Cumulant solution of the elastic Boltzmann transport equation in an infinite uniform medium

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We consider an analytical solution of the time-dependent elastic Boltzmann transport equation in an infinite uniform isotropic medium with an arbitrary phase function. We obtain (1) the exact distribution in angle, (2) the exact first and second spatial cumulants at any angle, and (3) an approximate combined distribution in position and angle and a spatial distribution whose central position and half-width of spread are always exact. The resulting Gaussian distribution has a center that advances in time, and an ellipsoidal contour that grows and changes shape providing a clear picture of the time evolution of the particle migration from near ballistic, through snakelike and into the final diffusive regime.

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I. INTRODUCTION

Scientists have tried for decades to develop exact or accurate analytical approximate solutions of the Boltzmann transport equation in various cases [1–3]. Any progress in this direction is a contribution to fundamental research in non-equilibrium statistical dynamics. An accurate analytical approximation may have applications in a broad range of fields, such as the atmosphere, medicine, and solid state physics. Photon migration in a highly scattering turbid medium is a good example. The solution of inverse problems in optical tomography, such as the location of a tumor in a woman's breast from the scattering of light pulses, requires the inversion of a weight matrix [4] obtained by convoluting two Green's functions of the forward scattering problem. The analytical solution of the photon diffusive equation in an infinite uniform medium has been broadly used as a background Green's function [4]. By introducing ''image sources,'' the solution can be extended to semi-infinite, slabs, and boxes geometry. The diffusion approximation fails at early times when the photon distribution is highly anisotropic. Solutions of the diffusion equation or the telegrapher's equation do not produce the correct ballistic limit of light propagation [5]. The Monte Carlo method can be used to simulate photon migration at early times; however, detailed solution of a five-dimensional Boltzmann transport equation using a predominately numerical approach, with the resolution good enough to check the analytical solution, leads to prohibitive CPU times.

Recently, Polishchuk *et al.* [6] and Perelman *et al.* [7] suggested different models of photon migration. They used the path integral approach and the time-dependent Green's function method to treat the photon migration problem. They consider only multiple small-angle scattering, based on the fact that the phase function (angular distribution of the scattering cross section) in many media has a very sharp forward peak. A solution of the steady transport equation based on the small angle approximation was also presented by Ishimaru [8]. However, it can be shown that the transport mean free path obtained by an average of $1-\cos\theta$ over small angles could be several times larger than that obtained by an average over all angles. Thus, the small angle scattering approximation is not quantitatively correct. Therefore, a procedure permitting wide-angle scattering is essential.

In this paper, we present analytical expressions for the distribution function and the density distribution of the solution of the elastic Boltzmann transport equation in an infinite uniform medium. The phase function is assumed to depend only on the scattering angle $P(\mathbf{s},\mathbf{s}_0)=P(\mathbf{s}\cdot\mathbf{s}_0)$. Under this assumption, the small angle approximation is avoided, and an arbitrary phase function can be handled. Our solution for the distribution in angle is exact, as are all first and second spatial cumulants at any angle as functions of time. After many scattering events have taken place, the central limit theorem guarantees that the spatial Gaussian distribution calculated will become accurate in detail, all cumulants higher than the second approach small values relative to the approximate power of the second cumulant. At early times, when the errors would be worst, the spatial distribution function at any angle is quantitatively accurate in the sense that it has the exact mean position (the first cumulant) and the exact and narrow half-width of spread (the second cumulant) as a function of time. Since the inverse scattering problem is done with instruments of finite resolution, in the presence of noise, finer detail is lost, and the first two cumulants may provide an adequate description of the scattered beam.

This paper is organized as follows. Section II describes the derivation of the formula, which includes (1) obtaining an exact solution of the distribution in angle, (2) obtaining an exact formal solution in position and angle, (3) using the cumulant approximation up to the second order that leads to a Gaussian spatial distribution, (4) obtaining exact first and second spatial cumulants based on the exact angular distribution. Section III provides the main results of the distribution function in position and angle, and the density distribution in position alone. Section IV makes a comparison of our result for the special case of isotropic scattering with that of the exact solution provided by Hauge [9]. A discussion of the effectiveness of the cumulant approximation is presented in Sec. V.

II. DERIVATION

Without loss of generality, we discuss the photon scattering problem with a given light speed in the medium c. Applying our result to an another particle elastic scattering problem, with the constant particle speed in the medium v is straightforward. The photon distribution function $I(\mathbf{r},\mathbf{s},t)$ as a function of time t, position $\mathbf{r}$ and direction $\mathbf{s}$, in an infinite uniform medium, from a point pulse light source $\delta(\mathbf{r}-\mathbf{r}_0)\delta(\mathbf{s}-\mathbf{s}_0)\delta(t-0)$ obeys the Boltzmann equation [3]

$$\begin{aligned}\partial I(\mathbf{r},\mathbf{s},t)/\partial t+c\mathbf{s}\cdot\nabla_{\mathbf{r}}I(\mathbf{r},\mathbf{s},t)+\mu_a I(\mathbf{r},\mathbf{s},t)\\ =\mu_s\int P(\mathbf{s},\mathbf{s}')[I(\mathbf{r},\mathbf{s}',t)-I(\mathbf{r},\mathbf{s},t)]d\mathbf{s}'\\ +\delta(\mathbf{r}-\mathbf{r}_0)\delta(\mathbf{s}-\mathbf{s}_0)\delta(t-0),\end{aligned}\tag{1}$$

where μ_s is the scattering rate, μ_a is the absorption rate, and $P(\mathbf{s}',\mathbf{s})$ is the phase function, normalized to $\int d\mathbf{s}'P(\mathbf{s}',\mathbf{s})=1$. When the phase function depends only on the scattering angle in an isotropic medium, we can expand the latter in Legendre polynomials

$$P(\mathbf{s},\mathbf{s}')=\frac{1}{4\pi}\sum_l a_l P_l(\mathbf{s}\cdot\mathbf{s}'),\tag{2}$$

and regard a_l as known, either from Mie theory [10], or a preliminary experiment.

We first study the dynamics of the photon distribution in the light direction space $F(\mathbf{s},\mathbf{s}_0,t)$, on a spherical surface for $\mathbf{s}$ of radius 1, which is equivalent to the velocity space in the elastic scattering case. The kinetic equation for $F(\mathbf{s},\mathbf{s}_0,t)$ can be obtained by integrating Eq. (1) over the whole space $\mathbf{r}$. The spatial independence of μ_s, μ_a, and $P(\mathbf{s},\mathbf{s}')$ retains translation invariance. Thus the integral of Eq. (1) obeys

$$\begin{aligned}\partial F(\mathbf{s},\mathbf{s}_0,t)/\partial t+\mu_a F(\mathbf{s},\mathbf{s}_0,t)\\ +\mu_s\left[F(\mathbf{s},\mathbf{s}_0,t)-\int P(\mathbf{s},\mathbf{s}')F(\mathbf{s}',\mathbf{s}_0,t)d\mathbf{s}'\right]\\ =\delta(\mathbf{s}-\mathbf{s}_0)\delta(t-0).\end{aligned}\tag{3}$$

Since the integral of the gradient term over all-space vanishes, in contrast to Eq. (1), if we expand $F(\mathbf{s},\mathbf{s}_0,t)$ in spherical harmonics, its components do not couple with each other. Therefore, it is easy to obtain the exact solution of Eq. (3) [11]:

$$F(\mathbf{s},\mathbf{s}_0,t)=\sum_l \frac{2l+1}{4\pi}\exp(-g_l t)P_l(\mathbf{s}\cdot\mathbf{s}_0)\exp(-\mu_a t),\tag{4}$$

where $g_l=\mu_s[1-a_l/(2l+1)]$. Two special values of g_l are $g_0=0$, which follows from the normalization of $P(\mathbf{s},\mathbf{s}')$ and $g_1=c/l_t$, where l_t is the transport mean free path, defined by $l_t=c/[\mu_s(1-\overline{\cos\theta})]$, where $\overline{\cos\theta}$ is the average of $\mathbf{s}\cdot\mathbf{s}'$ with $P(\mathbf{s},\mathbf{s}')$ as weight. Equation (4) serves as the exact Green's function of light propagation in the velocity (or angular) space. Since in an infinite uniform medium this function is independent of the source position $\mathbf{r}_0$, requirements for a Green's function are satisfied, especially, a Chapman-Kolmogorov condition is obeyed: $\int d\mathbf{s}'F(\mathbf{s}'',\mathbf{s}',t-t')F(\mathbf{s}',\mathbf{s},t'-t_0)=F(\mathbf{s}'',\mathbf{s},t-t_0)$. In fact, in an infinite uniform medium, this propagator determines all behavior of light migration, including its spatial distribution, because displacement is an integration of velocity over time. The photon distribution function $I(\mathbf{r},\mathbf{s},t)$, for the initial source direction $\mathbf{s}_0$ and the source position $\mathbf{r}_0=0$, is given by

$$I(\mathbf{r},\mathbf{s},t)=\left\langle \delta\left[\mathbf{r}-c\int_0^t \mathbf{s}(t')dt'\right]\delta[\mathbf{s}(t)-\mathbf{s}]\right\rangle,\tag{5}$$

where the angle brackets denote the ensemble average in the velocity space. The first δ function insures that the displacement, $\mathbf{r}-0$, is given by the path integral. The second δ function assures the correct final value of direction. Equation (5) is a formally exact solution, but can not be evaluated directly. We, hence, make a Fourier transform for the first δ function in Eq. (5) and make a cumulant expansion to the second order [12]. For an arbitrary random variable,

$$\langle e^A\rangle\approx\exp(\langle A\rangle)\exp(\langle A^2\rangle_c/2),\tag{6}$$

where index c denotes cumulant: $\langle A^2\rangle_c=\langle A^2\rangle-\langle A\rangle\langle A\rangle$. An exact result is valid only if A is Gaussian. In the following $\langle B\rangle_c$ is called the cumulant of B, while $\langle B\rangle$ is called the moment of B. Substituting this approximation into the Fourier transform of Eq. (5), we have

$$\begin{aligned}I(\mathbf{r},\mathbf{s},t)=F(\mathbf{s},\mathbf{s}_0,t)\frac{1}{(2\pi)^3}\int d\mathbf{k}\\ \times\exp\Bigg(ik_\alpha\left(r_\alpha-c\left\langle\int_0^t dt' s_\alpha(t')\right\rangle\right)\\ -\frac{1}{2}k_\alpha k_\beta c^2\left\{\left\langle\int_0^t dt'\int_0^t dt'' T[s_\alpha(t')s_\beta(t'')]\right\rangle\right.\\ \left.-\left\langle\int_0^t dt' s_\alpha(t')\right\rangle\left\langle\int_0^t dt' s_\beta(t')\right\rangle\right\}\Bigg),\end{aligned}\tag{7}$$

where T denotes time-ordered multiplication [13]. Integration over $\mathbf{k}$ in Eq. (7) directly leads to a Gaussian spatial distribution displayed in Eq. (10) below. Using a standard time-dependent Green's function approach, the ensemble average of the cumulants in Eq. (7) can be calculated. The components of the first cumulant, which is the average center position of the distribution, conditioned on $\mathbf{s}=\mathbf{s}_0$ at $t=0$ are given by

$$\begin{aligned}\left\langle\int_0^t dt' s_\alpha(t')\right\rangle=\frac{1}{F(\mathbf{s},\mathbf{s}_0,t)}\int_0^t dt'\int d\mathbf{s}'F(\mathbf{s},\mathbf{s}',t-t')\\ \times s'_\alpha F(\mathbf{s}',\mathbf{s}_0,t').\end{aligned}\tag{8}$$

The denominator appears because this is a conditional average. The components of the second moment, which is related to the second cumulant (average half-width of spread) of the distribution, conditioned on $\mathbf{s}=\mathbf{s}_0$ at $t=0$ are given by

$$\left\langle \int_0^t dt' \int_0^t dt'' T[s_\alpha(t')s_\beta(t'')] \right\rangle$$
$$= \frac{1}{F(\mathbf{s},\mathbf{s}_0,t)} \left\{ \int_0^t dt' \int_0^{t'} dt'' \int d\mathbf{s}' \times \int d\mathbf{s}'' F(\mathbf{s},\mathbf{s}',t-t') s'_\alpha F(\mathbf{s}',\mathbf{s}'',t'-t'') \times s''_\beta F(\mathbf{s}'',\mathbf{s}_0,t'') + (\text{t.c.}) \right\}, \tag{9}$$

where (t.c.) means the second term is obtained by exchanging the index α and β in the first term. Equation (7) is the only approximate formula used in our derivation. Formula for calculating the first two moments, Eqs. (8) and (9), are exact. In Eqs. (8) and (9), $F(\mathbf{s}_2,\mathbf{s}_1,t)$ is given by Eq. (4). Since Eq. (4) is exact, Eqs. (8) and (9) provide the exact first and second moments. Integrations in Eqs. (8) and (9) are tedious, but straightforward.

III. RESULTS

In the following, we set $\mathbf{s}_0$ along the z direction and denote $\mathbf{s}$ as (θ, ϕ). Our cumulant approximation to the photon distribution function is given by

$$I(\mathbf{r},\mathbf{s},t) = \frac{F(\mathbf{s},\mathbf{s}_0,t)}{(4\pi)^{3/2}} \frac{1}{(\det B)^{1/2}} \exp\left[-\frac{1}{4}(B^{-1})_{\alpha\beta} \times (r-r^c)_\alpha (r-r^c)_\beta \right], \tag{10}$$

with the center of the packet (the first cumulant), denoted by $\mathbf{r}^c$, located at

$$r_z^c = G \sum_l A_l P_l(\cos\theta)[(l+1)f(g_l-g_{l+1}) + l f(g_l-g_{l-1})], \tag{11a}$$

$$r_x^c = G \sum_l A_l P_l^{(1)}(\cos\theta)(\cos\phi) \times [f(g_l-g_{l-1}) - f(g_l-g_{l+1})], \tag{11b}$$

where $G = c\exp(-\mu_a t)/F(\mathbf{s},\mathbf{s}_0,t), A_l = (1/4\pi)\exp(-g_l t), g_l$ is defined after Eq. (4), and

$$f(g) = [\exp(gt)-1]/g. \tag{12}$$

r_y^c is obtained by replacing $\cos\phi$ in Eq. (11b) by $\sin\phi$.

As an example, we derive Eq. (11a) as follows:

$$r_z^c = \frac{c}{F(\mathbf{s},\mathbf{s}_0,t)} \int_0^t dt' \int d\mathbf{s}' F(\mathbf{s},\mathbf{s}',t-t') s'_z F(\mathbf{s}',\mathbf{s}_0,t'),$$

where $F(\mathbf{s}_2,\mathbf{s}_1,t)$ is given by Eq. (4). We denote $\mathbf{s} = [s_x,s_y,s_z] = [\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta]$. The spherical harmonics addition theorem is given by [14]

$$P_l(\mathbf{s}_1\cdot\mathbf{s}_2) = \sum_m \frac{\eta_m(l-m)!}{(l+m)!} P_l^{(m)}(\cos\theta_1) P_l^{(m)} \times (\cos\theta_2)\cos[m(\phi_1-\phi_2)], \tag{13}$$

where $\eta_0 = 1$ and $\eta_m = 2 (m>0)$, $P_l^{(m)}(\cos\theta)$ is the associated Legendre function. The recurrence relations of the spherical harmonics is given by

$$\cos\theta' P_l^{(m)}(\cos\theta') = \frac{1}{2l+1}[(l-m+1)P_{l+1}^{(m)}(\cos\theta') + (l+m)P_{l-1}^{(m)}(\cos\theta')]. \tag{14a}$$

$$\sin\theta' P_l^{(m)}(\cos\theta') = \frac{1}{2l+1}[P_{l+1}^{(m+1)}(\cos\theta') - P_{l-1}^{(m+1)}(\cos\theta')]. \tag{14b}$$

The orthogonality relation of the spherical harmonics is

$$\int_{-1}^1 d\cos\theta' P_l^{(m)}(\cos\theta') P_{l'}^{(m)}(\cos\theta') = \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{ll'}. \tag{15}$$

Using Eqs. (13)–(15) and making integrations, first over ϕ', then over θ', and last over t', Eq. (11a) is obtained. Using a similar procedure, all results in this section were obtained.

The square of the average spread width (the second cumulant) is determined by

$$B_{\alpha\beta} = cG\Delta_{\alpha\beta} - r_\alpha^c r_\beta^c/2, \tag{16}$$

with

$$\Delta_{zz} = \sum_l A_l P_l(\cos\theta)\left[\frac{l(l-1)}{2l-1}E_l^{(1)} + \frac{(l+1)(l+2)}{2l+3}E_l^{(2)} + \frac{l^2}{2l-1}E_l^{(3)} + \frac{(l+1)^2}{2l+3}E_l^{(4)} \right]. \tag{17a}$$

$$\Delta_{xx,yy} = \sum_l \frac{1}{2} A_l P_l(\cos\theta)\left[-\frac{l(l-1)}{2l-1}E_l^{(1)} - \frac{(l+1)(l+2)}{2l+3}E_l^{(2)} + \frac{l(l-1)}{2l-1}E_l^{(3)} + \frac{(l+1)(l+2)}{2l+3}E_l^{(4)} \right] \pm \sum_l \frac{1}{2} A_l P_l^{(2)}(\cos\theta) \times \cos(2\phi)\left[\frac{1}{2l-1}E_l^{(1)} + \frac{1}{2l+3}E_l^{(2)} - \frac{1}{2l-1}E_l^{(3)} - \frac{1}{2l+3}E_l^{(4)} \right], \tag{17b}$$

where $(+)$ corresponds to Δ_{xx} and $(-)$ corresponds to Δ_{yy},

$$\Delta_{xy}=\Delta_{yx}=\sum_l \frac{1}{2}A_l P_l^{(2)}(\cos\theta)\sin(2\phi)\left[\frac{1}{2l-1}E_l^{(1)}+\frac{1}{2l+3}E_l^{(2)}-\frac{1}{2l-1}E_l^{(3)}-\frac{1}{2l+3}E_l^{(4)}\right], \tag{17c}$$

$$\Delta_{xz}=\Delta_{zx}=\sum_l \frac{1}{2}A_l P_l^{(1)}(\cos\theta)(\cos\phi)\left[\frac{2(l-1)}{2l-1}E_l^{(1)}-\frac{2(l+2)}{2l+3}E_l^{(2)}+\frac{1}{2l-1}E_l^{(3)}+\frac{1}{2l+3}E_l^{(4)}\right]. \tag{17d}$$

Δ_{yz} is obtained by replacing $\cos\phi$ in Eq. (17d) by $\sin\phi$. In Eqs. (17a)–(17d)

$$E_l^{(1)}=[f(g_l-g_{l-2})-f(g_l-g_{l-1})]/(g_{l-1}-g_{l-2}), \tag{18a}$$

$$E_l^{(2)}=[f(g_l-g_{l+2})-f(g_l-g_{l+1})]/(g_{l+1}-g_{l+2}), \tag{18b}$$

$$E_l^{(3)}=[f(g_l-g_{l-1})-t]/(g_l-g_{l-1}), \tag{18c}$$

$$E_l^{(4)}=[f(g_l-g_{l+1})-t]/(g_l-g_{l+1}). \tag{18d}$$

A cumulant approximate expression for the photon density distribution is obtained from $N(\mathbf{r},t) =\langle \delta[\mathbf{r}-c\int_0^t \mathbf{s}(t')dt']\rangle$, where an average over the angular distribution is required. Using $\int d\mathbf{s}F(\mathbf{s},\mathbf{s}',t)=\exp(-\mu_a t)$, we have a Gaussian shape

$$N(\mathbf{r},t)=\frac{1}{(4\pi D_{zz}ct)^{1/2}}\frac{1}{4\pi D_{xx}ct}\exp\left[-\frac{(z-R_z)^2}{4D_{zz}ct}\right]\times\exp\left[-\frac{(x^2+y^2)}{4D_{xx}ct}\right]\exp(-\mu_a t), \tag{19}$$

with a moving center located at

$$R_z=c[1-\exp(-g_1 t)]/g_1 \tag{20}$$

and the corresponding diffusion coefficients are given by

$$D_{zz}=\frac{c}{3t}\left\{\frac{t}{g_1}-\frac{3g_1-g_2}{g_1^2(g_1-g_2)}[1-\exp(-g_1 t)]+\frac{2}{g_2(g_1-g_2)}[1-\exp(-g_2 t)]-\frac{3}{2g_1^2}[1-\exp(-g_1 t)]^2\right\}, \tag{21a}$$

$$D_{xx}=D_{yy}=\frac{c}{3t}\left\{\frac{t}{g_1}+\frac{g_2}{g_1^2(g_1-g_2)}[1-\exp(-g_1 t)]-\frac{1}{g_2(g_1-g_2)}[1-\exp(-g_2 t)]\right\}. \tag{21b}$$

In contrast to Eqs. (11) and (17), these results are independent of g_l for $l>2$. Figure 1 shows the moving center of photons, R_z [Eq. (20)], and the diffusion coefficients, D_{zz} and D_{xx} [Eqs. (21)], as function of time, where g_l are calculated by Mie theory [10] assuming (for this figure) water droplets with $r/\lambda=1$ are uniformly distributed in air, with r the radius of the droplet, λ the wavelength of light, and the index of refraction $m=1.33$.

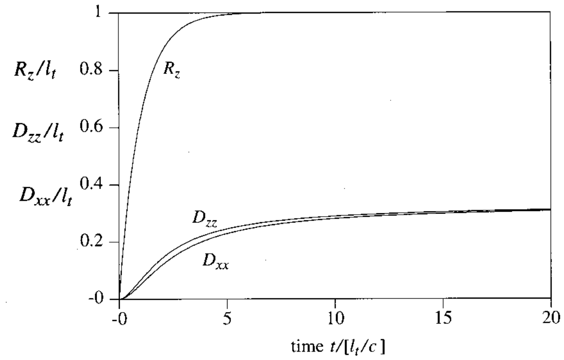

FIG. 1. The moving center of photon density function R_z [Eq. (20)] and the diffusion coefficients D_{zz} and D_{xx} [Eqs. (21)], as a function of time t.

Each distribution in Eq. (10) and Eq. (19) describes a photon ''cloud'' anisotropically spreading from a moving center, with time-dependent diffusion coefficients. At early time $t\to 0$, $f(g)\approx t+O(t^2)$ in Eq. (12), and $E_l^{(j)}=t^2/2+O(t^3)$ for $j=1,2,3,4$ in Eqs. (18). From Eqs. (11), Eqs. (17), and Eqs. (20) and (21), we see that for the density distribution, $N(\mathbf{r},t)$, and the dominant distribution function, that is $I(\mathbf{r},\mathbf{s},t)$ along $\mathbf{s}=\mathbf{s}_0$, the center moves as $ct\,\mathbf{s}_0$ and the $B_{\alpha\beta}$ in Eq. (16) are proportional to t^3 at $t\to 0$. A distribution function $I(\mathbf{r},\mathbf{s},t)$ along $\mathbf{s}\neq\mathbf{s}_0$ is small since $F(\mathbf{s},\mathbf{s}_0,t)\sim t$ when $t\to 0$. Its center moves at a certain direction with displacement proportional to ct, and the $B_{\alpha\beta}$ in Eq. (16) are proportional to t^2 at $t\to 0$. These results present a clear picture of nearly ballistic motion at $t\to 0$. Roughly speaking, this near ballistic motion maintains its speed up to $R_z\approx 0.6 l_t$ [see Eq. (20)]. This closely agrees with experimental results of optical coherent tomography (OCT) [15] that the range of good resolution extends to about 600 μm, in a tissue of $l_t\sim 1$ mm. With increase of time, the motion of the center slows down, and the diffusion coefficients increase from zero. This stage of photon migration is often called a ''snakelike mode.''

With further increase in time, the lth Legendre component in Eqs. (4), (11), and (17), exponentially decay with a rate related to g_l. The detailed decay rate, g_l, is determined by the shape of the phase function. Generally speaking, the very high lth components decays in a rate of order of μ_s, as long as its Legendre coefficient a_l distinctly smaller than $2l+1$. Even in the case that the phase function has a very sharp forward peak, in which there are nonzero a_l for very high lth rank, the a_l are, usually, much smaller than $2l+1$. Therefore, for the distribution function at time t after the ballistic stage is over, a truncation in the summation over l is available.

At large times, the distribution function tends to become isotropic. From Eqs. (19)–(21), the photon density, at $t\gg l_t/c$ and $r\gg l_t$, tends towards the conventional diffusion solution with the diffusive coefficient $l_t/3$. Therefore, our solution quantitatively describes how the photon migrates from nearly ballistic motion to diffusive motion.

IV. COMPARISON WITH AN EXACT SOLUTION IN THE ISOTROPIC SCATTERING CASE

A check of our angular distribution, Eq. (4), the first moments, Eq. (11), and the second moments, Eq. (17), for a special case of isotropic scattering is performed by comparing with the exact solution given by Hauge [9] and agreement is verified. Hauge has provided an exact solution for isotropic scattering in the form of a Fourier transform in space and Laplace transform in time, which is given by

$$I_{\mathbf{k}\zeta}(\mathbf{s})\equiv\int_0^\infty dt e^{-\zeta t}\int d\mathbf{r}e^{-i\mathbf{k}\cdot\mathbf{r}}I(\mathbf{r},\mathbf{s},t), \tag{22}$$

with

$$I_{\mathbf{k}\zeta}(\mathbf{s})=\frac{\mu}{\zeta+\mu+i\mathbf{k}\cdot c\mathbf{s}}\left[1-\frac{\mu}{|\mathbf{k}|c}\tan^{-1}\frac{|\mathbf{k}|c}{\zeta+\mu}\right]^{-1}$$
$$\times\frac{1}{4\pi}\,\frac{1}{\zeta+\mu+i\mathbf{k}\cdot c\mathbf{s}_0}+\frac{\delta(\mathbf{s}-\mathbf{s}_0)}{\zeta+\mu+i\mathbf{k}\cdot c\mathbf{s}_0}. \tag{23}$$

In order to compare, we set $\mu_a=0$ and $\mu_s\equiv\mu$ in this paper. In the case of isotropic scattering, $g_0=0$, and $g_l=\mu$, $l=1,2,\ldots$.

Equation (4) in the isotropic scattering case, reduces to

$$F(\mathbf{s},\mathbf{s}_0,t)=\frac{1}{4\pi}[1-e^{-\mu t}]+e^{-\mu t}\delta(\mathbf{s}-\mathbf{s}_0). \tag{24}$$

Its Laplace transform in time is given by

$$\mathcal{L}[F(\mathbf{s},\mathbf{s}_0,\zeta)]=\frac{1}{4\pi}\,\frac{\mu}{\zeta(\zeta+\mu)}+\frac{\delta(\mathbf{s}-\mathbf{s}_0)}{\zeta+\mu}. \tag{25}$$

If Eq. (23) is evaluated at $\mathbf{k}=0$, that means integration of $I(\mathbf{r},\mathbf{s},t)$ over $\mathbf{r}$, the result is the same as Eq. (25). Thus the exactness of $F(\mathbf{s},\mathbf{s}_0,t)$ is verified for the isotropic scattering case.

The first moments, Eqs. (11), without normalization, [without divided by $F(\mathbf{s},\mathbf{s}_0,t)$], for the isotropic scattering case, reduce by our procedure to

$$\overline{r_z^c}=c\left[\frac{1+\cos\theta}{4\pi}\left(\frac{1-e^{-\mu t}}{\mu}-te^{-\mu t}\right)+te^{-\mu t}\delta(\mathbf{s}-\mathbf{s}_0)\right]. \tag{26a}$$

$$\overline{r_x^c}=c\sin\theta\cos\phi\frac{1}{4\pi}\left[\frac{1-e^{-\mu t}}{\mu}-te^{-\mu t}\right]. \tag{26b}$$

These coordinates of the center have the Laplace transforms, given by

$$\mathcal{L}[\overline{r_z^c}]=c\left[\frac{1+\cos\theta}{4\pi}\,\frac{\mu}{\zeta(\zeta+\mu)^2}+\frac{\delta(\mathbf{s}-\mathbf{s}_0)}{(\zeta+\mu)^2}\right], \tag{27a}$$

$$\mathcal{L}[\overline{r_x^c}]=c(\sin\theta)(\cos\phi)\frac{1}{4\pi}\,\frac{\mu}{\zeta(\zeta+\mu)^2}. \tag{27b}$$

Since moments can be obtained by differentiation of characteristic functions, we evaluate $\partial/\partial(-ik_\alpha)\{Eq.(23)\}|_{\mathbf{k}=\mathbf{0}}$, that means integration over space of r_α with $I(\mathbf{r},\mathbf{s},t)$ as weight. The results are same as Eqs. (27). Thus, by a slight extension of Hauge's results we verify the exactness of our first moment in the isotropic scattering case.

For a check of the second moment, we notice that Eqs. (18) are obtained from

$$\int_0^t dt'\exp(at')\int_0^{t'}dt''\exp(bt'')$$
$$=\begin{cases}(1/b)[(e^{(a+b)t}-1)/(a+b)-(e^{at}-1)/a],\\(1/a)[(e^{at}-1)/a-t],\quad a=-b.\end{cases} \tag{28}$$

In the isotropic scattering case, the limit as $a\to0$, or $b\to0$, or both is needed.

Equation (17a), without normalization, in the isotropic scattering case reduce to

$$\overline{\Delta_{zz}^c}=c^2\frac{\cos^2\theta+\cos\theta}{4\pi}\left[\frac{1}{\mu^2}-e^{-\mu t}\frac{1}{\mu^2}-e^{-\mu t}\frac{t}{\mu}-e^{-\mu t}\frac{t^2}{2}\right]$$
$$+\frac{c^2}{12\pi}\left[\frac{t}{\mu}-e^{-\mu t}\frac{t}{\mu}-e^{-\mu t}t^2\right]+c^2\frac{t^2}{2}e^{-\mu t}\delta(\mathbf{s}-\mathbf{s}_0). \tag{29}$$

This moment based on our method has a Laplace transform, given by

$$\mathcal{L}[\overline{\Delta_{zz}^c}]=c^2\frac{\cos^2\theta+\cos\theta}{4\pi}\,\frac{\mu}{\zeta(\zeta+\mu)^3}+\frac{c^2}{12\pi}\,\frac{\mu^2+3\zeta\mu}{\zeta^2(\zeta+\mu)^3}$$
$$+\frac{c^2}{(\zeta+\mu)^3}\delta(\mathbf{s}-\mathbf{s}_0). \tag{30}$$

The corresponding result from Hauge's solution are obtained by $(1/2)\partial^2/\partial(-ik_z)\partial(-ik_z)\{Eq.(23)\}|_{\mathbf{k}=\mathbf{0}}$, which implies integration of $(r_zr_z)/2$ with $I(\mathbf{r},\mathbf{s},t)$ as weight over space. The same result as Eq. (30) is obtained. The similar proofs have been performed for $\overline{\Delta_{xx}^c}$, $\overline{\Delta_{yy}^c}$, $\overline{\Delta_{xz}^c}$, $\overline{\Delta_{yz}^c}$, and $\overline{\Delta_{xy}^c}$, verifying the exactness of our second moments. In evaluation of the value and the derivatives of $B\equiv\{1-(\mu/|\mathbf{k}|c)\tan^{-1}[|\mathbf{k}|c/(\zeta+\mu)]\}^{-1}$ at $\mathbf{k}=0$, we have $B=(\zeta+\mu)/\zeta$, $B_\alpha=0$, $B_{\alpha\alpha}=2\mu c^2/[3\zeta^2(\zeta+\mu)]$, and $B_{\alpha\beta}=0$ if $\alpha\neq\beta$.

In the above equations the term related to $e^{-\mu t}\delta(\mathbf{s}-\mathbf{s}_0)$, has cumulants $r_z^c=ct$ and $2\Delta_{zz}-(r_z^c)^2=0$. This spike represents the unscattered part of the light, which reduces its intensity as $\exp(-\mu t)$. The scattered part of light along the directions of $\mathbf{s}\neq\mathbf{s}_0$ has the correct mean positions and spreads, as has been proved.

V. DISCUSSION

The decoupling of harmonics is valid only for the angular distribution, $F(\mathbf{s},\mathbf{s}_0,t)$, because in Eq. (3) the term such as $c\mathbf{s}\cdot\nabla_{\mathbf{r}}I(\mathbf{r},\mathbf{s},t)$ in Eq. (1) disappears. This result is available only for an infinite uniform medium, otherwise Eq. (3) cannot be derived from Eq. (1). When the spatial related distribution, $I(\mathbf{r},\mathbf{s},t)$, is calculated, the coupling of the different harmonics remains, and is presented in Eqs. (8) and (9), through the recurrence relation of harmonics, Eq. (14), and explicitly shown in Eqs. (11) and (17), the results of the first two moments. Contrasting with the usual approach using angular moment expansion of Eq. (1), our cumulant approach has two remarkable features: (a) since the formula for calculating cumulants, Eqs. (8) and (9) (and possible extension to higher order cumulants), use the standard Green's function approach without making approximation and the Green's function, Eq. (4), is exact, the obtained cumulants, as far as the nth order concern, are exact. (b) The cumulants obtained appear as the arguments of the exponential functions in Eq. (7), that implies that an infinite series in the usual angular moment expansion has been included. Therefore, even though only derived by terminating at the second order cumulant, the distribution function obtained has the exact central position and the exact half-width as functions of time, and thus leads to the correct ballistic limit at $t \rightarrow 0$ and correct diffusive limit at large t. This result is not achieved for a general phase function in any known publication.

The cumulant expansion terminating at the second order is a standard method in statistics [12], which neglects all cumulants higher than second order, and leads to a Gaussian distribution. If we examine the spatial displacement after each collision event as an independent random variable, $\Delta \mathbf{r}_i$, the total displacement is $\Sigma \Delta \mathbf{r}_i (i=1,\ldots,N)$. The central limit theorem claims that if N is a large number, then the sum of N variables will have an essentially Gaussian distribution. Therefore, after enough collision events happened, the distributions we calculated become accurate in detail, not just having the correct center and spread. At early time, the photon spread is narrow, hence, in many applications the detailed shape is less important than the correct position and correct narrow width of the beam.

In case a more accurate distribution at early time is needed, the exact higher (than second) order cumulants can be analytically calculated, and Eq. (7) can be extended to higher order. Analytical expressions for exact spatial cumulants up to an arbitrary nth high order have been derived, and will be presented elsewhere [16]. However, a closed analytical form in space is unlikely to result, and a numerical Fourier transform over $\mathbf{k}$ would be required. We have therefore terminated the current calculation at second order in this paper.

In summary, we have derived an analytical solution of the distribution function, Eq. (10), and the density distribution, Eq. (19), for the elastic Boltzmann transport equation in an infinite uniform medium. This solution is quantitatively accurate up to the second order cumulant approximation and shows a clear picture of time evolution of particle migration from ballistic to snakelike, then to the diffusion regime. The first two position cumulants at any angle and the angular distribution are completely exact as functions of time.

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