Fokker-Planck description of particle transport in finite media: Boundary conditions

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Using the Fokker-Planck description of particle transport, which is valid when the scattering is forwardly peaked and the energy loss per scattering is small, the energy-dependent transport of electrons and photons in finite homogeneous media is studied. Treating the coupling between the angular and spatial dependence of the angular particle density as a small parameter, a modified diffusion equation for the particle number density $F(\mathbf{x},s)$ is obtained by a systematic perturbation expansion, and the appropriate boundary conditions on the outer surface of the medium are developed. As an application, the transport of photons in a half-infinite medium, for a pulsed coherent laser beam uniformly incident on the interface, is studied analytically and numerically. The spatial distribution of photons in the medium, as a function of the distance from the interface at different path lengths, as well as the path length distribution of the reflected photons, are obtained. Due to its importance in diffusive wave spectroscopy, the Laplace transform of the path length distribution of the reflected photons is calculated, and compared with the result obtained with the diffusion theory that assumes a fictitious isotropic pulsed light source at a distance z_0 from the surface of the medium. By matching the initial slopes, a value $1.67l^*$ is found for z_0, which enters the diffusion theory as an adjustable parameter. [S1063-651X(98)07810-6]

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I. INTRODUCTION

The conventional linear Boltzmann equation can be cast into the Fokker-Planck form when the scattering is forwardly peaked, and the energy change in scattering is small [1]:

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

where $n(\mathbf{x},E,\mathbf{\Omega},t)$ is the energy-dependent angular particle density; $S(E)$ is the energy loss per unit distance, or the stopping power; $\Sigma_a(E)$ is the macroscopic absorption cross section; $\overline{\Sigma}(E)=\Sigma_{tr}(E)-\Sigma_a(E)$ where $\Sigma_{tr}(E)$ is the transport cross section; L^2 is the total angular momentum operator defined by

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

the vector $\mathbf{\Omega}$ is the unit vector in the direction of particle velocity; $v(E)$ is the particle speed corresponding to the particle energy E; μ is the cosine of the polar angle describing the unit vector $\mathbf{\Omega}$, and ϕ is the corresponding azimuthal angle. The sign of L^2 is chosen such that its eigenfunction $Y_{lm}(\mathbf{\Omega})$, i.e., the spherical harmonics, satisfy

$$L^2 Y_{lm}(\mathbf{\Omega})=l(l+1)Y_{lm}(\mathbf{\Omega}). \quad (3)$$

The definitions of $S(E)$ and $\overline{\Sigma}(E)$ in terms of the differential cross section are

$$S(E)=\int_0^\infty dE'\int d\mathbf{\Omega}'(E-E')\Sigma_s(E\to E',\mathbf{\Omega}\cdot\mathbf{\Omega}'), \quad (4)$$

$$\overline{\Sigma}(E)=2\pi\int_0^\infty dE'\int_{-1}^1 d\mu(1-\mu)\Sigma_s(E\to E',\mu). \quad (5)$$

We have shown in an earlier paper [2], which will henceforth be referred to as "I," that, with the initial condition $n(\mathbf{x},E,\mathbf{\Omega},0)=\delta(E-E_0)f(\mathbf{x},\mathbf{\Omega},0)$, the angular density can be expressed as

$$n(\mathbf{x},E,\mathbf{\Omega},t)=\delta(E-\mathcal{E}(t))p(E)f(\mathbf{x},\mathbf{\Omega},t), \quad (6a)$$

where $p(E)$ is the nonabsorption probability defined by

$$p(E)=\exp\left[-\int_E^{E_0}dE'\frac{\Sigma_a(E')}{S(E')}\right] =\exp\left[-\int_0^t dt' v(t')\Sigma_a(t')\right], \quad (6b)$$

where $v(t)=v(\mathcal{E}(t))$ and $\Sigma_a(t)=\Sigma_a(\mathcal{E}(t))$. The function $\mathcal{E}(t)$ is the solution of

$$\frac{d\mathcal{E}(t)}{dt}=-v(\mathcal{E})S(\mathcal{E}), \quad (7a)$$

with the initial condition $\mathcal{E}(0)=E_0$. It is a known function of time. It proves convenient to rewrite this equation in terms of path length $s(t)$ using $ds=v(t)dt$ as

$$\frac{d\mathcal{E}(s)}{ds}=-S(\mathcal{E}), \quad (7b)$$

which is consistent with the meaning of $S(E)$ as the energy loss per unit distance. Henceforth, we shall use the path length variable s instead of the time variable t; these are transformed into each other through $ds=v(t)dt$, which is clearly just a change of variables. The function $f(\mathbf{x},\mathbf{\Omega},s)$, which is introduced in Eq. (6), satisfies

$$\frac{\partial}{\partial s} f(\mathbf{x},\mathbf{\Omega},s)+\mathbf{\Omega}\cdot\mathbf{\nabla} f=-\frac{\overline{\Sigma}(s)}{2} L^2 f, \tag{8}$$

where $\overline{\Sigma}(s)=\overline{\Sigma}(\mathcal{E}(s))$. The elimination of the energy variable in Eq. (1) enables one to reduce the original Fokker-Planck equation for the full energy-dependent angular density $n(\mathbf{x},E,\mathbf{\Omega},s)$ to the simpler form given in Eq. (8) for $f(\mathbf{x},\mathbf{\Omega},s)$. The latter can be interpreted as the one-speed Fokker-Planck equation for the angular particle density in the absence of absorption. In many problems one is not interested in the angular information, and tries to obtain an approximate equation (diffusion approximation) for the number density defined by

$$F(\mathbf{x},s)=\int d\mathbf{\Omega}\ f(\mathbf{x},\mathbf{\Omega},s). \tag{9}$$

In I, we have shown, by using an elimination procedure based on the projection operator formalism in which the coupling operator $L_1=-\mathbf{\Omega}\cdot\mathbf{\nabla}$ in Eq. (8) is treated as small, that $F(\mathbf{x},s)$ satisfies the following diffusion equation up to second order in L_1:

$$\frac{\partial F(\mathbf{x},s)}{\partial s}=-m(s)\ \frac{\partial F}{\partial z}+D_{\parallel}(s)\ \frac{\partial^2 F}{\partial z^2}+D_T(s)\left(\frac{\partial^2 F}{\partial x^2}+\frac{\partial^2 F}{\partial y^2}\right). \tag{10}$$

In deriving this equation, the initial condition for the angular density is taken to be monodirectional, i.e., $f(\mathbf{x},\mathbf{\Omega},0)=\delta(\mathbf{\Omega}-\mathbf{\Omega}_0)F(\mathbf{x},0)$, and the z axis is chosen parallel to $\mathbf{\Omega}_0$. In this equation, $D_{\parallel}(s)$ and $D_T(s)$ denote, respectively, the s-dependent parallel and transverse diffusion coefficients. $D_{\parallel}(s)$ characterizes the diffusion of particles parallel to the initial direction, $\mathbf{\Omega}_0$, whereas $D_T(s)$ characterizes diffusion on a plane perpendicular to $\mathbf{\Omega}_0$. The expressions of $D_{\parallel}(s)$, $D_T(s)$, and $m(s)$, which are presented in I, as well as an earlier paper [3], will not be needed in the following derivations.

The diffusion equation in Eq. (10) was solved in I and in Refs. [3,4] in an infinite medium, and its application to dose calculations in tissue resulting from an electron beam was discussed [3,4]. The possibility of using Eq. (10) in diffusive wave spectroscopy (DWS), where the number density $F(\mathbf{x},s)$ is interpreted as the path length distribution of photons arriving at the detector, was also mentioned in I.

It is clear that, in such applications, the finiteness of the medium in which the particles are transported must be taken into account: in the case of dose calculations, an electron beam is directed to the tissue from outside; in the case of DWS the intensity correlations of either the backscattered light, or of the transmitted light through a slab are considered. Therefore, for realistic applications of Eq. (10), we have to obtain solutions in a finite medium, such as a semi-infinite or a finite slab. To obtain solutions of Eq. (10) in finite media we have to first establish the appropriate boundary conditions consistent with the approximations used in the derivation of Eq. (10). This is the main theme of this paper.

The organization of the paper is as follows. In Sec. II we present an alternative and more physical derivation of Eq. (10) without resorting to the general and abstract method of elimination of fast variables (the direction variable $\mathbf{\Omega}$ in our application), which was presented in I. Such a simpler derivation is now possible because we already know from I that Eq. (10) is obtained by ignoring the terms of third and higher order in a power series expansion in the coupling operator $L_1=-\mathbf{\Omega}\cdot\mathbf{\nabla}$. However, the purpose of Sec. II is not only to provide an alternative derivation of a known result: the new derivation is based on an expansion of $f(\mathbf{x},\mathbf{\Omega},s)$ into spherical harmonics, which enables us to calculate the partial currents needed to establish the appropriate boundary conditions. The details of these calculations, and the boundary conditions themselves, are presented in Sec. III. Section IV illustrates an implementation of the boundary conditions in the case of a half-infinite medium, where the angular distribution of the albedo current is explicitly calculated. The implication of the results of Sec. IV in DWS, as well as conclusions, are discussed in Sec. V.

II. AN ALTERNATIVE DERIVATION OF EQ. (10)

We start with Eq. (8) and rewrite it as

$$\frac{\partial f(\mathbf{x},\mathbf{\Omega},s)}{\partial s}+\varepsilon\mathbf{\Omega}\cdot\mathbf{\nabla} f(\mathbf{x},\mathbf{\Omega},s)=-\frac{1}{2}\overline{\Sigma}(s)L^2 f(\mathbf{x},\mathbf{\Omega},s), \tag{11}$$

where we have put the smallness parameter ε in evidence, as suggested by the derivation in I. We solve this equation assuming that the initial angular distribution is separable in space and angle:

$$f(\mathbf{x},\mathbf{\Omega},0)=P(\mathbf{\Omega},0)F(\mathbf{x},0), \tag{12}$$

where $P(\mathbf{\Omega},0)$ is the initial angular distribution, and hence normalized

$$\int d\mathbf{\Omega}\ P(\mathbf{\Omega},0)=1.$$

The $F(\mathbf{x},0)$ is the initial value of the spatial distribution, or the scalar number density, defined for all s by

$$F(\mathbf{x},s)=\int d\mathbf{\Omega}\ f(\mathbf{x},\mathbf{\Omega},s). \tag{13}$$

The separability assumption in Eq. (12) is satisfied in the problems we will be interested in. The angular distribution $f(\mathbf{x},\mathbf{\Omega},s)$ cannot remain separable for $s>0$ because of the streaming operator $\varepsilon\mathbf{\Omega}\cdot\mathbf{\nabla}$ in Eq. (11), which couples the angular and spatial evolution of f. In the absence of this term, the angular distribution would evolve in s according to

$$\frac{\partial}{\partial s} P(\mathbf{\Omega},s)+\frac{1}{2}\overline{\Sigma}(s)L^2 P(\mathbf{\Omega},s)=0, \tag{14}$$

which is easily solved as

$$P(\mathbf{\Omega},s)=e^{-(1/2)\Theta(s)L^2}P(\mathbf{\Omega},0), \tag{15a}$$

where

$$\Theta(s)=\int_0^s ds'\bar{\Sigma}(s'). \tag{15b}$$

We mention for future use that, when the initial angular distribution is isotropic, i.e., when $P(\mathbf{\Omega},0)=1/4\pi$, $P(\mathbf{\Omega},s)=1/4\pi$ for all s because $L^2 1=0$. The expression of $P(\mathbf{\Omega},s)$ for initially monodirectional particles, i.e., for $P(\mathbf{\Omega},0)=\delta(\mathbf{\Omega}-\mathbf{\Omega}_0)$, will be given in Sec. III [cf. Eq. (33)]. The first angular moment of $P(\mathbf{\Omega},s)$ follows from Eq. (15a) as

$$\langle\mathbf{\Omega}(s)\rangle=e^{-\Theta(s)}\langle\mathbf{\Omega}(0)\rangle. \tag{16}$$

In obtaining Eq. (16), we have used the fact that L^2 is self-adjoint, and $L^2\mathbf{\Omega}=2\mathbf{\Omega}$.

Returning to the nonseparability of $f(\mathbf{x},\mathbf{\Omega},s)$ for $s>0$, we have found that $f(\mathbf{x},\mathbf{\Omega},s)$ is separable for all $s>0$ in the absence of the streaming term in the Fokker-Planck equation, and hence can be written as $f(\mathbf{x},\mathbf{\Omega},s)=P(\mathbf{\Omega},s)F(\mathbf{x},0)$ at all times. In order to take into account the coupling between the evolution of $\mathbf{x}$ and $\mathbf{\Omega}$, caused by the streaming operator, we expand $f(\mathbf{x},\mathbf{\Omega},s)-P(\mathbf{\Omega},s)F(\mathbf{x},s)$ into spherical harmonics as follows:

$$f(\mathbf{x},\mathbf{\Omega},s)=P(\mathbf{\Omega},s)F(\mathbf{x},s)+A(\mathbf{x},s)+\frac{3}{4\pi}\,\mathbf{J}_D(\mathbf{x},s)\cdot\mathbf{\Omega} + (\text{higher-order terms}), \tag{17a}$$

where $F(\mathbf{x},s)$, $A(\mathbf{x},s)$, and $\mathbf{J}_D(\mathbf{x},s)$ are the expansion coefficients to be determined, and the higher-order terms in the expansion consist of second- and higher-order spherical harmonics. Integration of Eq. (17a) over angles then yields $A(\mathbf{x},s)=0$, so that the expansion reduces to

$$f(\mathbf{x},\mathbf{\Omega},s)=P(\mathbf{\Omega},s)F(\mathbf{x},s)+\frac{3}{4\pi}\,\mathbf{J}_D(\mathbf{x},s)\cdot\mathbf{\Omega} + (\text{higher-order terms}). \tag{17b}$$

Our strategy can be outlined as follows. In Eq. (17b), the first term is of zeroth order in ε. The remaining terms are at least of first order in ε, because they vanish when $\varepsilon=0$. We determine only the second term in the lowest order in ε, although the terms involving higher-order spherical harmonics also contribute to $f(\mathbf{x},\mathbf{\Omega},s)$ at the same order. The reason for neglecting the contributions of higher-order terms is that our aim in this paper is only to modify and extend the diffusion approximation in order to include the initial ballistic evolution of a monodirectional particle beam. The inclusion of the contributions from the higher-order spherical harmonics would lead to a systematic extension of the P_N approximation.

The $\mathbf{J}_D(\mathbf{x},s)$ can be related to the usual current density $\mathbf{J}(\mathbf{x},s)$, which is defined by

$$\mathbf{J}(\mathbf{x},s)\equiv\int d\mathbf{\Omega}\;\mathbf{\Omega}f(\mathbf{x},\mathbf{\Omega},s), \tag{18}$$

by multiplying Eq. (17b) by $\mathbf{\Omega}$, and then integrating over $\mathbf{\Omega}$ we arrive at

$$\mathbf{J}(\mathbf{x},s)=\langle\mathbf{\Omega}(s)\rangle F(\mathbf{x},s)+\mathbf{J}_D(\mathbf{x},s). \tag{19}$$

The first term in Eq. (19) represents the effect of the initial angular distribution, whereas $\mathbf{J}_D(\mathbf{x},s)$ accounts for the usual diffusion current, and satisfies Fick's law with an s-dependent diffusion constant, as we show below.

Since the first term in Eq. (17b) at $s=0$ is exactly equal to $f(\mathbf{x},\mathbf{\Omega},0)$ by construction, $\mathbf{J}_D(\mathbf{x},0)=0$. In order to obtain equations for $F(\mathbf{x},s)$ and $\mathbf{J}_D(\mathbf{x},s)$ for $s>0$, we substitute the expansion in Eq. (17b) into the Fokker-Planck equation (11), and take the zeroth and first angular moments of the resulting equation yielding

$$\frac{\partial F(\mathbf{x},s)}{\partial s}=-\varepsilon\nabla\cdot[\langle\mathbf{\Omega}(s)\rangle F(\mathbf{x},s)+\mathbf{J}_D(\mathbf{x},s)], \tag{20}$$

$$\frac{\partial \mathbf{J}_D(\mathbf{x},s)}{\partial s}+\bar{\Sigma}(s)\mathbf{J}_D(\mathbf{x},s)=-\varepsilon\,\delta\mathbf{\Phi}(s)\cdot\nabla F(\mathbf{x},s). \tag{21}$$

The first equation is the continuity equation, and exact. The second equation is approximate because we have neglected in its derivation the term $\varepsilon\langle\mathbf{\Omega}(s)\rangle\nabla\cdot\mathbf{J}_D(\mathbf{x},s)$, which is of second order in the coupling constant ε because $\mathbf{J}_D(\mathbf{x},s)$ itself is of order ε. In Eq. (21) we have introduced the variance matrix $\delta\mathbf{\Phi}(s)$, which is defined by

$$\delta\mathbf{\Phi}(s)=\int d\mathbf{\Omega}\;\mathbf{\Omega}\mathbf{\Omega}P(\mathbf{\Omega},s)-\langle\mathbf{\Omega}(s)\rangle\langle\mathbf{\Omega}(s)\rangle =\langle\mathbf{\Omega}(s)\mathbf{\Omega}(s)\rangle-\langle\mathbf{\Omega}(s)\rangle\langle\mathbf{\Omega}(s)\rangle, \tag{22}$$

and was calculated explicitly earlier [2,3]. We do not need to present the expression of $\delta\mathbf{\Phi}(s)$ in the subsequent derivations.

Equation (21) can be solved for $\mathbf{J}_D(\mathbf{x},s)$ as

$$\mathbf{J}_D(\mathbf{x},s)=-\varepsilon\int_0^s du\; e^{-[\Theta(s)-\Theta(u)]}\delta\mathbf{\Phi}(u)\cdot\nabla F(\mathbf{x},u), \tag{23}$$

where we have used the initial condition $\mathbf{J}_D(\mathbf{x},0)=0$. Substitution of $\mathbf{J}_D(\mathbf{x},s)$ from Eq. (23) into the continuity equation (20) yields an integro-differential equation for the number density $F(\mathbf{x},s)$:

$$\frac{\partial F(\mathbf{x},s)}{\partial s}=-\varepsilon\langle\mathbf{\Omega}(s)\rangle\cdot\nabla F(\mathbf{x},s) +\varepsilon^2\int_0^s du\; e^{-[\Theta(s)-\Theta(u)]}\nabla\cdot\delta\mathbf{\Phi}(u)\cdot\nabla F(\mathbf{x},u). \tag{24}$$

We can obtain either the diffusion equation or the telegrapher's equation from Eq. (24): to obtain the diffusion equation, we treat $F(\mathbf{x},u)$ in Eq. (24) as a slowly varying function of u, replace it by $F(\mathbf{x},s)$, and take it outside the u integral. This step is justified because the Taylor series expansion of $F(\mathbf{x},u)$ about s contains $\partial F(\mathbf{x},s)/\partial s$, which is at least of order ε according to the continuity equation (20). With this simplification, Eq. (24) reduces to

$$\frac{\partial F(\mathbf{x},s)}{\partial s} = -\varepsilon\langle\mathbf{\Omega}(s)\rangle\cdot\frac{\partial F}{\partial \mathbf{x}} + \varepsilon^2\nabla\cdot\mathbf{D}(s)\cdot\nabla F, \quad (25)$$

which is the desired modified diffusion equation in matrix form. In Eq. (25), we have introduced the diffusion matrix $\mathbf{D}(s)$ as

$$\mathbf{D}(s) = \int_0^s du\ e^{-[\Theta(s)-\Theta(u)]}\delta\mathbf{\Phi}(u). \quad (26)$$

The calculation of $\mathbf{D}(s)$, also, was presented in two earlier papers [2,3]. Equation (25) is the same as Eq. (10), but without the assumption that the initial distribution is monodirectional. The accuracy of the diffusion equation in powers of ε is explicitly displayed in Eq. (25). The simplification used in obtaining Eq. (25) is equivalent to approximating the diffusion current $\mathbf{J}_D(\mathbf{x},s)$ in Eq. (20) by the usual Fick law

$$\mathbf{J}_D(\mathbf{x},s) = -\varepsilon\mathbf{D}(s)\cdot\nabla F(\mathbf{x},s). \quad (27)$$

In order to obtain the telegrapher's equation, we differentiate Eq. (24) with respect to s, and then eliminate the memory integral in it in favor of the first time derivative of $F(\mathbf{x},s)$. After some algebra, we obtain

$$\frac{\partial^2 F(\mathbf{x},s)}{\partial s^2} + \overline{\Sigma}(s)\frac{\partial F(\mathbf{x},s)}{\partial s} = \varepsilon^2\nabla\cdot\mathbf{\Phi}(s)\cdot\nabla F(\mathbf{x},s), \quad (28)$$

where $\mathbf{\Phi}(s) = \langle\mathbf{\Omega}(s)\mathbf{\Omega}(s)\rangle$ [see Eq. (22)]. Since we shall not use the telegrapher's equation in this paper, we do not present the intermediate steps of its derivation.

III. PARTIAL CURRENTS AND BOUNDARY CONDITIONS

The partial currents for a given direction $\hat{\mathbf{n}}$ are defined in the usual way by integrating $\hat{\mathbf{n}}\cdot\mathbf{\Omega}f(\mathbf{x},\mathbf{\Omega},s)$ over a half range:

$$J_+^{\hat{\mathbf{n}}}(\mathbf{x},s) = \int_{\hat{\mathbf{n}}\cdot\mathbf{\Omega}>0} d\mathbf{\Omega}\ \hat{\mathbf{n}}\cdot\mathbf{\Omega}f(\mathbf{x},\mathbf{\Omega},s) \quad (29a)$$

and

$$J_-^{\hat{\mathbf{n}}}(\mathbf{x},s) = -\int_{\hat{\mathbf{n}}\cdot\mathbf{\Omega}<0} d\mathbf{\Omega}\ \hat{\mathbf{n}}\cdot\mathbf{\Omega}f(\mathbf{x},\mathbf{\Omega},s). \quad (29b)$$

Substituting the expansion of $f(\mathbf{x},\mathbf{\Omega},s)$ obtained in Sec. II, i.e.,

$$f(\mathbf{x},\mathbf{\Omega},s) = P(\mathbf{\Omega},s)F(\mathbf{x},s) + \frac{3}{4\pi}\mathbf{J}_D(\mathbf{x},s)\cdot\mathbf{\Omega}, \quad (30)$$

into Eqs. (29), we obtain

$$J_\pm^{\hat{\mathbf{n}}}(\mathbf{x},s) = \langle\hat{\mathbf{n}}\cdot\mathbf{\Omega}(s)\rangle_\pm F(\mathbf{x},s) \pm \tfrac{1}{2}\hat{\mathbf{n}}\cdot\mathbf{J}_D(\mathbf{x},s), \quad (31)$$

where $\langle\hat{\mathbf{n}}\cdot\mathbf{\Omega}(s)\rangle_\pm$ denote

$$\langle\hat{\mathbf{n}}\cdot\mathbf{\Omega}(s)\rangle_+ = \int_{\hat{\mathbf{n}}\cdot\mathbf{\Omega}>0} d\mathbf{\Omega}\ \hat{\mathbf{n}}\cdot\mathbf{\Omega}P(\mathbf{\Omega},s) \quad (32a)$$

and

$$\langle\hat{\mathbf{n}}\cdot\mathbf{\Omega}(s)\rangle_- = -\int_{\hat{\mathbf{n}}\cdot\mathbf{\Omega}<0} d\mathbf{\Omega}\ \hat{\mathbf{n}}\cdot\mathbf{\Omega}P(\mathbf{\Omega},s). \quad (32b)$$

In the special case of an isotropic initial distribution, $P(\mathbf{\Omega},s) = 1/4\pi$, and hence we obtain $\langle\hat{\mathbf{n}}\cdot\mathbf{\Omega}(s)\rangle_\pm = \frac{1}{4}$, so that Eq. (31) reduces to the conventional expression of the partial currents in the conventional diffusion theory.

As another limiting case, we consider initially monodirectional particles so that $P(\mathbf{\Omega},0) = \delta(\mathbf{\Omega}-\mathbf{\Omega}_0)$, and choose $\hat{\mathbf{n}}$ in the direction of $\mathbf{\Omega}_0$. In this case, $\langle\hat{\mathbf{n}}\cdot\mathbf{\Omega}(0)\rangle_+ = 1$, and $\langle\hat{\mathbf{n}}\cdot\mathbf{\Omega}(0)\rangle_- = 0$. For $s\neq 0$, we first obtain $P(\mathbf{\Omega},s)$, given in Eq. (15a) with the initial distribution $P(\mathbf{\Omega},0) = \delta(\mathbf{\Omega}-\mathbf{\Omega}_0)$. Representing the δ function in terms of spherical harmonics, we obtain

$$P(\mathbf{\Omega},s) = \sum_{l,m} e^{-(1/2)\Theta(s)l(l+1)}Y_{lm}(\mathbf{\Omega})Y_{lm}^*(\mathbf{\Omega}_0)$$
$$= \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}P_l(\mathbf{\Omega}\cdot\mathbf{\Omega}_0)e^{-(1/2)\Theta(s)l(l+1)}. \quad (33)$$

[We point out for future reference that $P(\mathbf{\Omega},s)$ becomes isotropic in the limit of $\Theta(s)\to\infty$, because in this limit only the $l=0$ term survives in Eq. (33), and hence $P(\mathbf{\Omega},s)\to 1/4\pi$.]

To calculate $\langle\hat{\mathbf{n}}\cdot\mathbf{\Omega}(s)\rangle_+$, we write Eq. (32a) explicitly

$$\langle\hat{\mathbf{n}}\cdot\mathbf{\Omega}(s)\rangle_+ = \int_0^1 d\mu\ \mu\int_0^{2\pi}d\varphi\ P(\mathbf{\Omega},s). \quad (34)$$

To perform the integrals in Eq. (34), we choose $\hat{\mathbf{n}}$ in the direction of $\mathbf{\Omega}_0$, so that in Eq. (33) $\mathbf{\Omega}\cdot\mathbf{\Omega}_0 = \mu$, the polar angle of $\mathbf{\Omega}$, and obtain

$$\langle\hat{\mathbf{n}}\cdot\mathbf{\Omega}(s)\rangle_+ = \sum_{l=0}^{\infty}\frac{2l+1}{2}e^{-(1/2)\Theta(s)l(l+1)}\int_0^1 d\mu\ \mu P_l(\mu). \quad (35)$$

We verify in passing the value of $\langle\hat{\mathbf{n}}\cdot\mathbf{\Omega}(0)\rangle_+$,

$$\langle\hat{\mathbf{n}}\cdot\mathbf{\Omega}(0)\rangle_+ = \int_0^1 d\mu\ \mu\sum_{l=0}^{\infty}\frac{2l+1}{2}P_l(\mu)$$
$$= \int_0^1 d\mu\ \mu\delta(\mu-1) = 1.$$

The integral in Eq. (35) is known [5],

$$\int_0^1 d\mu\ \mu P_l(\mu) = \frac{\sqrt{\pi}}{4}\frac{1}{\Gamma(\frac{3}{2}-l/2)\Gamma(2+l/2)}. \quad (36)$$

We observe from this formula that the integral vanishes for all odd l except for $l=1$, i.e., for odd l

$$\int_0^1 d\mu\ \mu P_l(\mu) = \tfrac{1}{3}\delta_{l,1},$$

which can be verified directly by observing that $\mu P_l(\mu)$ is even when l is odd, and extending the range of integration to $(-1,1)$. Hence, Eq. (35) can be written as

$$\langle \hat{\mathbf{n}}\cdot \mathbf{\Omega}(s)\rangle_+ = \frac{1}{2} e^{-\Theta(s)} + \frac{\sqrt{\pi}}{8} \sum_{l(\mathrm{even})=0}^{\infty} \frac{2l+1}{\Gamma(\frac{3}{2}-l/2)\Gamma(2+l/2)} \times e^{-\Theta(s) l(l+1)/2}. \quad (37)$$

The alternating series in Eq. (37) is rapidly convergent. To demonstrate this assertion, we consider the limit of $s=0$. Since we know that $\langle \hat{\mathbf{n}}\cdot \mathbf{\Omega}(0)\rangle_+ = 1$ in this limit, we must have

$$\frac{\sqrt{\pi}}{8} \sum_{l(\mathrm{even})=0}^{\infty} \frac{2l+1}{\Gamma(\frac{3}{2}-l/2)\Gamma(2+l/2)} = \frac{1}{2}.$$

The sum of the first three terms is 0.467, which is indeed close to 0.5.

We now calculate $\langle \hat{\mathbf{n}}\cdot \mathbf{\Omega}(s)\rangle_-$. Since

$$\langle \hat{\mathbf{n}}\cdot \mathbf{\Omega}(s)\rangle = e^{-\Theta(s)}$$

and $\langle \hat{\mathbf{n}}\cdot \mathbf{\Omega}(s)\rangle = \langle \hat{\mathbf{n}}\cdot \mathbf{\Omega}(s)\rangle_+ - \langle \hat{\mathbf{n}}\cdot \mathbf{\Omega}(s)\rangle_-$, we obtain $\langle \hat{\mathbf{n}}\cdot \mathbf{\Omega}(s)\rangle_-$ as

$$\langle \hat{\mathbf{n}}\cdot \mathbf{\Omega}(s)\rangle_- = \langle \hat{\mathbf{n}}\cdot \mathbf{\Omega}(s)\rangle_+ - \langle \hat{\mathbf{n}}\cdot \mathbf{\Omega}(s)\rangle \quad (38a)$$

or explicitly as

$$\langle \hat{\mathbf{n}}\cdot \mathbf{\Omega}(s)\rangle_- = -\frac{1}{2} e^{-\Theta(s)} + \frac{\sqrt{\pi}}{8} \sum_{l(\mathrm{even})=0}^{\infty} \times \frac{2l+1}{\Gamma(\frac{3}{2}-l/2)\Gamma(2+l/2)} e^{-\Theta(s) l(l+1)/2}. \quad (38b)$$

We verify, as a check, that both $\langle \hat{\mathbf{n}}\cdot \mathbf{\Omega}(s)\rangle_\pm$ approach $\frac{1}{4}$ in the limit of $\Theta(s)\to\infty$, because in this limit, $P(\mathbf{\Omega},s)$ becomes isotropic as we have already pointed out after Eq. (33). Indeed, as $\Theta(s)\to\infty$, the first terms in Eqs. (37) and (38b) vanish, and only the term $l=0$ survives in the second terms. The latter is $\frac{1}{4}$ because $\Gamma(\frac{3}{2}) = \sqrt{\pi}/2$ and $\Gamma(2)=1$, proving the assertion.

The boundary condition for a specified geometry can now be implemented in terms of the partial currents in the usual way, as Sec. IV demonstrates.

IV. IMPLEMENTATION OF THE BOUNDARY CONDITION IN A SEMI-INFINITE MEDIUM

We consider a semi-infinite medium, and a normally incident beam of particles on its interface with vacuum as indicated in Fig. 1. Since the problem is one dimensional, the diffusion equation to be solved is

$$\frac{\partial F(x,s)}{\partial s} = -m(s) \frac{\partial F}{\partial x} + D(s) \frac{\partial^2 F}{\partial x^2}, \quad (39)$$

where

$$m(s) = \langle \hat{\mathbf{x}}\cdot \mathbf{\Omega}(s)\rangle = e^{-\Theta(s)},$$

and $D(s) = D_\parallel(s)$. The parallel diffusion coefficient was calculated earlier [2,3]:

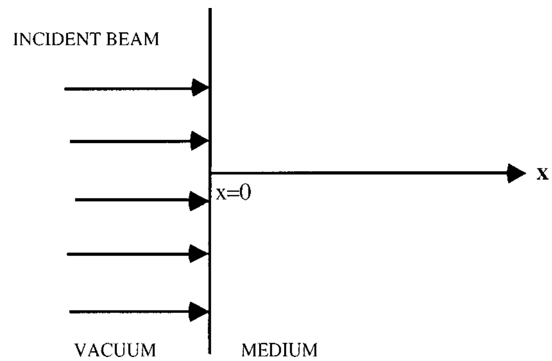

FIG. 1. Normal incidence on the interface of a half-infinite sample.

$$D_\parallel(s) = \tfrac{1}{3} e^{-\Theta(s)} \int_0^s ds' [e^{\Theta(s')} - 3e^{-\Theta(s')} + 2e^{-2\Theta(s')}]. \quad (40)$$

We shall solve Eq. (39) for a burst of monodirectional particles (one particle/cm^2) in the x direction, introduced at $x=0^+$ and $s=0$. This source condition corresponds to an initial angular density $f(x,\mu,s=0) = \delta(\mu-1)\delta(x-0^+)$. Integrating over μ, we obtain the initial condition for $F(x,s)$ as $F(x,0) = \delta(x-0^+)$. The appropriate boundary conditions are $F(x\to\infty,s)=0$ at infinity, and $J_+(0,s) = \delta(s)$ at $x=0$, i.e.,

$$m_+(s)F(0,s) - \frac{1}{2} D(s) \left. \frac{\partial F(x,s)}{\partial x} \right|_{x=0} = \delta(s), \quad (41a)$$

where $m_+(s) = \langle \hat{\mathbf{x}}\cdot \mathbf{\Omega}(s)\rangle_+$, which is defined in Eq. (37). This condition shows that $F(0,s)$ has a singularity at $s=0$, which can be removed by introducing $F_1(0,s) = F(0,s) - \delta(s)$. Since $D(0)=0$ and $m_+(0)=1$, the boundary condition for the nonsingular part becomes

$$m_+(s)F_1(0,s) - \frac{1}{2} D(s) \left. \frac{\partial F_1(x,s)}{\partial x} \right|_{x=0} = 0. \quad (41b)$$

It is clear that $F_1(0,s) = F(0,s)$ for all $s>0$.

The solution of Eq. (39) is constructed by first taking its one-sided Fourier transform with respect to x:

$$\frac{\partial \overline{F}(k,s)}{\partial s} = -[D(s)k^2 + ikm(s)]\overline{F}(k,s) + R(k,s), \quad (42)$$

where

$$\overline{F}(k,s) = \int_0^\infty dx\, F(x,s) e^{-ikx}, \quad (43a)$$

$$F(x,s) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, \overline{F}(k,s) e^{ikx}, \quad (43b)$$

and

$$R(k,s) = [m(s) - ikD(s)]F(0,s) - D(s)\partial F(x,s)/\partial x|_{x=0}. \quad (44a)$$

Clearly, $R(k,s)$ contains the unknown boundary conditions $F(0,s)$ and $\partial F(x,s)/\partial x|_{x=0}$. The latter can be expressed in terms of $F(0,s)$ by invoking the boundary condition in Eq. (41b):

$$R(k,s)=[m(s)-2m_+(s)-ikD(s)]F(0,s)+2\delta(s). \tag{44b}$$

Since $m(s)=m_+(s)-m_-(s)$, we further simplify Eq. (44b) as

$$R(k,s)=-[M(s)+ikD(s)]F(0,s)+2\delta(s), \tag{44c}$$

where we have introduced $M(s)=m_+(s)+m_-(s)$, which is explicitly given by

$$M(s)=\frac{\sqrt{\pi}}{4}\sum_{l(\text{even})=0}^{\infty}\frac{2l+1}{\Gamma(\frac{3}{2}-l/2)\Gamma(2+l/2)}\,e^{-(1/2)\Theta(s)l(l+1)} \tag{45}$$

[see Eqs. (37) and (38b) for $m_+(s)$ and $m_-(s)$]. The substitution of Eq. (44c) into Eq. (42) results in the following inhomogeneous equation:

$$\frac{\partial\overline{F}(k,s)}{\partial s}=-[D(s)k^2+ikm(s)]\overline{F}(k,s)-[M(s)+ikD(s)]F(0,s)+2\delta(s). \tag{46a}$$

We eliminate the singular part of $F(0,s)$ by using $F(0,s)=F_1(0,s)+\delta(s)$ to obtain

$$\frac{\partial\overline{F}(k,s)}{\partial s}=-[D(s)k^2+ikm(s)]\overline{F}(k,s)-[M(s)+ikD(s)]F_1(0,s)+\delta(s). \tag{46b}$$

We should emphasize here that because $x=0$ is to the left of the source located at $x=0^+$, $F_1(0,s)$ is not the limit of $F(x,s)$ as $x\rightarrow 0$ from the right. This discontinuity, which does not arise in ordinary diffusion theory, is due to the fact that $D(s)\rightarrow 0$ rapidly as $s\rightarrow 0$, reflecting the initial ballistic motion of the particles in the modified diffusion equation (39).

The δ function in Eq. (46b) determines the initial condition for $\overline{F}(k,s)$ as $\overline{F}(k,0)=1$, which is consistent with the initial condition $F(x,0)=\delta(x-0^+)$. The solution of Eq. (46b) with this initial condition is then obtained for $s>0$ as

$$\overline{F}(k,s)=\overline{F}_\infty(k,s)-\int_0^s ds'\,\overline{G}_\infty(k;s,s')\times[M(s')+ikD(s')]F_1(0,s'), \tag{47}$$

where

$$\overline{F}_\infty(k,s)=\exp\{-[\tfrac{1}{2}\sigma^2(s)k^2+ik\overline{m}(s)]\}, \tag{48a}$$

and

$$\overline{G}_\infty(k;s,s')=\exp(-\{\tfrac{1}{2}[\sigma^2(s)-\sigma^2(s')]k^2+ik[\overline{m}(s)-\overline{m}(s')]\}), \tag{48b}$$

which is equal to $\overline{F}_\infty(k,s)/\overline{F}_\infty(k,s')$. One can easily verify that $\overline{F}_\infty(k,s)$ is the infinite medium solution of Eq. (39) in Fourier space with the initial condition $\overline{F}_\infty(k,0)=1$, corresponding to a monodirectional unit pulse source of particles at $x=0$. In Eq. (48) we have introduced

$$\overline{m}(s)=\int_0^s ds'\,m(s') \tag{49}$$

and

$$\sigma^2(s)=2\int_0^s ds'\,D(s'). \tag{50}$$

It is clear that $\overline{m}(s)$ is the mean particle position $\langle x(s)\rangle$ of the pulse for the case of an infinite medium, and $\sigma^2(s)$ is the variance $\langle x^2\rangle-\langle x(s)\rangle^2$ of the particle positions for an infinite medium. The properties of this solution were discussed in detail elsewhere [2–4].

The inverse Fourier transform of Eq. (47) gives the semi-finite medium solution as

$$F(x,s)=F_\infty(x,s)-\int_0^s ds'[G_\infty(x;s,s')M(s')+G'_\infty(x;s,s')D(s')]F_1(0,s'), \tag{51}$$

where

$$F_\infty(x,s)=\frac{1}{(2\pi)^{1/2}\sigma(s)}\exp\left\{-\frac{[x-\overline{m}(s)]^2}{2\sigma^2(s)}\right\}, \tag{52a}$$

$$G_\infty(x;s,s')=\frac{1}{(2\pi)^{1/2}[\sigma^2(s)-\sigma^2(s')]^{1/2}}\times\exp\left\{-\frac{\{x-[\overline{m}(s)-\overline{m}(s')]\}^2}{2[\sigma^2(s)-\sigma^2(s')]}\right\}, \tag{52b}$$

and $G'_\infty(x;s,s')=\partial G_\infty(x;s,s')/\partial x$. The $F_1(0,s)$ in Eq. (51) is still unknown.

By evaluating Eq. (51) at $x=0$, we obtain a consistency relation, from which $F_1(0,s)$ can be obtained,

$$F_1(0,s)=F_\infty(0,s)-\int_0^s ds'[G_\infty(0;s,s')M(s')+G'_\infty(0;s,s')D(s')]F_1(0,s'),\quad s>0. \tag{53}$$

Although not in a closed form, Eqs. (51) and (53) express the semi-infinite solution in terms of the known infinite medium solution.

Once $F(x,s)$ is obtained by solving Eqs. (51) and (53), the partial current $J_-(x,s)$ can be obtained from

$$J_-(x,s)=m_-(s)F(x,s)+\frac{1}{2}D(s)\frac{\partial F(x,s)}{\partial x}. \tag{54}$$

The backscattered current $J_{-}(0,s)$ is of particular interest in diffusive wave spectroscopy [6]. Evaluating Eq. (54) at $x=0$, and combining the result with the boundary condition in Eq. (41a), we obtain

$$J_{-}(0,s)=M(s)F(0,s)-\delta(s)=M(s)F_1(0,s), \quad (55)$$

where $M(s)=m_{+}(s)+m_{-}(s)$, and is given in Eq. (45). Thus it is sufficient to solve only the integral equation (53) for $F_1(0,s)$ in order to determine the reflected current $J_{-}(0,s)$.

One can verify, as a consistency check, that

$$\int_0^\infty ds J_{-}(0,s)=1$$

as it should be because only one particle is introduced into the medium initially. Since it is normalized to unity, $J_{-}(0,s)$ is the path length distribution of backscattered photons.

A. Numerical computation of $F(x,s)$

We must first solve the integral equation, Eq. (53), for $F_1(s)=F_1(0,s)$. To do so, we note that $F_1(0)=0$ and interpolate $F_1(s)$ on a grid of s values $\{s_0,s_1,\ldots\}$ using an expansion in a cardinal basis set $C_i(s)$ as

$$F_1(s)\approx\sum_{i=0}^{\infty} F_iC_i(s), \quad (56)$$

where $C_i(s_j)=\delta_{ij}$ and $F_i\approx F_1(s_i)$. Substitution of this expansion into Eq. (53) results in a system of linear equations to solve for the coefficients F_i,

$$F_k=F_\infty(0,s_k)-\sum_{i=0}^{\infty} F_i\int_0^{s_k}ds' K(0;s_k,s')C_i(s'), \quad (57)$$

where

$$K(x;s,s')=G_\infty(x;s,s')\left[M(s')+D(s')\,\frac{\overline{m}(s)-\overline{m}(s')-x}{\sigma^2(s)-\sigma^2(s')}\right] \quad (58)$$

is the kernel from Eq. (51) written in a slightly different form.

If the interpolation functions $C_i(s)$ are selected so that $C_i(s)=0$ for $s<s_i$ then, using $F_1(0)=F_0=0$, the system of equations, i.e., Eq. (57), is lower diagonal, and can be trivially solved for F_k as

$$F_k=\frac{F_\infty(0,s_k)-\sum_{i=1}^{k-1} F_i\int_0^{s_k}ds' K(0;s_k,s')C_i(s')}{1+\int_0^{s_k}ds' K(0;s_k,s')C_i(s')}. \quad (59)$$

Computing F_k for $k=1,2,3,\ldots$ is then simply a matter of numerically computing the values of the integrals

$$\int_0^{s_k}ds' K(0;s_k,s')C_i(s'), \quad k=1,2,\ldots .$$

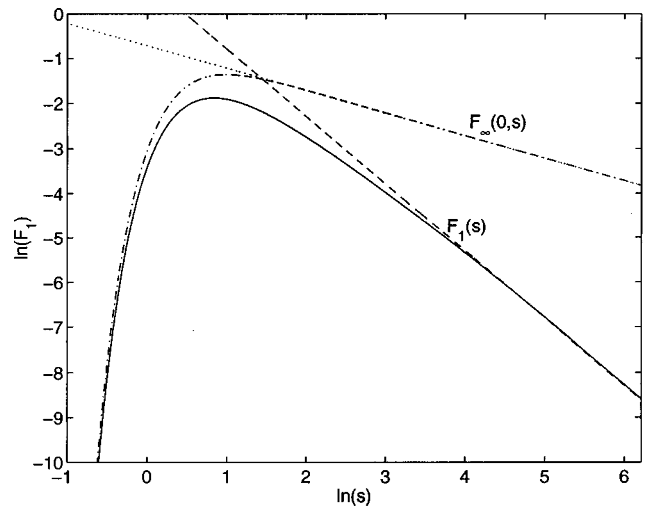

FIG. 2. The nonsingular part of the distribution function, $F_1(s)$, in the finite medium (solid line), compared with the infinite medium solution, $F_\infty(0,s)$ (dashed-dotted line), for path lengths up to $500/\overline{\Sigma}$. The asymptotic behavior of both curves is also indicated by dashed and dotted lines.

Once the F_k are obtained, it is also possible to compute

$$F_1(x,s_k)=F_\infty(x,s_k)-\sum_{i=1}^{k-1} F_i\int_0^{s_k}ds' K(x;s_k,s')C_i(s'), \quad (60)$$

by evaluating some integrals numerically.

We select the piecewise-constant cardinal basis

$$C_i(s)=\begin{cases}1, & s_i\leqslant s<s_{i+1}\\ 0 & \text{otherwise.}\end{cases} \quad (61)$$

This choice leads to a truncation error in the integral equation that is of order $\Delta s^{3/2}$, where $\Delta s=\min_i(s_{i+1}-s_i)$ is the mesh spacing of the grid. The fractional power arises because of the square-root singularity in the kernel as $s'\to s\neq 0$. Because of this truncation error we can afford to approximate the integrals in Eq. (59) with a similar error. This can be done by changing the variable of integration to $\sigma^2(s')$, averaging the regular part of the integrand over an interval $[\sigma^2(s_i),\sigma^2(s_{i+1})]$, and performing the integral of the singular part exactly. Only as $s_i\to 0$ is any care required, but in this limit the exponential goes to zero very rapidly, so there is in fact no difficulty there.

Figure 2 shows the function $F_1(s)=F_1(0,s)$ for $0\leqslant s\leqslant 10$ (solid line); also shown, for comparison, is the function $F_\infty(0,s)$, which is the infinite medium solution, and is given analytically by Eq. (52a). In this figure, and in all that follow, $\overline{\Sigma}$ is taken to be independent of path length, and path length itself is measured in units of $1/\overline{\Sigma}$, and hence unitless. One can show analytically that $F_\infty(s)$ and $F_1(s)$ approach asymptotically to, respectively, $\sqrt{3/4\pi}/s^{1/2}$ and $c/s^{3/2}$ as $s\to\infty$, which are also plotted in the figure with $c\approx 2.04$. The numerical value of c is obtained through curve fitting. It is observed that $F_1(s)$ attains its asymptotic behavior more slowly than $F_\infty(s)$ does.

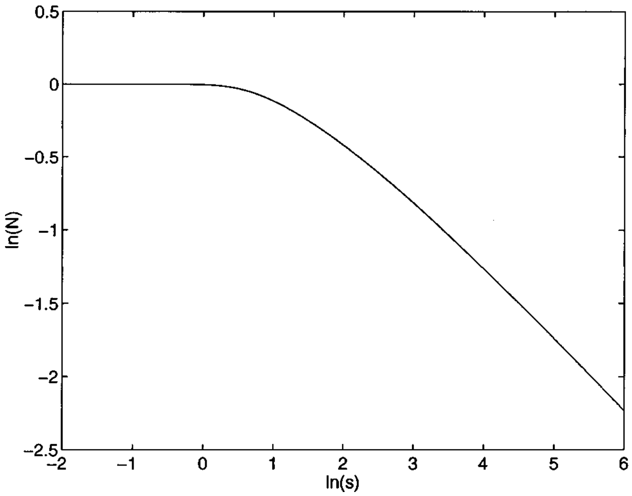

FIG. 3. The variation of the total number of particles $N(s)$ in the medium as a function of the path length s.

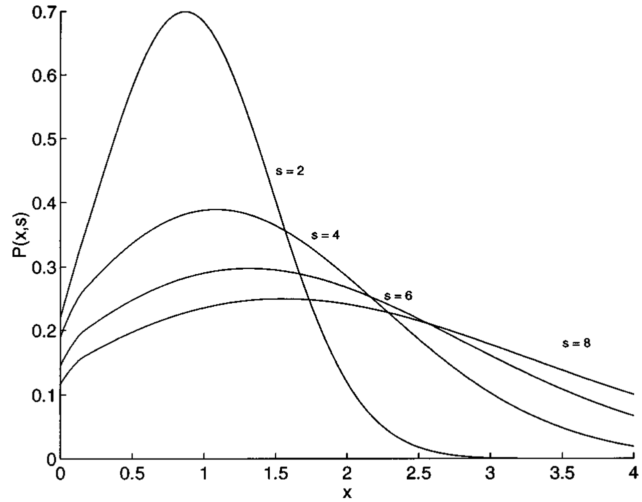

FIG. 4. The variation of the spatial probability distribution, $P(x;s)$ as a function of the distance from the interface for four values of the path length s.

From $F_1(s)$ we can compute all other quantities of interest, such as $F(x,s)$, which is given in Eq. (60), and the probability distribution $P(x;s)$ of finding a particle, which is introduced into the medium at $x=0$ at $s=0$, in a unit interval about x after having traversed a path length s:

$$P(x;s)=\frac{1}{N(s)}F(x,s), \tag{62}$$

where $N(s)$ is the number of particles remaining in the medium at a path length s, i.e.,

$$\begin{aligned} N(s)&=\int_0^\infty dx\; F(x,s)\\ &=1-\int_0^s ds' M(s')F_1(s')\\ &=\int_s^\infty ds' M(s')F_1(s'). \end{aligned} \tag{63}$$

The second line, which expresses $N(s)$ directly in terms of $F_1(s)$, follows from the expression of the outgoing partial current given in Eq. (55). Figure 3 shows a log plot of $N(s)$. In this plot we see that at large path lengths s the number of particles in the system decays algebraically; fitting a line to this data suggests that $N(s)\sim s^{-0.5}$. Using the asymptotic behavior of $M(s)F_1(s)\to c/2s^{3/2}$ for large s in Eq. (63), we indeed find that $N(s)\to c/s^{1/2}$ where $c\approx 2.04$.

The variation of the probability distribution $P(x;s)$ as a function of distance from the interface is presented in Fig. 4 for four values of s. We note in this figure that $\lim_{x\to 0}P(x;s)\neq F_1(0,s)/N(s)$ for small s. This is because of the presence of the pulsed source $\delta(x-0^+)\delta(s)$, the influence of which persists even for $s>0$. [See the comment following Eq. (46b).]

It is also of some interest to compute the mean position of the particles in the medium

$$\langle x\rangle(s)=\int_0^\infty dx\; xP(x;s). \tag{64}$$

This can also be expressed in terms of $F_1(s)$ directly. Multiplying Eq. (39) by x, integrating over x, and evaluating various integrals by parts yields

$$\frac{d}{ds}N(s)\langle x\rangle(s)=m(s)N(s)+D(s)F_1(0,s). \tag{65}$$

In the last term we used $D(s)F(0,s)=D(s)[\delta(s)+F_1(0,s)]=D(s)F_1(0,s)$ and $D(0)=0$. Integration over s, and using $\langle x\rangle(0)=0$ yields

$$\langle x\rangle(s)=\frac{1}{N(s)}\left[\int_0^s ds' m(s')N(s')+\int_0^s ds' D(s')F_1(s')\right]. \tag{66}$$

Figure 5 shows $\langle x\rangle(s)$ as computed from the $F_1(s)$ presented in Fig. 2. We observe from this plot that those particles that remain in the medium penetrate more and more deeply, with their mean position traveling initially at almost the particle speed. Indeed, for small s, the first term in Eq.

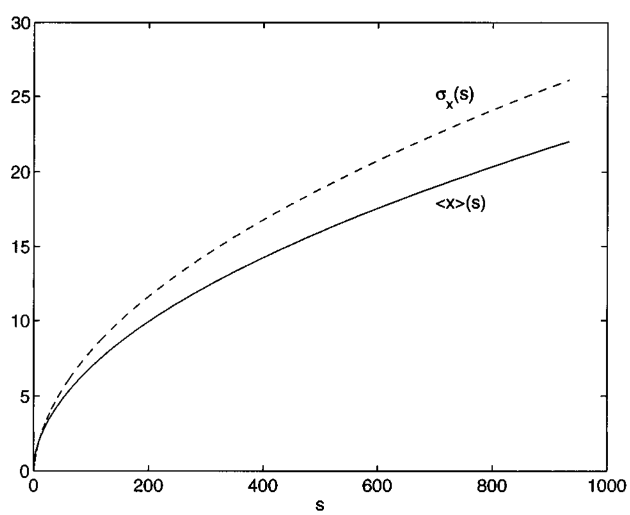

FIG. 5. The variation of the mean particle position $\langle x\rangle(s)$ and the standard deviation $\sigma_x(s)$ with path length s.

(66) dominates, and since $N(s)$ and $m(s)$ tend to unity as $s \to 0$, we obtain $\langle x \rangle(s) \to s$. The behavior of $\langle x \rangle(s)$ for large s can also be determined from Eq. (66): since the integrals on the right hand side are convergent, it is $1/N(s)$ that dictates the asymptotic behavior of $\langle x \rangle(s)$. Hence, one finds $\langle x \rangle(s) \to (K/c)\sqrt{s}$, where

$$K = \int_0^\infty ds\ m(s)N(s) + \int_0^\infty ds\ D(s)F_1(s),$$

and $c \approx 2.04$. This behavior of $\langle x \rangle(s)$ is very different from the mean particle position in an infinite medium solution, which asymptotically approaches $\langle x \rangle = 1$, the penetration distance, as discussed in an earlier paper [2]. This difference is mainly due to the fact that in the finite medium there are very few particles traveling to the left, because those particles quickly leave the medium and cease to contribute to the mean position. It is interesting to note that the first spatial moment of the particle density $F_1(x,s)$, which is equal to $N(s)\langle x \rangle(s)$, approaches the value $K \approx 1.56$.

Figure 5 also shows the variation of the standard deviation $\sigma_x(s) = \{\langle [x - \langle x \rangle(s)]^2 \rangle\},^{1/2}$ as a function of s. The expression of the second moment $\langle x^2 \rangle(s)$ is obtained by multiplying Eq. (39) by x^2, integrating over x, and evaluating various integrals by parts as it was done to obtain Eqs. (65) and (66); the result is

$$\langle x^2 \rangle(s) = \frac{2}{N(s)} \int_0^s ds' [m(s')N(s')\langle x \rangle(s') + D(s')N(s')]. \tag{67}$$

For small s, the first term dominates. Since $N(s)$ and $m(s)$ tend to unity, and $\langle x \rangle(s) \to s$ as $s \to 0$, we find $\langle x^2 \rangle(s) \to s^2$, and $\sigma_x^2(s) \to 0$ in this limit. This is expected because the particles predominantly stream for small s. For large s, the second term in Eq. (67) dominates; this diverges as $4s/3$ because $D(s \to \propto) = \frac{1}{3}$ and $N(s \to \infty) \to c/\sqrt{s}$. Thus, since $\langle x \rangle(s) \to (K/c)\sqrt{s}$ as $s \to \infty$, the variance behaves as $\sigma_x^2(s \to \infty) \to [\frac{4}{3} - (K/c)^2]\ s \approx 0.75s$ implying a diffusion motion of particles about their mean position. The numerical value 0.75 is close to $\frac{2}{3}$, as one expects from the mean square displacement $2Ds$ due to diffusion with the diffusion coefficient $\frac{1}{3}$.

B. Application to diffusive wave spectroscopy

The path length distribution $P(s)$ of the backscattered particles in the absence of absorption in the medium is equal to the outgoing partial current $J_-(0,s)$ at the interface, i.e.,

$$P(s) = M(s)F_1(s). \tag{68}$$

The variation of $P(s)$ with path length is shown in Fig. 6. The probability that a particle will emerge from the medium with a path length less than $s = 0.5$ is virtually zero due to the forwardness of scattering. The probability peaks at about $s = 2.2$ with a value of approximately 0.08, decreases very gradually thereafter, approaching asymptotically to $c/s^{3/2}$. This implies that most of the particles are backscattered after having traversed path lengths larger than $s = 2$. In diffusive wave spectroscopy the measured intensity correlation function is expressed in terms of the Laplace transform of $P(s)$ [6,7]. Figure 7 shows the variation of

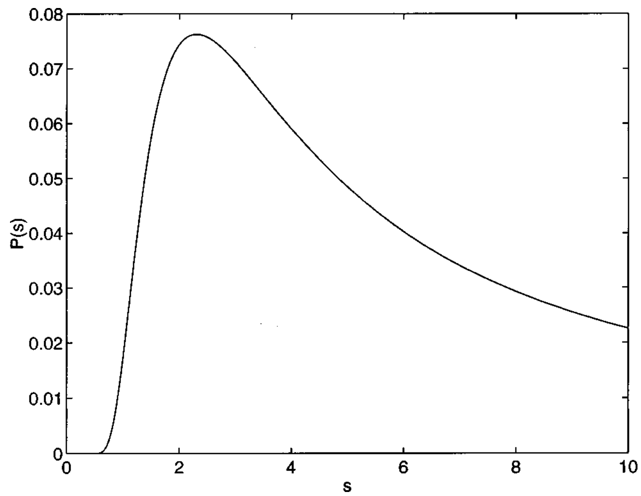

FIG. 6. The variation of the path length distribution of the reflected particles as a function of path length s.

$$g_1(q) = \int_0^\infty ds\ e^{-qs} P(s), \tag{69}$$

with q. One can verify analytically that $g_1(q)$ behaves for small q as

$$g_1(q) \to \frac{e^{-\sqrt{3q}}}{1 + \sqrt{(16/3)q}}. \tag{70}$$

This tendency is indicated in Fig. 7 as the initial slope of $g_1(q)$.

Although the actual light source in an optical measurement is a coherent laser beam, which is uniformly incident on the interface of the medium, the calculation of the path length distribution by using the diffusion theory in diffusive

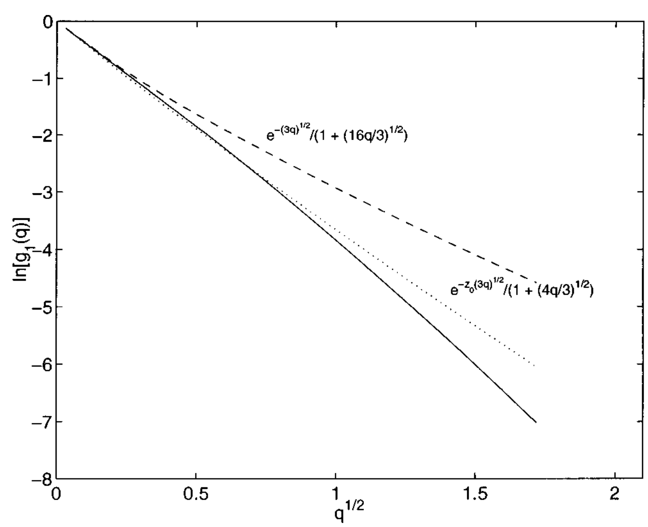

FIG. 7. The variation of $g_1(q)$, the Laplace transform of the path length distribution $P(s)$, with the Laplace variable q (solid curve). The dotted curve shows $g_1(q)$ as calculated with the diffusion theory assuming a fictitious isotropic plane light source located at $z_0 = 1.67$ from the interface in the medium.

wave spectroscopy assumes a fictitious isotropic light source located at some distance z_0 inside the *sample*. The value of z_0 is taken to be approximately the transport mean free path to allow the coherent light entering the medium to become diffusive as a result of a sufficient number of collisions. When the reflection of the photons from inside at the interface back into the medium is neglected, the diffusion theory yields [6,7] the following expression for $g_1(q)$:

$$g_1(q)\to\frac{e^{-z_0\sqrt{3q}}}{1+\sqrt{(4/3)q}}\quad\text{(diffusion theory)}. \tag{71}$$

By matching the initial slope $-[z_0+(\frac{2}{3})]\sqrt{3}$ of this expression to $-[1+(\frac{4}{3})]\sqrt{3}$ of Eq. (70), we obtain $z_0=1+(\frac{2}{3})=1.67$.

The comparison of the results for $g_1(q)$, obtained with the modified diffusion theory developed in this paper, and those obtained with the diffusion theory are shown in Fig. 7. The difference is due to the fact that the modified diffusion theory treats the transition from the initial coherent behavior to the diffusive regime more accurately than traditional diffusion theory with an isotropic source inside the medium. We do not pursue this point any further, because we intend to apply the modified diffusion theory to a slab sample with finite thickness, and investigate the angular dependence of the intensity correlation function of the reflected light at the front surface, as well as that of transmitted light as a function of the slab thickness in a separate publication.

V. DISCUSSIONS AND CONCLUSIONS

Once $F(\mathbf{x},s)$ is obtained approximately by solving the modified diffusion equation (25) in a specified geometry with the appropriate boundary conditions, we can construct the full solution of the original Fokker-Planck equation (1) for the energy-dependent angular number density, $n(\mathbf{x},E,\mathbf{\Omega},t)$, by substituting the expansion of $f(\mathbf{x},\mathbf{\Omega},s)$ in Eq. (12) into Eq. (6a):

$$n(\mathbf{x},E,\mathbf{\Omega},s)=\delta(E-\mathcal{E}(s))p(s)\times\left[P(\mathbf{\Omega},s)F(\mathbf{x},s)+\frac{3}{4\pi}\mathbf{J}_D(\mathbf{x},s)\cdot\mathbf{\Omega}\right], \tag{72}$$

where the functions $\mathcal{E}(s)$, $p(s)$, $P(\mathbf{\Omega},s)$, and $\mathbf{J}_D(\mathbf{x},s)$ are given, respectively, by Eqs. (7b), (6b), (15a), and (27). The energy-dependent number density and the particle current are obtained from Eq. (72) as

$$n(\mathbf{x},E,s)=\delta(E-\mathcal{E}(s))p(s)F(\mathbf{x},s), \tag{73a}$$

$$\mathbf{J}(\mathbf{x},E,s)=\delta(E-\mathcal{E}(s))p(s)v(s)[\langle\mathbf{\Omega}(s)\rangle F(\mathbf{x},s)+\mathbf{J}_D(\mathbf{x},s)]. \tag{73b}$$

The partial currents along a direction $\hat{\mathbf{n}}$ follow as

$$J_{\pm}^{\hat{\mathbf{n}}}(\mathbf{x},E,s)=\delta[E-\mathcal{E}(s)]p(s)v(s)\times[\langle\hat{\mathbf{n}}\cdot\mathbf{\Omega}(s)\rangle_{\pm}F(\mathbf{x},s)\pm\tfrac{1}{2}\hat{\mathbf{n}}\cdot\mathbf{J}_D(\mathbf{x},s)], \tag{73c}$$

where $\langle\hat{\mathbf{n}}\cdot\mathbf{\Omega}(s)\rangle_{\pm}$ are given by Eqs. (37) and (38b). In particular, the reflected current in the case of the semi-infinite medium as discussed in Sec. IV is obtained from Eq. (12) as

$$\mathbf{J}_{-}(0,E,s)=\delta[E-\mathcal{E}(s)]p(s)v(s)M(s)F_1(0,s). \tag{74}$$

We plan to use these results, in the future, to calculate the path length distribution of reflected photons, which enters in the interpretation of the intensity correlation function of the reflected light in diffusive wave spectroscopy.

The weak-coupling expansion described in this paper is also applicable to the one-speed transport equation:

$$\frac{\partial}{\partial s}n(\mathbf{x},\mathbf{\Omega},s)+\varepsilon\mathbf{\Omega}\cdot\mathbf{\nabla}n=-\Sigma_t n+\int d\mathbf{\Omega}'\Sigma_s(\mathbf{\Omega}\cdot\mathbf{\Omega}')n(\mathbf{x},\mathbf{\Omega}',s), \tag{75}$$

where $s=vt$ is the path length, and $\Sigma_t=\Sigma_{a+}\Sigma_s$. The approximate solution can be constructed as in Eq. (72),

$$n(\mathbf{x},\mathbf{\Omega},s)=p(s)\left[P(\mathbf{\Omega},s)F(\mathbf{x},s)+\frac{3}{4\pi}\mathbf{J}_D(\mathbf{x},s)\cdot\mathbf{\Omega}\right], \tag{76}$$

where $p(s)=\exp[-\Sigma_a s]$, and $P(\mathbf{\Omega},s)$ is the solution of

$$\frac{\partial}{\partial s}P(\mathbf{\Omega},s)=-\Sigma_s P(\mathbf{\Omega},s)+\int d\mathbf{\Omega}'\Sigma_s(\mathbf{\Omega}\cdot\mathbf{\Omega}')P(\mathbf{\Omega}',s) \tag{77}$$

instead of Eq. (14). This is the only difference between the Fokker-Planck and the one-speed transport descriptions. Whereas the exact solution of Eq. (14) is available in a closed form, as presented in Eq. (15a), an analytical solution of Eq. (77) is not readily forthcoming. However, we can still obtain the first and second moments of $P(\mathbf{\Omega},s)$ in terms of the Legendre polynomial expansion of $\Sigma_s(\mathbf{\Omega}\cdot\mathbf{\Omega}')$ [4]. For example, the mean follows from Eq. (77) as

$$\frac{d\langle\mathbf{\Omega}(s)\rangle}{ds}=-\bar{\Sigma}\langle\mathbf{\Omega}(s)\rangle,$$

where $\bar{\Sigma}=\Sigma_s[1-\langle\mu\rangle]$.

In this case the number density $F(\mathbf{x},s)$ still satisfies the same modified diffusion equation [see Eq. (25)] as in the case of Fokker-Planck description:

$$\frac{\partial F(\mathbf{x},s)}{\partial s}=-\langle\mathbf{\Omega}(s)\rangle\cdot\frac{\partial F}{\partial\mathbf{x}}+\mathbf{\nabla}\cdot\mathbf{D}(s)\cdot\mathbf{\nabla}F. \tag{78}$$

Since the solution of this equation in an infinite medium is Gaussian, the approximation inherent in this equation, i.e., keeping the terms up to second order in the coupling parameter ε, is referred to as the Gaussian approximation in Ref. [4], and introduced as a model in the moment method.

When the scattering is forwardly peaked, the one-speed transport approach reduces to the Fokker-Planck description. However, the latter description takes into account energy degradation in scattering in the continuous slowing-down approximation.

In the limit of isotropic scattering, we expect the small-coupling approximation, based on Eq. (78), to be not as accurate as the ordinary diffusion approximation with the first collision distributed source representing the effect of the initial monodirectional beam.

In conclusion, the Fokker-Planck description in finite media with the weak-coupling expansion seems to be well suited to the study of electron and photon transport, especially near boundaries when the scattering is forwardly peaked.

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