde{f} must satisfy the equation

$$\frac{d}{ds} \tilde{f}(s) = \mathcal{L}(s)\tilde{f}(s), \quad (18)$$

with

$$\mathcal{L}(s) = U(s)^{-1}L_c(s)U(s), \quad (19)$$

where $U(s)^{-1}$ denotes the inverse of $U(s)$.

Because our interest in the system will be satisfied by a knowledge of the reduced distribution $F(s)$, we shall introduce a projection of the distribution $Pf(s)$ that is easily related to $F(s)$. In particular, the projection acts on any function of \mathbf{a} and \mathbf{b} according to

$$Ph(\mathbf{a}, \mathbf{b}) = g(\mathbf{b}) \int h(\mathbf{a}, \mathbf{b}) d\mathbf{b}, \quad (20)$$

where g is a function of \mathbf{b} only and satisfies $\int g(\mathbf{b}) d\mathbf{b} = 1$, so that $P^2 = P$ is satisfied. The choice of the function g shall be dictated by the initial condition on f , as described below. This projection has the property that $PL_{\mathbf{a}} = L_{\mathbf{a}}P$, and we shall assume also that $PL_{\mathbf{b}}(s) = 0$, which is the case for our application.

Let $Q = I - P$ be the complement of the projection P , and let us represent the solution of Eq. (18) as $\tilde{f} = P\tilde{f} + Q\tilde{f}$. Equation (18) can then be written as the pair of coupled equations

$$\frac{dP\tilde{f}}{ds} = P\mathcal{L}(s)P\tilde{f} + P\mathcal{L}(s)Q\tilde{f}, \quad (21)$$

$$\frac{dQ\tilde{f}}{ds} = Q\mathcal{L}(s)P\tilde{f} + Q\mathcal{L}(s)Q\tilde{f}. \quad (22)$$

At this stage we require that the initial distribution function $f(0)$ satisfies $Pf(0) = f(0)$; this implies that

$$f(\mathbf{a}, \mathbf{b}, 0) = g(\mathbf{b}) \int f(\mathbf{a}, \mathbf{b}, 0) d\mathbf{b} = g(\mathbf{b})F(\mathbf{a}, 0).$$

We are thus assuming that the initial data $f(0)$ is separable in \mathbf{a} and \mathbf{b} , and that the function g appearing in the projection operator is the normalized initial distribution of the \mathbf{b} variables. In contrast Grigolini and Marchesoni make the choice $g = g^{\text{eq}}$ where $L_{\mathbf{b}}g^{\text{eq}} = 0$; this they could do because their operator $L_{\mathbf{b}}$ did not depend on time. Our projection integrates out the \mathbf{b} dependence and replaces it with that of the initial distribution, rather than the decoupled equilibrium distribution of \mathbf{b} variables.

With our choice of g it then follows that $P\tilde{f}(0) = f(0)$, and we thus have $Q\tilde{f}(0) = 0$. We therefore solve Eq. (22) for $Q\tilde{f}(s)$ with zero initial data, yielding

$$Q\tilde{f} = \int_0^s U(s, s') Q\mathcal{L}(s') P\tilde{f}(s') ds', \quad (23)$$

where $U(s, s')$ is the operator satisfying

$$\frac{d}{ds} U(s, s') = Q\mathcal{L}(s)U(s, s'), \quad (24)$$

with data $U(s', s') = I$. Using this expression $Q\tilde{f}$ in Eq. (21) yields an equation for the function $P\tilde{f}$

$$\frac{dP\tilde{f}}{ds} = P\mathcal{L}(s)P\tilde{f} + \int_0^s P\mathcal{L}(s)U(s, s') Q\mathcal{L}(s') P\tilde{f}(s') ds'. \quad (25)$$

The value of this equation lies in our ability to convert it into an equation for Pf , rather than for $P\tilde{f}$. This is possible when $PL_{\mathbf{b}}(s) = 0$, and P and $L_{\mathbf{a}}$ commute, as we required above, for in this case P commutes with $U_{\mathbf{a}}$ and $dPU_{\mathbf{b}}/ds = 0$ by Eq. (17). This latter implies that $PU_{\mathbf{b}}(s) = PU_{\mathbf{b}}(0) = P$, and therefore $PU_{\mathbf{a}}U_{\mathbf{b}} = U_{\mathbf{a}}P$. Hence $Pf = PU\tilde{f} = U_{\mathbf{a}}P\tilde{f}$, and we can thus uniquely relate \tilde{f} to Pf .

If we differentiate $Pf = U_{\mathbf{a}}P\tilde{f}$ with respect to time s , and use the definition of $U_{\mathbf{a}}$ we discover that

$$\begin{aligned} \frac{dPf}{ds} &= L_{\mathbf{a}}U_{\mathbf{a}}(s)P\tilde{f} + U_{\mathbf{a}}(s)P\mathcal{L}(s)P\tilde{f} \\ &+ \int_0^s U_{\mathbf{a}}(s)P\mathcal{L}(s)U(s, s')Q\mathcal{L}(s')P\tilde{f}(s') ds'. \end{aligned} \quad (26)$$

Now use $Pf = U_{\mathbf{a}}P\tilde{f}$, the definition of $\mathcal{L}(s)$ from Eq. (19), the relation $PU^{-1}(s) = U_{\mathbf{a}}^{-1}P$ and the fact that $UU_{\mathbf{a}}^{-1} = U_{\mathbf{b}}$ so that this equation can be rewritten as an equation for Pf

$$\begin{aligned} \frac{dPf}{ds} &= L_{\mathbf{a}}Pf + PL_c(s)U_{\mathbf{b}}Pf + \int_0^s PL_c(s)U(s, s') \\ &\times QU^{-1}(s')L_c(s')U_{\mathbf{b}}(s')Pf(s') ds'. \end{aligned} \quad (27)$$

Thus we have now arrived at an exact equation for the evolution of the projection of the distribution onto the relevant variables. This equation may be, indeed will be, useful because we can make approximations to the memory term to arrive at a simplified model of the interaction between the variables \mathbf{a} and \mathbf{b} .

We can now use Eq. (27) to derive an exact equation for the evolution of the reduced distribution function F . In order to organize the resulting equation we define

$$g(s) = U_{\mathbf{b}}(s)g, \quad (28)$$

which is the evolution of the \mathbf{b} dependant part of the initial distribution when it is uncoupled to the \mathbf{a} variables. We also introduce $Q(s) = U(s)QU^{-1}(s)$ as the time-dependent complementary projection, which has the explicit representation

$$Q(s) = I - g(s) \int d\mathbf{b}. \quad (29)$$

Also let $Z(s, s') = U(s)U(s, s')U^{-1}(s')$ be the operator that satisfies

$$\frac{d}{ds} Z(s, s') = [L_{\mathbf{a}} + L_{\mathbf{b}}(s) + Q(s)L_c(s)]Z(s, s'), \quad (30)$$

with $Z(s', s') = I$. Using $g(s)$ and $Q(s)$ in Eq. (27) and noting that $Pf(s) = g(0)F(s)$ then yields

$$\frac{dF}{ds} = L_{\mathbf{a}}F + \bar{L}_c(s)F + \int_0^s M(s, s')F(s') ds', \quad (31)$$

where the operators \bar{L}_c and M are defined by

$$\bar{L}_c(s)F(s) = \int L_c(s)(g(s)F(s))d\mathbf{b} \quad (32)$$

and

$$M(s,s')F(s') = \int L_c(s)Z(s,s') \times Q(s')L_c(s')(g(s')F(s'))d\mathbf{b}. \quad (33)$$

Note that $\bar{L}_c(s)$ is the average of $L_c(s)$ against the distribution $g(s)$. Equation (31) is an exact equation for the evolution of the reduced distribution function; it is the main result of the elimination method based on the projection operator formalism in the interaction representation. It reduces to the form given by Grigolini and Marchesoni when $L_b(s)$ and $L_c(s)$ are independent of time, and g is chosen as the equilibrium distribution g^{eq} .

B. Application to the Fokker-Planck equation

The general elimination procedure described in the preceding subsection can now be applied to the reduced Fokker-Planck equation, Eq. (10), in order to develop a diffusion equation for the position dependent number density $F(\mathbf{x},s)$. To do so, we identify \mathbf{b} of the preceding section with the directional variable $\hat{\mathbf{\Omega}}$, and \mathbf{a} with the position variable \mathbf{x} . By comparing Eqs. (14) and (10), we see that in our problem

$$L_a = 0, \quad (34)$$

$$L_b(s) = -\frac{\bar{\Sigma}(\mathcal{E}(s))}{2} L^2 \quad (35)$$

and identify the coupling operator as

$$L_c = -\hat{\mathbf{\Omega}} \cdot \nabla. \quad (36)$$

We consider separable initial data $f(\mathbf{x},\hat{\mathbf{\Omega}},0) = g(\hat{\mathbf{\Omega}},0)F(\mathbf{x},0)$ with $1 = \int_{4\pi} g(\hat{\mathbf{\Omega}},0)d\hat{\mathbf{\Omega}}$, and compute the evolution of $g(\hat{\mathbf{\Omega}},0)$ from

$$\frac{\partial g}{\partial s} = -\frac{\bar{\Sigma}(\mathcal{E}(s))}{2} L^2 g.$$

This yields

$$g(\hat{\mathbf{\Omega}},s) = \exp\left[-\frac{\theta(s)}{2} L^2\right] g(\hat{\mathbf{\Omega}},0), \quad (37)$$

where

$$\theta(s) = \int_0^s \bar{\Sigma}(\mathcal{E}(s')) ds' \quad (38)$$

is the distance in penetration lengths $l(E) = 1/\bar{\Sigma}(E)$ that the particle has traveled. Note that $g(\hat{\mathbf{\Omega}},s)$ can be expanded in to spherical harmonics, if desired; this is not needed in the following derivations. From the expression for $g(\hat{\mathbf{\Omega}},s)$ we easily compute the second term on the right-hand side of Eq. (31) as

$$\bar{L}_c(s) = \bar{\mathbf{\Omega}}(s) \cdot \nabla \quad (39)$$

where

$$\bar{\mathbf{\Omega}}(s) = \int \hat{\mathbf{\Omega}} g(\hat{\mathbf{\Omega}},s) d\hat{\mathbf{\Omega}} = e^{-\theta(s)} \bar{\mathbf{\Omega}}(0) \quad (40)$$

is the mean of the direction after the particle has traveled a path length s . Note that this mean of the direction is zero if the initial distribution, $g(\hat{\mathbf{\Omega}},0)$, is isotropic, and in all cases decays to zero as the particles travel farther and farther through the medium, reflecting the increasing isotropy of the particle distribution in the absence of coupling to the spatial variable. To obtain Eq. (40) we have exploited that fact the L^2 is self-adjoint, and $L^2 \hat{\mathbf{\Omega}} = 2\hat{\mathbf{\Omega}}$; this latter fact follows from the fact that the spherical components of $\hat{\mathbf{\Omega}}$ are proportional to Y_{1m} .

The final task is to compute the memory term, the third term of Eq. (31). However, in order to do so, we must compute the operator $Z(s,s')$ satisfying Eq. (30), which is still a difficult problem. We write this operator as $Z(s,s') = Z^0(s,s') + Z^c(s,s')$, where $Z^0(s,s')$ satisfies

$$\frac{d}{ds} Z^0(s,s') = -\frac{\bar{\Sigma}(\mathcal{E}(s))}{2} L^2 Z^0(s,s'), \quad (41)$$

with $Z^0(s',s') = I$, and

$$\begin{aligned} \frac{d}{ds} Z^c(s,s') &= -\frac{\bar{\Sigma}(\mathcal{E}(s))}{2} L^2 Z^c(s,s') - Q(s) \hat{\mathbf{\Omega}} \cdot \nabla Z^c(s,s') \\ &\quad - Q(s) \hat{\mathbf{\Omega}} \cdot \nabla Z^0(s,s'), \end{aligned} \quad (42)$$

with $Z^c(s',s') = 0$. We can then at least solve for

$$Z^0(s,s') = e^{-1/2[\theta(s) - \theta(s')]L^2}, \quad (43)$$

even though finding $Z^c(s,s')$ remains difficult. However, it is clear from the zero initial condition on $Z^c(s,s')$ and Eq. (42) that $Z^c(s,s')$ will be first order in the coupling operator, $L_c = -\hat{\mathbf{\Omega}} \cdot \nabla$.

We now use the decomposition $Z(s,s') = Z^0(s,s') + Z^c(s,s')$ to induce a similar decomposition of $M(s,s') = M^2(s,s') + M^c(s,s')$. Here $M^2(s,s')$ is defined by

$$\begin{aligned} M^2(s,s')F(s') &= \int_{4\pi} \hat{\mathbf{\Omega}}_j \frac{\partial}{\partial x_j} Z^0(s,s') \\ &\quad \times Q(s') \hat{\mathbf{\Omega}}_i \frac{\partial}{\partial x_i} g(\hat{\mathbf{\Omega}},s') F(\mathbf{x},s') d\hat{\mathbf{\Omega}}, \end{aligned} \quad (44)$$

where the superscript denotes the order of the operator in powers of the coupling operator, and $M^c(s,s')$ is defined by

$$\begin{aligned}
M^c(s, s')F(s') &= \int_{4\pi} \hat{\Omega}_j \frac{\partial}{\partial x_j} Z^c(s, s') \\
&\quad \times Q(s') \hat{\Omega}_i \frac{\partial}{\partial x_i} g(\hat{\Omega}, s') F(\mathbf{x}, s') d\hat{\Omega}, \tag{45}
\end{aligned}$$

where $\hat{\Omega}_i$ denotes the i th component of $\hat{\Omega}$, and where the summation convention is in effect. Because $Z^0(s, s')$ does not act on the spatial variable \mathbf{x} and because $g(\hat{\Omega}, s')$ is independent of \mathbf{x} , we can rewrite $M^2(s, s')F(s')$ as

$$\begin{aligned}
M^2(s, s')F(s') &= \left[\int_{4\pi} \hat{\Omega}_j Z^0(s, s') \right. \\
&\quad \left. \times Q(s') \hat{\Omega}_i g(\hat{\Omega}, s') d\hat{\Omega} \right] \frac{\partial^2}{\partial x_i \partial x_j} F(\mathbf{x}, s'). \tag{46}
\end{aligned}$$

This quantity, once integrated over s in Eq. (31), will, therefore, generate a diffusion term under the history integral.

Now let

$$\mathcal{D}_{ji}(s, s') = \int_{4\pi} \hat{\Omega}_j Z^0(s, s') Q(s') \hat{\Omega}_i g(\hat{\Omega}, s') d\hat{\Omega}. \tag{47}$$

We shall evaluate these quantities in stages, starting with

$$Q(s') \hat{\Omega}_i g(\hat{\Omega}, s') = (\hat{\Omega}_i - \bar{\Omega}_i(s')) g(\hat{\Omega}, s'). \tag{48}$$

where we have used Eq. (29) for $Q(s')$. We now apply $Z^0(s, s')$ to this and use Eq. (37) to thereby compute

$$\begin{aligned}
Z^0(s, s') Q(s') \hat{\Omega}_i g(\hat{\Omega}, s') &= [Z^0(s, s') \hat{\Omega}_i g(\hat{\Omega}, s') \\
&\quad - \bar{\Omega}_i(s') g(\hat{\Omega}, s)], \tag{49}
\end{aligned}$$

where we have used $Z^0(s, s') g(\hat{\Omega}, s') = g(\hat{\Omega}, s)$ [from Eqs. (37) and (43)]. Thus

$$\begin{aligned}
\mathcal{D}_{ji}(s, s') &= \int_{4\pi} [\hat{\Omega}_j Z^0(s, s') \hat{\Omega}_i g(\hat{\Omega}, s') \\
&\quad - \bar{\Omega}_i(s') \hat{\Omega}_j g(\hat{\Omega}, s)] d\hat{\Omega}. \tag{50}
\end{aligned}$$

The integral over particle directions consists of two terms, the second of which is immediately seen to be the product of the mean particle directions at the path lengths s and s'

$$\begin{aligned}
\int_{4\pi} \bar{\Omega}_i(s') \hat{\Omega}_j g(\hat{\Omega}, s) d\hat{\Omega} &= \bar{\Omega}_i(s') \bar{\Omega}_j(s) \\
&= \bar{\Omega}_i(0) \bar{\Omega}_j(0) e^{-\theta(s) - \theta(s')}. \tag{51}
\end{aligned}$$

On the other hand, the first term is

$$\begin{aligned}
&\int \hat{\Omega}_j Z^0(s, s') \hat{\Omega}_i g(\hat{\Omega}, s') \\
&= \int_{4\pi} \hat{\Omega}_j e^{-1/2[\theta(s) - \theta(s')] L^2} \hat{\Omega}_i g(\hat{\Omega}, s') \\
&= \int_{4\pi} \hat{\Omega}_i g(\hat{\Omega}, s') e^{-1/2[\theta(s) - \theta(s')] L^2} \hat{\Omega}_j \\
&= \int_{4\pi} \hat{\Omega}_i g(\hat{\Omega}, s') e^{-[\theta(s) - \theta(s')] L^2} \hat{\Omega}_j \\
&= e^{-[\theta(s) - \theta(s')] L^2} \int_{4\pi} \hat{\Omega}_i \hat{\Omega}_j g(\hat{\Omega}, s'), \tag{52}
\end{aligned}$$

where the facts that L^2 is self-adjoint and $L^2 \hat{\Omega} = 2\hat{\Omega}$ have once again been used. We write this as

$$\int_{4\pi} \hat{\Omega}_j Z^0(s, s') \hat{\Omega}_i g(\hat{\Omega}, s') d\hat{\Omega} = e^{-[\theta(s) - \theta(s')] L^2} \Phi_{ij}(s'), \tag{53}$$

where

$$\Phi_{ij}(s') = \int_{4\pi} \hat{\Omega}_j \hat{\Omega}_i g(\hat{\Omega}, s') d\hat{\Omega}, \tag{54}$$

and we see that it describes the decay of the correlation between the particle directions at time s' and the later time s . In terms of these quantities we now have

$$\mathcal{D}_{ji}(s, s') = e^{-[\theta(s) - \theta(s')] L^2} \Phi_{ij}(s') - \bar{\Omega}_i(0) \bar{\Omega}_j(0) e^{-\theta(s) - \theta(s')}. \tag{55}$$

In order to evaluate the matrix Φ in general we first express the Cartesian components of $\hat{\Omega}$ in polar coordinates, with μ the cosine of the polar angle and ϕ the azimuthal angle. Differentiating the zz component of Eq. (54) yields

$$\frac{d\Phi_{zz}}{ds} = -\frac{1}{2} \bar{\Sigma}(\mathcal{E}(s)) \int_{4\pi} g(\hat{\Omega}, s) L^2 \mu^2 d\hat{\Omega}, \tag{56}$$

and evaluating the action of L^2 on μ^2 then yields

$$\begin{aligned}
\frac{d\Phi_{zz}}{ds} &= \bar{\Sigma}(\mathcal{E}(s)) \int_{4\pi} g(\hat{\Omega}, s) (1 - 3\mu^2) d\hat{\Omega} \\
&= \bar{\Sigma}(\mathcal{E}(s)) (1 - 3\Phi_{zz}). \tag{57}
\end{aligned}$$

Solving this gives us

$$\Phi_{zz}(s) = \frac{1}{3} + e^{-3\theta(s)} [\Phi_{zz}(0) - \frac{1}{3}], \tag{58}$$

which clearly decays to the isotropic value $1/3$ as $s \rightarrow \infty$.

A similar calculation will show that

$$\begin{aligned}
&\int_{4\pi} g(\hat{\Omega}, s) (1 - \mu^2) \cos(2\phi) d\hat{\Omega} \\
&= e^{-3\theta(s)} \int_{4\pi} g(\hat{\Omega}, 0) (1 - \mu^2) \cos(2\phi) d\hat{\Omega}, \tag{59}
\end{aligned}$$

which is a useful result because differentiating the yy component of Eq. (54) yields

$$\begin{aligned} \frac{d\Phi_{yy}}{ds} &= \frac{\bar{\Sigma}(\mathcal{E}(s))}{2} \int_{4\pi} g(\hat{\mathbf{\Omega}}, s) (-1 + 3\mu^2) d\hat{\mathbf{\Omega}} \\ &+ \frac{3\bar{\Sigma}(\mathcal{E}(s))}{2} \int_{4\pi} g(\hat{\mathbf{\Omega}}, s) (1 - \mu^2) \cos(2\phi) d\hat{\mathbf{\Omega}}. \end{aligned} \quad (60)$$

It is easy to confirm that $\int g(\hat{\mathbf{\Omega}}, s) d\hat{\mathbf{\Omega}} = 1$ (because it was so at $s=0$), and so

$$\frac{d\Phi_{yy}}{ds} = \frac{\bar{\Sigma}(\mathcal{E}(s))}{2} (-1 + 3\Phi_{zz}) + \frac{3\bar{\Sigma}(\mathcal{E}(s))}{2} \psi(0) e^{-3\theta(s)}, \quad (61)$$

where

$$\psi(0) = \int_{4\pi} g(\hat{\mathbf{\Omega}}, 0) (1 - \mu^2) \cos(2\phi) d\hat{\mathbf{\Omega}} \quad (62)$$

is a measure of the azimuthal asymmetry of the initial angular distribution. Thus,

$$\Phi_{yy}(s) = \Phi_{yy}(0) + \frac{1}{6} (1 - e^{-3\theta(s)}) [3\Phi_{zz}(0) - 1 + 3\psi(0)], \quad (63)$$

which does not necessarily approach $1/3$ as $s \rightarrow \infty$, although if the initial distribution $g(\hat{\mathbf{\Omega}}, 0)$ is isotropic then $\Phi_{yy} = 1/3$ for all s , as it should be.

Similarly we can find that

$$\frac{d\Phi_{xx}}{ds} = \frac{\bar{\Sigma}(\mathcal{E}(s))}{2} (-1 + 3\Phi_{zz}) - \frac{3\bar{\Sigma}(\mathcal{E}(s))}{2} \psi(0) e^{-3\theta(s)} \quad (64)$$

and discover

$$\Phi_{xx}(s) = \Phi_{xx}(0) + \frac{1}{6} (1 - e^{-3\theta(s)}) [3\Phi_{zz}(0) - 1 - 3\psi(0)]; \quad (65)$$

this element also can decay to a value different from $\frac{1}{3}$. More calculations like those above will yield the cross terms

$$\Phi_{xy}(s) = e^{-3\theta(s)} \phi_{xy}(0), \quad (66)$$

$$\Phi_{xz}(s) = e^{-3\theta(s)} \phi_{xz}(0), \quad (67)$$

$$\Phi_{yz}(s) = e^{-3\theta(s)} \phi_{yz}(0), \quad (68)$$

all of which decay to zero as $s \rightarrow \infty$.

Since the medium is isotropic the only preferred directions are those suggested by the initial distribution; when this is azimuthally symmetric about $\hat{\mathbf{\Omega}}(0)$ the matrix $\Phi(s)$ is diagonal in the coordinate frame in which $\hat{\mathbf{\Omega}}(0)$ defines the z direction

$$\Phi(s) = \begin{bmatrix} \Phi_{\perp}(s) & 0 & 0 \\ 0 & \Phi_{\perp}(s) & 0 \\ 0 & 0 & \Phi_{\parallel}(s) \end{bmatrix}, \quad (69)$$

where

$$\begin{aligned} \Phi_{\perp}(s) &= \int_{4\pi} \hat{\Omega}_x \hat{\Omega}_x g(\hat{\mathbf{\Omega}}, s) d\hat{\mathbf{\Omega}} = \Phi_{xx}(0) + \frac{1}{6} (1 - e^{-3\theta(s)}) \\ &\times [3\Phi_{zz}(0) - 1] \end{aligned} \quad (70)$$

and

$$\Phi_{\parallel}(s) = \int_{4\pi} \hat{\Omega}_z \hat{\Omega}_z g(\hat{\mathbf{\Omega}}, s) d\hat{\mathbf{\Omega}} = \frac{1}{3} + e^{-3\theta(s)} [\Phi_{\parallel}(0) - \frac{1}{3}]. \quad (71)$$

On the other hand, when the initial distribution is isotropic $g(\hat{\mathbf{\Omega}}, s) = 1/4\pi$ for all s and there is no preferred direction; in this case the Φ matrix is diagonal with elements $\frac{1}{3}$ on the diagonal in any coordinate frame. Thus for azimuthally symmetric initial data we can always work in a frame where Φ is diagonal, and we shall do so when convenient.

The final result then is an exact delay-diffusion equation for the evolution of the direction independent density $F(\mathbf{x}, s)$

$$\begin{aligned} \frac{\partial F}{\partial s} &= -\bar{\Omega}(s) \cdot \nabla F + \int_0^s \mathcal{D}_{ij}(s, s') \frac{\partial^2}{\partial x_i \partial x_j} F(\mathbf{x}, s') ds' \\ &+ \int_0^s M^c(s, s') F(s', \mathbf{x}) ds', \end{aligned} \quad (72)$$

where only the operator $M^c(s, s')$ is unknown. While this equation is exact, it is not in closed form because we cannot evaluate the operator Z^c that appears in M^c . However, because Z^c is first order in L_c , this equation is in a form suitable for expansion in powers of the coupling operator. We shall take up this approximation in Sec. V.

V. APPROXIMATE CLOSED-FORM ELIMINATION OF THE ANGULAR VARIABLE

In order to develop a tractable, closed-form diffusionlike equation for the description of the penetration of particles through the medium we note that Eq. (72) implies that $\partial F / \partial s$ is first order in the coupling operator. Thus we can write

$$F(\mathbf{x}, s') = F(\mathbf{x}, s) + O(L_c)(s - s'). \quad (73)$$

But the first history term of Eq. (72) is already of second order in L_c , while the third term, which contains Z^c , is of third order. Therefore, we can write

$$\frac{\partial F}{\partial s} = -\bar{\Omega}(s) \cdot \nabla F + \int_0^s \mathcal{D}_{ij}(s, s') ds' \frac{\partial^2}{\partial x_i \partial x_j} F(\mathbf{x}, s) \quad (74)$$

correct through terms of second order in the coupling operator. Writing this in a coordinate frame with $\hat{\mathbf{\Omega}}(0)$ along the z axis, and assuming azimuthally symmetric initial data for simplicity, we have

$$\frac{\partial F}{\partial s} = -m(s) \frac{\partial F}{\partial z} + D_{\parallel}(s) \frac{\partial^2 F}{\partial z^2} + D_{\perp}(s) \left[\frac{\partial^2 F}{\partial x^2} + \frac{\partial^2 F}{\partial y^2} \right], \quad (75)$$

where

$$m(s) = \|\bar{\mathbf{\Omega}}(0)\| e^{-\theta(s)} \quad (76)$$

is a time-dependent mobility, and

$$D_{\parallel}(s) = \frac{e^{-\theta(s)}}{3} \int_0^s [e^{\theta(s')} + e^{-2\theta(s')} [3\Phi_{\parallel}(0) - 1] - 3\|\bar{\mathbf{\Omega}}(0)\|^2 e^{-\theta(s')}] ds' \quad (77)$$

and

$$D_{\perp}(s) = \frac{e^{-\theta(s)}}{3} \int_0^s [3\Phi_{\perp}(0) e^{\theta(s')} + \frac{1}{2} [e^{\theta(s')} - e^{-2\theta(s')}] \times [3\Phi_{\parallel}(0) - 1]] ds'. \quad (78)$$

Equation (75) was first presented by Akcasu and Larsen as a phenomenological diffusion equation that exactly reproduces the first two spatial moments $\langle \mathbf{x}(s) \rangle$ and $\langle \mathbf{x}(s) \mathbf{x}(s)^T \rangle$ in an infinite homogeneous medium, although they assumed that $g(\hat{\mathbf{\Omega}}, 0) = \delta(\hat{\mathbf{\Omega}} - \hat{\mathbf{\Omega}}_0)$, so that $\Phi_{\parallel}(0) = 1$, $\|\bar{\mathbf{\Omega}}(0)\| = 1$, $\Phi_{\perp}(0) = 0$. The systematic derivation of Eq. (75) as the first two terms in an expansion in powers of the coupling operator is considered to be the main contribution of this paper. The formalism of course allows us to calculate the next term in this expansion, although we do not attempt to do so here.

VI. SPECIAL CASES AND LIMITING BEHAVIORS

In order to illustrate the physical implications of the above results quantitatively, we assume that the transport cross section for electrons is independent of the incident energy, but still allows energy transfer to the scatterer. In this special case $\theta(s) = \bar{\Sigma}s$. This simple model, however, is more realistic in the case of photon transport because photon scattering (under the circumstances typical of diffusive wave experiments) is quasielastic, and the energy loss on scattering, expressed as a change in the frequency of the incident photon, is neglected [9,10]. This means that the energy loss per unit length $S(E)$ is zero in the above general formulation, and that photons maintain their initial energy E_0 . Although the photon scattering cross section is strongly energy dependent, it is always evaluated at the initial energy E_0 , so that $\bar{\Sigma}(\mathcal{E}(s')) = \bar{\Sigma}(E_0)$, and $\theta(s) = \bar{\Sigma}(E_0)s$, as in the case of electrons. In this special case, and also assuming an initial δ distribution in direction along the z axis, the diffusion coefficients reduce to

$$D_{\parallel}(s) = \frac{1}{3\bar{\Sigma}} \left[1 - 3e^{-\bar{\Sigma}s} + 3e^{-2\bar{\Sigma}s} - e^{-3\bar{\Sigma}s} = \frac{(e^{\bar{\Sigma}s} - 1)^3}{3e^{3\bar{\Sigma}s}\bar{\Sigma}} \right], \quad (79)$$

$$D_{\perp}(s) = \frac{1}{3\bar{\Sigma}} \left[1 - \frac{3}{2} e^{-\bar{\Sigma}s} + \frac{1}{2} e^{-3\bar{\Sigma}s} \right]. \quad (80)$$

We shall make use of these expressions in our examples later.

The asymptotic behavior of the diffusion coefficients for small and large s are also of interest, as they help us understand how the transport process represented by Eq. (75) transforms from the Fermi-Eyges behavior to isotropic diffusion. Again for the case of a δ function distribution of initial directions, we expand the expressions in Eqs. (77) and (78) for small s to find

$$D_{\parallel} \sim \frac{1}{3} \bar{\Sigma}(E_0)^2 s^3, \quad (81)$$

$$D_{\perp} \sim \frac{1}{3} \bar{\Sigma}(E_0) s^2. \quad (82)$$

We observe that $D_{\parallel}(s)$ vanishes faster than $D_{\perp}(s)$, and, hence, can be ignored in Eq. (75) in the small- s limit. Since $m(s) \sim 1$ in this limit, the initial evolution (Fermi-Eyges) of the beam is described by

$$\frac{\partial F}{\partial s} = -\frac{\partial F}{\partial z} + D_{\perp}(s) \left[\frac{\partial^2 F}{\partial x^2} + \frac{\partial^2 F}{\partial y^2} \right]. \quad (83)$$

This equation represents streaming along the z direction, which is parallel to the beam axis, accompanied by a spread of the beam on a plane perpendicular to the z axis, as described by the second term. This transverse motion, however, is not a diffusion process because $D_{\perp}(s)$ is not independent of s , and the mean-square displacement on a transverse plane is not proportional to s , but rather behaves as

$$\langle \mathbf{x}_{\perp}^2 \rangle \sim \frac{2}{3} \bar{\Sigma}(E_0) s^3. \quad (84)$$

We compare this result to the short time limit of the mean-square displacement in the z direction, which follows from Eq. (81) as:

$$\langle \mathbf{x}_{\parallel}^2 \rangle \sim \frac{1}{6} \bar{\Sigma}(E_0)^2 s^4. \quad (85)$$

Thus we find that the transverse spread of the beam is larger than the longitudinal spread in the early stages of beam penetration, that is, where $\bar{\Sigma}(\mathcal{E}(0))s \ll 1$.

The large- s limits of $D_{\parallel}(s)$ and $D_{\perp}(s)$ are obtained by assuming that $\theta(s)$ diverges as $s \rightarrow \infty$, and then applying L'Hôpital's rule to the indeterminate ratio obtained after replacing the first factor $e^{-\theta(s)}$ by $1/e^{\theta(s)}$ in Eqs. (77) and (78), again in the case $g(\mathbf{b}, 0) = \delta(\hat{\mathbf{\Omega}} - \hat{\mathbf{\Omega}}_0)$. One finds that both diffusion coefficients approach the same limit

$$D_{\parallel}(s) \sim D_{\perp}(s) \sim \frac{1}{3\bar{\Sigma}(s)} \equiv D(s) \quad \text{as } s \rightarrow \infty \quad (86)$$

On the other hand, the mobility $m(s)$ vanishes exponentially in this limit, and so Eq. (75) reduces to

$$\frac{\partial F}{\partial s} = D(s) \nabla^2 F \quad (87)$$

which describes isotropic diffusion. Thus we see that Eq. (75) will describe the transition from the Fermi-Eyges theory used in electron transport-dose calculations to the isotropic diffusion behavior assumed in photon diffusive wave spectroscopy.

When the initial distribution is isotropic, $\Phi_{\parallel}(0)=1/3$, $\bar{\Omega}(0)=0$, $\Phi_{\perp}(0)=0$ and $\psi(0)=0$. Equations (77) and (78) then tell us that the diffusion coefficients are equal, although still s dependent

$$D_{\parallel}(s)=D_{\perp}(s)\equiv D_0(s)=\frac{1}{3}e^{-\theta(s)}\int_0^s e^{\theta(s')}ds' \quad (88)$$

and Eq. (75) reduces to the isotropic diffusion equation with a time-dependent diffusion coefficient $D_0(s)$. When $\theta(s)=s\bar{\Sigma}$ this latter becomes

$$D_0(s)=\frac{1}{3\bar{\Sigma}}(1-e^{-s\bar{\Sigma}}). \quad (89)$$

It is interesting to note that the modified diffusion equation (75) differs from the conventional diffusion theory, even in this case of an isotropic source, for distances less than the penetration depth $l^*=1/\bar{\Sigma}$.

VII. SOLUTION IN AN INFINITE MEDIUM

A. Pulsed source

The general solution of Eq. (75) for an arbitrary initial directional distribution of particles located initially at $\mathbf{x}_0(0,0,z_0)$, and with $\bar{\Omega}(0)$ once again defining the z axis, is easily constructed in an infinite medium as

$$F_{\infty}(\mathbf{x},s)=\frac{1}{(2\pi)^{3/2}\sigma_{\perp}^2(s)\sigma_{\parallel}(s)}\times\exp\left\{-\frac{[z-\langle z(s)\rangle]^2}{2\sigma_{\parallel}^2(s)}-\frac{x^2+y^2}{2\sigma_{\perp}^2(s)}\right\}, \quad (90)$$

where $\langle z(s)\rangle$ denotes the mean position

$$\langle z(s)\rangle=z_0+\int_0^s m(s')ds' \quad (91)$$

and where σ_{\parallel}^2 and σ_{\perp}^2 denote parallel and transverse spatial variances, respectively, i.e., $\sigma_{\parallel}^2(s)=\langle z^2-\langle z(s)\rangle^2\rangle$ and $\sigma_{\perp}^2(s)=\langle x^2\rangle=\langle y^2\rangle$, and are given by

$$\sigma_{\parallel}^2(s)=2\int_0^s D_{\parallel}(s')ds', \quad (92)$$

$$\sigma_{\perp}^2(s)=2\int_0^s D_{\perp}(s')ds'. \quad (93)$$

As expected from the isotropy of the medium, the mean position $\langle z(s)\rangle$ of the particles moves in the initial direction with a exponentially decreasing velocity $e^{-\theta(s)}$. When the cross section is independent of energy in electron transport, and when the scattering is elastic in the case of photon transport, $\theta(s)=s\bar{\Sigma}$, and Eq. (91) becomes

$$\langle z(s)\rangle=z_0+\frac{1-e^{-s\bar{\Sigma}}}{\bar{\Sigma}}, \quad (94)$$

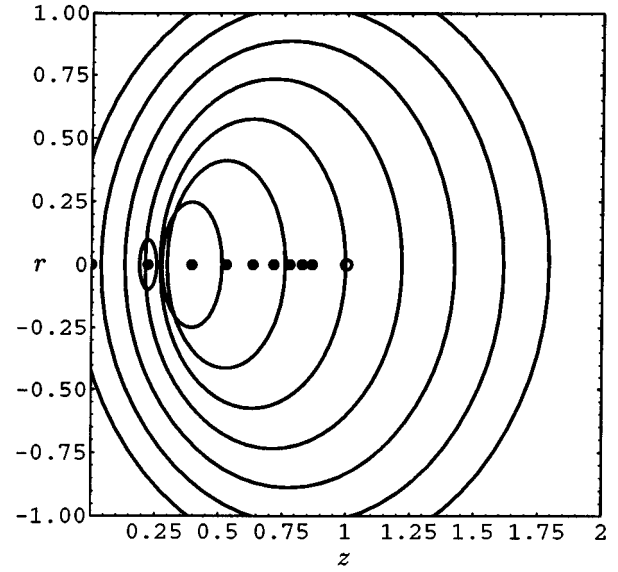


FIG. 1. The evolution of a cloud of particles injected into an infinite medium with constant penetration cross section $\bar{\Sigma}$. Each ellipse contains 50% of the total number of particles at different total path lengths s , with s running from 0 to 2 in steps of 0.25. The solid dots show the mean particle position, which approaches the point marked with a circle as $s\rightarrow\infty$. The outer ellipse corresponds to $s=2.0$; the path length for the other ellipses are easily identifiable by counting in from the outer one in steps of 0.25.

which shows that the mean position of the particle stops at $z_0+1/\bar{\Sigma}$ in the limit of $s\rightarrow\infty$. Hence, $l^*=1/\bar{\Sigma}$ can be interpreted as the penetration distance of the beam. The asymptotic isotropic diffusion, described by Eq. (87), takes place about this mean position. In contrast, at finite times the particle displays an anisotropic diffusion motion around $\langle\mathbf{x}(s)\rangle=\langle z(s)\rangle$, with different, time-dependent, longitudinal, and transverse diffusion coefficients.

Thus, the physical content of the infinite medium solution in Eq. (90) can be summarized as follows: We start with a large burst of particles all located at a single point, and moving in the z direction. As time elapses, these particles begin diffusing anisotropically, forming a cloud which looks like an oblate rotational ellipsoid about the z axis. The center of the cloud moves along the z axis while its size grows anisotropically as it moves. The center of the cloud eventually stops at the penetration point, a distance $l^*=1/\bar{\Sigma}$ (for $\bar{\Sigma}$ constant as described above) from the injection point. The shape of the cloud gradually becomes spherical as time passes. In the asymptotic regime, the particles execute an isotropic diffusion motion about the penetration point, and the size of the cloud continues growing, becoming increasingly spherical with a mean-square radius that grows like $\langle R(s)^2\rangle=2l^*s$.

In Fig. 1 we plot, as a function of path length traveled, the ellipse that contains half of the particles which were initially injected by a monodirectional, monoenergetic, point source at $(z,r)=(0,0)$, where $r^2=x^2+y^2$. All of the particles initially travel in the positive z direction. Each ellipse contains 50% of the total number of particles at different total path lengths s , with s running from 0 to 2 in steps of 0.25, where the units of distance are $1/\bar{\Sigma}$, which is taken to be independent of energy. The dots, at the center of each ellipse, show

the mean particle position as it penetrates into the medium. At long times this mean particle position comes to a stop at $(z, r) = (1, 0)$, which is marked with a small circle. At $s = 2.0$, the last path length shown, the mean position has reached $z = 0.865$.

The expression of F_∞ given in Eq. (90) is, with a proper normalization [9,10] the path-length distribution of particles arriving at a point \mathbf{x} in an infinite medium. This path-length distribution plays a central role in diffusive wave spectroscopy [9,10].

B. Steady state solutions

In this section we calculate the energy-dependent scalar particle density $n_\infty(x, E)$ due to a constant point source of electrons $\delta(\mathbf{x} - \mathbf{x}_0)\delta(E - E_0)\delta(\hat{\mathbf{\Omega}} - \hat{\mathbf{\Omega}}_0)$ in an infinite medium. The particle density, or more usefully the particle flux, is important because it enters in the dose calculations in nuclear medicine applications. We start with $n(\mathbf{x}, E, t)$, which is obtained by integrating Eq. (7) over $\hat{\mathbf{\Omega}}$

$$n(\mathbf{x}, E, t) = p(E)\delta(E - E(t))F(\mathbf{x}, t), \quad (95)$$

where $E(t) = \mathcal{E}(s(t))$ and satisfies $dE(t)/dt = -v(E)S(E)$. The only unknown in Eq. (95) is $F(\mathbf{x}, t)$; hence, if $F(\mathbf{x}, t)$ is determined for a pulsed point source in the medium with appropriate boundary conditions, then $n(\mathbf{x}, E, t)$ can be interpreted as the time-Green's function, and the steady state solution can be constructed as

$$n(\mathbf{x}, E) = \int_0^\infty n(\mathbf{x}, E, t) dt = p(E) \int_0^\infty F(\mathbf{x}, t) \delta(E - E(t)) dt. \quad (96)$$

Changing the integration variable in this equation from t to E using $dE(t)/dt = -v(E)S(E)$ yields

$$n(\mathbf{x}, E) = p(E) \int_0^{E_0} \frac{F(\mathbf{x}, t(E')) \delta(E - E')}{v(E')S(E')} dE'. \quad (97)$$

In obtaining this result we have used $E(0) = E_0$, and $E(t) \rightarrow 0$ as $t \rightarrow \infty$. Evaluating the integral in Eq. (97) and introducing the scalar flux $\varphi(\mathbf{x}, E) = v(E)n(\mathbf{x}, E)$, we find, in general

$$S(E)\varphi(\mathbf{x}, E) = p(E)F(\mathbf{x}, t(E)) = p(E)F(\mathbf{x}, s(E)). \quad (98)$$

Thus, we can obtain all the properties of the steady state flux explicitly from the knowledge of $F(\mathbf{x}, s)$, for which we have already derived exact and approximate equations; we simply replace s in the latter by $s(E)$, the path length traveled by the particle in slowing down from the energy E_0 to the energy E . An approximation to $F(\mathbf{x}, s)$ has already been constructed (in the preceding section) for an infinite medium, so we can now obtain explicitly all the properties of the flux.

However, it is sometimes more convenient to start with a diffusion equation for the flux, especially in applications involving finite geometries. We obtain such an equation by differentiating both sides of Eq. (98) with respect to E , yielding

$$\frac{\partial}{\partial E} S\varphi = \Sigma_a \varphi + p \left. \frac{\partial F}{\partial s} \right|_{s=s(E)} \frac{ds}{dE}. \quad (99)$$

Using $ds/dE = -1/S$ and Eq. (72) we can then derive an exact equation for the steady state flux. More usefully for the case of a monoenergetic, monidirectional point source, we can use the approximate diffusion equation Eq. (75) to eliminate $\partial F/\partial s$ and arrive at the slowing down equation

$$\frac{\partial}{\partial E} S\varphi - \Sigma_a \varphi = m(E) \frac{\partial \varphi}{\partial z} - \mathcal{D}_\parallel \frac{\partial^2 \varphi}{\partial z^2} - \mathcal{D}_\perp \left[\frac{\partial \varphi}{\partial x^2} + \frac{\partial \varphi}{\partial y^2} \right]. \quad (100)$$

The coefficients in this equation denote $m(E) = m(s(E))$, $\mathcal{D}_\parallel(E) = \mathcal{D}_\parallel(s(E))$, and $\mathcal{D}_\perp(E) = \mathcal{D}_\perp(s(E))$. They can easily be obtained from Eqs. (76), (77), and (78). These expressions all contain the function $\theta(s)$, defined by Eq. (38). By changing the variable from s' to E' we obtain $\Theta(E) = \theta(s(E))$ as

$$\Theta(E) = \int_E^{E_0} \frac{\bar{\Sigma}(E')}{S(E')} dE'. \quad (101)$$

The same procedure is used to obtain

$$m(E) = e^{-\Theta(E)}, \quad (102)$$

$$\begin{aligned} \mathcal{D}_\parallel(E) = & \frac{1}{3} e^{-\Theta(E)} \int_E^{E_0} \frac{1}{S(E')} [e^{\Theta(E')} - 3e^{-\Theta(E')} \\ & + 2e^{-2\Theta(E')}] dE', \end{aligned} \quad (103)$$

$$\mathcal{D}_\perp(E) = \frac{1}{3} e^{-\Theta(E)} \int_E^{E_0} \frac{1}{S(E')} [e^{\Theta(E')} - e^{-2\Theta(E')}] dE' \quad (104)$$

and we thereby have explicit expressions for the mobility and diffusion coefficients in the slowing down equation (100).

For small energy losses, for which $E_0 - E$ is treated as a small parameter, $\Theta(E)$ can be approximated as $\Theta(E) \approx (E_0 - E)\bar{\Sigma}(E)/S(E)$. Hence, in the lowest order in $E_0 - E$,

$$m(E) \approx 1 - (E - E_0) \frac{\bar{\Sigma}(E)}{S(E)}, \quad (105)$$

$$\mathcal{D}_\parallel(E) \approx \int_E^{E_0} \frac{1}{S(E')} \left[(E_0 - E') \frac{\bar{\Sigma}(E')}{S(E')} \right]^2 dE', \quad (106)$$

and

$$\mathcal{D}_\perp(E) \approx \int_E^{E_0} (E_0 - E') \frac{\bar{\Sigma}(E')}{S^2(E')} dE'. \quad (107)$$

Since $\mathcal{D}_\parallel(E)$ is of third order in $E - E_0$, the slowing down equation (100), reduces for small energy losses to

$$\frac{\partial}{\partial E} S\varphi - \Sigma_a \varphi = m(E) \frac{\partial \varphi}{\partial z} - \mathcal{D}_\perp \left[\frac{\partial \varphi}{\partial x^2} + \frac{\partial \varphi}{\partial y^2} \right]. \quad (108)$$

When $m(E)$ is replaced by unity, and absorption is neglected, this equation reduces to the Fermi-Eyges result [1,2].

But, whereas, this latter result is valid only in the lowest order in $E - E_0$, the slowing down equation (100) is valid at all energies; thus it does indeed extend the Fermi-Eyges result to the full energy range. It is worth remembering that the only approximation required to derive the slowing down equation (100) from the Fokker-Planck equation (1), was the expansion of the memory kernel in powers of the coupling operator. Its validity or accuracy can, therefore, be examined by looking at the magnitude of the coupling term.

The full solution of the slowing down equation in an infinite medium without absorption is just

$$S(E)\varphi_\infty(E) = \frac{1}{(2\pi)^{3/2}\sigma_\perp^2(E)\sigma_\parallel(E)} \times e^{-[(z-z(E))^2/2\sigma_\perp^2(E)] + [x^2+y^2/2\sigma_\perp^2(E)]}, \quad (109)$$

where

$$\sigma_\parallel^2(E) = 2 \int_E^{E_0} \frac{1}{S(E')} \mathcal{D}_\parallel(E') dE', \quad (110)$$

$$\sigma_\perp^2(E) = 2 \int_E^{E_0} \frac{1}{S(E')} \mathcal{D}_\perp(E') dE', \quad (111)$$

and

$$\bar{z}(E) = \int_E^{E_0} \Theta(E') dE'. \quad (112)$$

is the mean position of the particles after they have slowed down to energy E .

The calculation of dose rates in a medium due to both a pulsed point source and a constant point source of particles in terms of corresponding density $F_\infty(\mathbf{x}, s)$ is straightforward [4], and will not be discussed here.

VIII. CONCLUSIONS

The purpose of this paper was to develop a new derivation of the approximate diffusionlike equation (75) for the particle density $F(\mathbf{x}, s)$. This derivation begins from the Fokker-Planck description of particle transport, which is itself an approximation that is valid when the scattering is forwardly peaked and the energy change in scattering is small. The new derivation was based on the elimination of the direction variable $\hat{\Omega}$ through an elimination scheme based on Zwanzig's projection operator formalism in the interaction representation. The elimination procedure closely follows the one described by Grigolini and Marchesoni [8], but with a different projection operator which is more appropriate to the transport problem at hand.

The approximate diffusion equation is obtained from an exact equation for the density Eq. (72), which is valid for arbitrary separable initial distributions, by expanding the usual memory function in the projection operator formalism in powers of the coupling operator L_c between the direction and spatial variables, and then retaining terms through second order in L_c . The result of this is Eq. (74). When the initial angular distribution is azimuthally symmetric this equation reduces to Eq. (75), which was first derived in Ref. [3] by a different method. The longitudinal and transverse diffusion coefficients, and the mobility in this equation are time dependent, and contain information regarding the initial angular distribution of particles during the early stages of particle penetration where they still maintain their pencil-beam distribution. This information gradually decays away so that at later stages the particles execute increasingly isotropic diffusion about their mean position. This situation is different from the conventional treatment of monodirectional beams in terms of an uncollided flux that is separated from an isotropic collision source. Since in the present problem the scattering is forwardly peaked, the initial direction is remembered even after many collisions.

We solved the new diffusion equation exactly for the particle density $F_\infty(\mathbf{x}, s)$ in a homogeneous infinite medium for a monoenergetic and monodirectional burst of particles at the origin. This solution was used to study the penetration and the transverse and longitudinal spread of the particle cloud as they are transported into the medium. The evolution of the shape of the particle cloud from pencil-like to spherical is quantitatively displayed in the figure.

The modified diffusion equation obtained in this paper is applicable to the calculation of the path-length distribution, which plays a central role in diffusive wave spectroscopy [9,10]. With proper normalization $F_\infty(\mathbf{x}, s)$ is the path-length distribution of particles arriving at point \mathbf{x} via different paths through an infinite medium [9,10]. It has been calculated until now by assuming that particles that are actually inserted at the origin instead appear instantaneously at the penetration point located l^* away, and by then solving the ordinary isotropic diffusion equation for an isotropic point source located at this displaced point. Therefore, those results are valid only at linear distances $|\mathbf{x}|$ from the origin that are much larger than l^* . Since the solution of the modified diffusion equation obtained in this paper is valid at all distances, the path-length distribution can be calculated without the above restriction. In future work we intend to compare the path-length distributions obtained by these two approaches quantitatively.

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