Green's function of the time-dependent radiative transport equation in terms of rotated spherical harmonics

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(Received 25 June 2012; published 17 September 2012)

The time-dependent radiative transport equation is solved for the three-dimensional spatially uniform infinite medium which is illuminated by a point unidirectional source using a spherical harmonics transform under rotation. Apart from the numerical evaluation of a spherical Hankel transform which connects the spatial distance with the radial distance in Fourier space, the dependence on all variables is found analytically. For the special case of a harmonically modulated source, even the spherical Hankel transform can be carried out analytically. Additionally, a special solution for the isotropically scattering infinite medium is given. The Monte Carlo method is used for a successful verification of the derived solution.

DOI: 10.1103/PhysRevE.86.036603 PACS number(s): 95.30.Jx, 29.30.Dn, 44.40.+a, 02.30.Uu

I. INTRODUCTION

The radiative transport equation (RTE) has a central importance in many areas of physics for studying the propagation of particles in random media, such as in astrophysics, nuclear physics, biophotonics, heat transfer, computer graphics, and climate research [1–5]. Due to the lack of analytical solutions of the RTE even for relatively simple cases like the infinite medium numerical methods or approximations such as the diffusion equation were considered. However the well-known restrictions of the diffusion theory lead in many applications for example the solution of inverse problems to unsatisfactory results. The Monte Carlo method is the most often used approach for solving the RTE numerically [6–8], but also other techniques like the finite element [9], the finite-difference [10], or the discrete-ordinate method [11] were applied. However, the simulation of Green's function of the time-independent RTE, e.g., with the Monte Carlo method, requires very long calculation times until accurate results are received. In the case of isotropic scattering media there exists an exact analytical solution to the three-dimensional time-independent RTE in Fourier space. However the corresponding solution in spatial coordinates involves the numerical evaluation of a complicated three-dimensional Fourier integral [3]. Regarding the time-dependent RTE the above mentioned solution for isotropic scattering media is not available with an analytical dependence on time resulting in the evaluation of a four-dimensional Fourier integral for finding the solution in space and time [12]. Recently, analytical solutions and methods regarding the three-dimensional time-independent RTE were derived for the infinite space, the half-space, and the slab geometry [13–17]. Faris [18] derived the solution of the RTE in the frequency domain for an isotropic point source in the infinite medium. Subsequently, the derived solution was applied for measurements of strongly absorbing media [19]. Regarding the time-dependent RTE for the three-dimensional infinite medium, there exists a cumulant solution [20] which involves a three-dimensional Fourier integral that has to be evaluated numerically. Further, a continued fraction solution dealing with a special case of the three-dimensional infinite medium was presented [21]. The final formula is given in the transformed space for both the time and one spatial coordinate. Furthermore, Gershenson [22] developed a higher-order spherical-harmonic approximation of the time-dependent radiative transfer equation to reduce the well-known breakdown of the diffusion theory at early times and short distances.

Recently, we derived the infinite space Green's function to the time-dependent RTE for the isotropic point source [23]. In this paper we present the derivation of the general Green's function to the time-dependent RTE of a three-dimensional anisotropically scattering medium for a point unidirectional source. The solution contains no approximations and is given in terms of analytical functions. The derived solution in Fourier space is dependent analytically on all variables whereas Green's function in real space involves a spherical Hankel transform which must be evaluated numerically. The obtained Green's function has most likely the maximal possible analytical dependence on its variables taking into account that no approximations are made. In addition, the corresponding Green's function for a harmonically modulated source is derived. Furthermore, the special case of isotropic scattering is considered. The found solutions were successfully verified by comparisons with Monte Carlo simulations.

II. THEORY

The three-dimensional time-dependent RTE for the specific intensity $\psi = \psi(\mathbf{r},\hat{\mathbf{s}},t)$ caused by the source $S = S(\mathbf{r},\hat{\mathbf{s}},t)$ in Cartesian coordinates is given by

$$\frac{1}{c}\frac{\partial\psi}{\partial t} + \hat{\mathbf{s}}\cdot\nabla\psi + \mu_t\psi = \mu_s\int f(\hat{\mathbf{s}}\cdot\hat{\mathbf{s}}')\psi(\mathbf{r},\hat{\mathbf{s}}',t)d^2s' + S, \tag{1}$$

where $\mu_t = \mu_a + \mu_s$ is the total attenuation coefficient, μ_a the absorption coefficient, μ_s the scattering coefficient, and c denotes the velocity of particles in the scattering medium. The unit vector $\hat{\mathbf{s}}$ specifies the direction of the wave propagation, and the phase function $f(\hat{\mathbf{s}}\cdot\hat{\mathbf{s}}')$ which is assumed to be rotationally invariant describes the probability that a particle coming from direction $\hat{\mathbf{s}}'$ is scattered into direction $\hat{\mathbf{s}}$. For illustration, Fig. 1 shows schematically the geometry of the problem for the special case of a point unidirectional source which is placed at the origin and is illuminating in the positive

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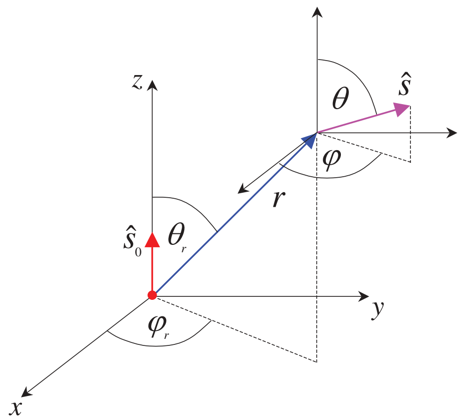

FIG. 1. (Color online) Illustrating the geometry of the problem including the spatial and angular variables.

z direction. The resulting specific intensity is evaluated at the position $\mathbf{r}$ in direction $\hat{\mathbf{s}}$.

Green's function of Eq. (1) is given by its solution for the point unidirectional source $S(\mathbf{r},\hat{\mathbf{s}},t) = \delta(\mathbf{r}-\mathbf{r}_0)\delta(\hat{\mathbf{s}}-\hat{\mathbf{s}}_0)\delta(t)$. Taking into account that the specific intensity and the source can be expanded in form of the Fourier integral

$$\psi(\mathbf{r},\hat{\mathbf{s}},t) = \int \frac{d^3k}{(2\pi)^3}\psi(\mathbf{k},\hat{\mathbf{s}},t)\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{r}), \tag{2}$$

the RTE (1) transforms into the spatially independent equation

$$\left(\frac{1}{c}\frac{\partial}{\partial t} + \mathrm{i}\mathbf{k}\cdot\hat{\mathbf{s}} + \mu_t\right)\psi(\mathbf{k},\hat{\mathbf{s}},t) = \mu_s\int f(\hat{\mathbf{s}}\cdot\hat{\mathbf{s}}')\psi(\mathbf{k},\hat{\mathbf{s}}',t)d^2s' + S(\mathbf{k},\hat{\mathbf{s}},t). \tag{3}$$

Next, the quantities of Eq. (3) are expanded in terms of spherical harmonics (SH) which are rotated about the azimuthal and polar angles of the wave vector $\hat{\mathbf{k}}$ leading to the series

$$\psi(\mathbf{k},\hat{\mathbf{s}},t) = \sum_{l=0}^{\infty}\sum_{M=-l}^{l}\psi_{lM}(\mathbf{k},t)Y_{lM}(\hat{\mathbf{s}};\hat{\mathbf{k}}), \tag{4}$$

where the corresponding "forward" transform is

$$\psi_{lM}(\mathbf{k},t) = \int \psi(\mathbf{k},\hat{\mathbf{s}},t)Y_{lM}^*(\hat{\mathbf{s}};\hat{\mathbf{k}})d^2s. \tag{5}$$

The SH $Y_{lM}(\hat{\mathbf{s}};\hat{\mathbf{k}})$ under rotation are given as a linear combination of $2l+1$ conventional spherical functions $Y_{lm}(\hat{\mathbf{s}}) = Y_{lm}(\hat{\mathbf{s}};\hat{\mathbf{z}})$:

$$Y_{lM}(\hat{\mathbf{s}};\hat{\mathbf{k}}) = \sum_{m=-l}^{l}\exp(-\mathrm{i}m\varphi_{\mathbf{k}})d_{mM}^{l}(\theta_{\mathbf{k}})Y_{lm}(\hat{\mathbf{s}}), \tag{6}$$

where $d_{mM}^{l}(\theta_{\mathbf{k}})$ is the Wigner d function with the closed-form expression [24]

$$d_{mM}^{l}(\theta_{\mathbf{k}}) = (-1)^{m+M}\sqrt{(l+m)!(l-m)!(l+M)!(l-M)!} \times \sum_{k}(-1)^k\frac{(1+\cos\theta_{\mathbf{k}})^{l-k-\frac{M-m}{2}}(1-\cos\theta_{\mathbf{k}})^{k+\frac{m-M}{2}}}{2^l k!(l-m-k)!(l+M-k)!(m-M+k)!} \tag{7}$$

and $\max(M-m,0) \leqslant k \leqslant \min(l-m,l+M)$. In accordance with the conventional SH [25], the rotated functions satisfy the relation

$$(\hat{\mathbf{k}}\cdot\hat{\mathbf{s}})Y_{lM}(\hat{\mathbf{s}};\hat{\mathbf{k}}) = \sqrt{\frac{l^2-M^2}{4l^2-1}}Y_{l-1,M}(\hat{\mathbf{s}};\hat{\mathbf{k}}) + \sqrt{\frac{(l+1)^2-M^2}{4(l+1)^2-1}}Y_{l+1,M}(\hat{\mathbf{s}};\hat{\mathbf{k}}). \tag{8}$$

The rotationally invariant phase function depends only on the cosine $\hat{\mathbf{s}}\cdot\hat{\mathbf{s}}'$ and becomes in SH decomposition the form

$$f(\hat{\mathbf{s}}\cdot\hat{\mathbf{s}}') = \sum_{l=0}^{\infty}\sum_{M=-l}^{l}f_l Y_{lM}(\hat{\mathbf{s}};\hat{\mathbf{k}})Y_{lM}^*(\hat{\mathbf{s}}';\hat{\mathbf{k}}), \tag{9}$$

where f_l are the expansion coefficients. Upon substitution of all series in Eq. (3), one obtains the following block-diagonal systems of first order differential equations parameterized by $M \in \mathbb{Z} \wedge l \geqslant |M|$:

$$\frac{1}{c}\frac{d}{dt}|\psi_M(\mathbf{k},t)\rangle + \mathbf{A}_M(k)|\psi_M(\mathbf{k},t)\rangle = |q_M(\mathbf{k},t)\rangle, \tag{10}$$

with the complex symmetric tridiagonal matrix

$$\mathbf{A}_M(k) = \begin{pmatrix} \sigma_l & \mathrm{i}k\beta_{lM} & 0 & 0 & \cdots & 0 \\ \mathrm{i}k\beta_{lM} & \sigma_{l+1} & \mathrm{i}k\beta_{l+1,M} & 0 & \cdots & \vdots \\ 0 & \mathrm{i}k\beta_{l+1,M} & \ddots & \ddots & \cdots & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \cdots & \cdots & \ddots & \sigma_{N-1} & \mathrm{i}k\beta_{NM} \\ 0 & \cdots & 0 & 0 & \mathrm{i}k\beta_{NM} & \sigma_N \end{pmatrix}, \tag{11}$$

$\beta_{lM} = \sqrt{(l^2-M^2)/(4l^2-1)}$ and $\sigma_l = \mu_a + (1-f_l)\mu_s$. Here $|\psi_M(\mathbf{k},t)\rangle$ and $|q_M(\mathbf{k},t)\rangle$ are infinite-dimensional vectors with components $\psi_{lM}(\mathbf{k},t)$ and $\exp(-\mathrm{i}\mathbf{k}\cdot\mathbf{r}_0)Y_{lM}^*(\hat{\mathbf{s}}_0;\hat{\mathbf{k}})\delta(t)$, respectively. The solution of the above differential equations is given for $t > 0$ by

$$|\psi_M(\mathbf{k},t)\rangle = c\exp[-\mathbf{A}_M(k)ct]|q_M(\mathbf{k},t)\rangle, \tag{12}$$

where $\exp[-\mathbf{A}_M(k)ct]$ is the matrix exponential with elements $\chi_{ll'}^{M}(k,t)$ for $l,l' \geqslant |M|$. Therefore, the time-dependent Green's function in Fourier space is obtained as

$$\psi(\mathbf{k},\hat{\mathbf{s}},\hat{\mathbf{s}}_0,t) = c\exp(-\mathrm{i}\mathbf{k}\cdot\mathbf{r}_0)\sum_{M=-\infty}^{\infty}\sum_{l,l'=|M|}^{\infty}Y_{l'M}^*(\hat{\mathbf{s}}_0;\hat{\mathbf{k}}) \times \chi_{ll'}^{M}(k,t)Y_{lM}(\hat{\mathbf{s}};\hat{\mathbf{k}}). \tag{13}$$

At this stage the solution is in principle completed and must be integrated according to the Fourier integral (2). In the Appendix readers will find some information regarding the inverse Fourier transform. Once the integration regarding the angular variables has been carried out analytically, we arrive at Green's function of the RTE (1) in terms of rotated SH

$$\psi(\mathbf{r},\hat{\mathbf{s}},\mathbf{r}_0,\hat{\mathbf{s}}_0,t) = \sum_{m=-\infty}^{\infty}\sum_{l,l'=|m|}^{\infty}Y_{l'm}^*(\hat{\mathbf{s}}_0;\hat{\mathbf{R}})\psi_{ll'}^{m}(R,t)Y_{lm}(\hat{\mathbf{s}};\hat{\mathbf{R}}), \tag{14}$$

with matrix elements

$$\psi_{ll'}^{m}(R,t) = c(-1)^m \sum_{M=-\bar{l}}^{\bar{l}} (-1)^M \sum_{L=|l-l'|}^{l+l'} C_{l,m,l',-m}^{L,0} C_{l,M,l',-M}^{L,0} \frac{\mathrm{i}^L}{2\pi^2} \times \int_0^\infty \chi_{ll'}^{M}(k,t) j_L(kR) k^2 dk, \quad (15)$$

where $\bar{l} = \min(l,l')$ and $\mathbf{R} = \mathbf{r} - \mathbf{r}_0$. Here $j_L(x)$ is the spherical Bessel function of the first kind and $C_{l_1,m_1,l_2,m_2}^{l_3,m_3}$ are the Clebsch-Gordan coefficients [26]. For the comparisons shown in the Sec. III, the integral is evaluated using the Gauß quadrature method. Green's function for the particle density is obtained via integration of the specific intensity resulting in a simple Legendre polynomial series

$$\Phi(\mathbf{r},\mathbf{r}_0,\hat{\mathbf{s}}_0,t) = \int \psi(\mathbf{r},\hat{\mathbf{s}},\mathbf{r}_0,\hat{\mathbf{s}}_0,t) d^2 s = c \sum_{l=0}^{\infty} \sqrt{2l+1}\, \chi_{0l}^{0}(R,t) P_l(\hat{\mathbf{s}}_0 \cdot \hat{\mathbf{R}}), \quad (16)$$

with coefficients

$$\chi_{0l}^{0}(R,t) = \frac{\mathrm{i}^l}{2\pi^2} \int_0^\infty \chi_{0l}^{0}(k,t) j_l(kR) k^2 dk. \quad (17)$$

In some cases it is desirable to separate the ballistic component of the RTE,

$$\psi_b(\mathbf{r},\hat{\mathbf{s}},\mathbf{r}_0,\hat{\mathbf{s}}_0,t) = c \frac{\exp(-\mu_t ct)}{R^2} \delta(R-ct) \delta(\hat{\mathbf{R}} - \hat{\mathbf{s}}_0) \delta(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0), \quad (18)$$

from the derived solution. In SH decomposition its matrix elements can be obtained as

$$\gamma_{ll'}^{M}(R,t) = c\sqrt{(2l+1)(2l'+1)} \exp(-\mu_t ct) \frac{\delta(R-ct)}{4\pi R^2} \delta_{M0}. \quad (19)$$

The elimination of the ballistic component can be accomplished either by modifying the source term in Eq. (1) or via subtraction of matrix elements before carrying out the spherical Hankel transform in the final solution (14). To this end we also expand the ballistic component in Fourier space,

$$\psi_b(\mathbf{k},\hat{\mathbf{s}},\hat{\mathbf{s}}_0,t) = c \exp(-\mu_t ct) \exp[-\mathrm{i}\mathbf{k} \cdot (\mathbf{r}_0 + ct\hat{\mathbf{s}}_0)] \delta(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0), \quad (20)$$

in terms of rotated SH according to Eq. (13). Note that in this case the diagonal elements of all block matrices (26) become $\sigma_l = \mu_t$. Due to this fact the infinite-dimensional matrix exponentials $\exp[-\mathbf{A}_M(k)ct]$ can be evaluated analytically for all $M \in \mathbb{Z}$ where the elements are obtained as

$$\gamma_{ll'}^{M}(k,t) = \exp(-\mu_t ct)(-1)^M \sqrt{(2l+1)(2l'+1)} \times \sum_{L=|l-l'|}^{l+l'} (-\mathrm{i})^L j_L(kct) C_{l,0,l',0}^{L,0} C_{l,M,l',-M}^{L,0}. \quad (21)$$

The derived elements can now be subtracted from Green's function in Eq. (14). Note that for the isotropic scattering medium the matrix elements $\chi_{ll'}^{M}(k,t)$ are exactly the same as that for the ballistic components $\gamma_{ll'}^{M}(k,t)$ if $|M| \geqslant 1$. At the end of the next section we also give an exact formula for the more complicated matrix exponential $\exp[-\mathbf{A}_0(k)ct]$.

A. Harmonically modulated source

Another important form of time-resolved measurements is performed in the frequency domain in which the amplitude of the source is modulated harmonically at a given angular frequency ω and the phase shift as well as the amplitude at that frequency is measured at the detector position. In that case the source term in the RTE (1) becomes

$$S(\mathbf{r},\hat{\mathbf{s}},t) = \delta(\mathbf{r} - \mathbf{r}_0)\delta(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0)\exp(\mathrm{i}\omega t). \quad (22)$$

The specific intensity caused by a time-harmonic source takes also the form

$$\psi(\mathbf{r},\hat{\mathbf{s}},\mathbf{r}_0,\hat{\mathbf{s}}_0,t) = \psi(\mathbf{r},\hat{\mathbf{s}},\mathbf{r}_0,\hat{\mathbf{s}}_0)\exp(\mathrm{i}\omega t), \quad (23)$$

where the complex amplitude is given by the solution of the time-independent RTE

$$[\hat{\mathbf{s}} \cdot \nabla + \mu_t + \mathrm{i}\omega/c]\psi(\mathbf{r},\hat{\mathbf{s}},\mathbf{r}_0,\hat{\mathbf{s}}_0) = \mu_s \int f(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}')\psi(\mathbf{r},\hat{\mathbf{s}}',\mathbf{r}_0,\hat{\mathbf{s}}_0) d^2 s' + \delta(\mathbf{r} - \mathbf{r}_0)\delta(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0). \quad (24)$$

We now proceed in the same way as already done from Eq. (4) until Eq. (9). Here we do not get systems of differential equations but the following systems of linear equations for $M \in \mathbb{Z} \wedge l \geqslant |M|$:

$$[\mathbf{A}_M(k) + \mathrm{i}\omega/c\mathbf{I}_M]|\psi_M(\mathbf{k})\rangle = |q_M(\mathbf{k})\rangle, \quad (25)$$

where $\mathbf{I}_M$ is the identity matrix and the components of $|q_M(k)\rangle$ are given by $\exp(-\mathrm{i}\mathbf{k} \cdot \mathbf{r}_0) Y_{lM}^{*}(\hat{\mathbf{s}}_0;\hat{\mathbf{k}})$. Now, the real quantities σ_l after Eq. (11) before become the complex numbers $\sigma_l = \mu_a + (1 - f_l)\mu_s + \mathrm{i}\omega/c$. For a given angular modulation frequency ω, we are indented to obtain the unknown vector $|\psi_M(\mathbf{k})\rangle$ with an analytical dependence on the wave number k. This task can be accomplished by performing an eigenvalue decomposition (EVD) of matrices $\mathbf{B}_M = \mathbf{B}_{-M}$ for $M \geqslant 0$ which have the form

$$\mathbf{B}_M = \begin{pmatrix} 0 & b_{lM} & 0 & 0 & \cdots & 0 \\ b_{lM} & 0 & b_{l+1,M} & 0 & \cdots & \vdots \\ 0 & b_{l+1,M} & \ddots & \ddots & \cdots & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \cdots & \cdots & \ddots & 0 & b_{NM} \\ 0 & \cdots & 0 & 0 & b_{NM} & 0 \end{pmatrix}, \quad (26)$$

where $l = M+1, M+2, \ldots$ and the complex quantities

$$b_{lM} = \sqrt{\frac{l^2 - M^2}{(4l^2 - 1)\sigma_{l-1}\sigma_l}}. \quad (27)$$

Here it is assumed that the EVD of all block matrices leads to the eigenvalues $\Lambda = \{\lambda_1, \lambda_2, \ldots\}$ with the corresponding eigenvectors $|u\rangle$. Furthermore we define the block diagonal matrix $\mathbf{U}$ where the column vectors of individual block matrices $\mathbf{U}_M$ contain the eigenvectors of $\mathbf{B}_M$. The inverse to this matrix is also block diagonal and denoted with $\mathbf{U}^{-1} = \mathbf{V}$. Note that apart from the special case $\omega = 0$ when all matrices are real and symmetric, we must be aware that in general $\mathbf{U}^{-1} \neq \mathbf{U}^{\mathrm{T}}$. In addition, the eigenvector components are denoted as $\langle l|u_i\rangle$ whereas $\langle v_i|l'\rangle$ are the row vector components of the inverse matrix $\mathbf{V} = \mathbf{U}^{-1}$, where $l,l' \geqslant |M|$. Upon the EVD of the matrices $\mathbf{B}_M$ the solution of the corresponding set of linear equations from Eq. (25) is obtained as

$$\psi_{lM}(\mathbf{k}) = \exp(-\mathrm{i}\mathbf{k}\cdot\mathbf{r}_0) \sum_{l'=|M|}^{\infty} \sum_{\mu} \frac{\langle l|u_\mu\rangle\langle v_\mu|l'\rangle}{1+\mathrm{i}k\lambda_\mu} \frac{Y^*_{l'M}(\hat{\mathbf{s}}_0;\hat{\mathbf{k}})}{\sqrt{\sigma_l\sigma_{l'}}}, \tag{28}$$

where $\mu = (M,i)$ is a composite index. For a fixed value M the inner summation regarding μ runs only over eigenvalues and vectors arising from the corresponding block matrix $\mathbf{B}_M$. Additionally, in the case of the harmonically modulated source the matrices $\mathbf{B}_M$ depend only on the angular modulation frequency ω but not on the wave number k. Thus the complete EVD must be performed once only. The performance of the inverse Fourier transform according to Eq. (2) and the consideration of symmetry properties of the vector components leads to the complex amplitude of the time-harmonic specific intensity from Eq. (23):

$$\psi(\mathbf{r},\hat{\mathbf{s}},\mathbf{r}_0,\hat{\mathbf{s}}_0) = \sum_{m=-\infty}^{\infty} \sum_{l,l'=|m|}^{\infty} Y^*_{l'm}(\hat{\mathbf{s}}_0;\hat{\mathbf{R}})\psi^m_{ll'}(R)Y_{lm}(\hat{\mathbf{s}};\hat{\mathbf{R}}), \tag{29}$$

with matrix elements

$$\psi^m_{ll'}(R) = \frac{c(-1)^m}{2\pi\sqrt{\sigma_l\sigma_{l'}}} \sum_{M=-\bar{l}}^{\bar{l}} (-1)^M \sum_{L=|l-l'|}^{l+l'} C^{L,0}_{l,m,l',-m} C^{L,0}_{l,M,l',-M} \times \sum_n \frac{\langle l|u_n\rangle\langle v_n|l'\rangle}{\lambda_n^3} k_L(R/\lambda_n), \tag{30}$$

where $k_l(x)$ is the spherical Bessel function of the second kind. The composite index n is practically the same as μ from Eq. (28) with the restriction that only eigenvalues λ_i with property $\mathrm{Re}(\lambda_i) > 0$ are considered.

B. Isotropic scattering

In the Introduction we have already mentioned that there exists an exact analytical Green's function to the three-dimensional steady-state RTE for isotropic scattering. The corresponding expression is only available in Fourier space and given by Ref. [12]

$$\psi(\mathbf{k},\hat{\mathbf{s}}) = \frac{\delta(\hat{\mathbf{s}}-\hat{\mathbf{s}}_0)}{\mu_t + \mathrm{i}\mathbf{k}\cdot\hat{\mathbf{s}}_0} + \frac{\mu_s}{4\pi} \frac{1}{(\mu_t+\mathrm{i}\mathbf{k}\cdot\hat{\mathbf{s}})(\mu_t+\mathrm{i}\mathbf{k}\cdot\hat{\mathbf{s}}_0)} \times \left[1 - \frac{\mu_s}{k}\arctan\frac{k}{\mu_t}\right]^{-1}, \tag{31}$$

where the left-hand side term represents the ballistic component. If no special symmetry is considered, the corresponding inverse Fourier transform must be carried out numerically over three dimensions which is not easy to perform. It is possible to reduce the inverse Fourier transform to a one-dimensional integral by writing the above specific intensity in SH decomposition according to Eq. (13). After that we can proceed in the same way as shown in the Appendix. If we take advantage of the relation

$$\frac{1}{\mu_t + \mathrm{i}\mathbf{k}\cdot\hat{\mathbf{s}}} = \frac{\mathrm{i}}{k} \sum_{l=0}^{\infty} (2l+1) Q_l(\mathrm{i}\mu_t/k) P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{s}}), \tag{32}$$

where $\mathrm{Re}(\mu_t) > 0$ and $Q_l(x)$ is the associated Legendre function of the second kind, we obtain an alternative expression for the specific intensity given in Eq. (31):

$$\psi(\mathbf{k},\hat{\mathbf{s}}) = \frac{\delta(\hat{\mathbf{s}}-\hat{\mathbf{s}}_0)}{\mu_t + \mathrm{i}\mathbf{k}\cdot\hat{\mathbf{s}}_0} + \sum_{l,l'=0}^{\infty} Y^*_{l'0}(\hat{\mathbf{s}}_0;\hat{\mathbf{k}}) I_{ll'}(k) Y_{l0}(\hat{\mathbf{s}};\hat{\mathbf{k}}), \tag{33}$$

with matrix elements

$$I_{ll'}(k) = -\frac{\mu_s}{k^2}\sqrt{(2l+1)(2l'+1)}\, Q_l(\mathrm{i}\mu_t/k) Q_{l'}(\mathrm{i}\mu_t/k) \times \left[1 - \frac{\mu_s}{k}\arctan\frac{k}{\mu_t}\right]^{-1}. \tag{34}$$

Note that the addition of the elements of the time-independent ballistic component for $M = 0$,

$$\gamma^M_{ll'}(k) = \mathrm{i}\frac{(-1)^M}{k}\sqrt{(2l+1)(2l'+1)} \times \sum_{L=|l-l'|}^{l+l'} Q_L(\mathrm{i}\mu_t/k) C^{L,0}_{l,0,l',0} C^{L,0}_{l,M,l',-M}, \tag{35}$$

to that of Eq. (34) results exactly in the elements of the infinite-dimensional inverse matrix $\mathbf{A}_0(k)$ from Eq. (10). Now we can give the exact solution for the elements $\chi^0_{ll'}(k,t)$ of the matrix exponential $\exp[-\mathbf{A}_0(k)ct]$ by replacing μ_t by $\mu_t + s$ in Eq. (34) and performing

$$\chi^0_{ll'}(k,t) = \gamma^0_{ll'}(k,t) + \frac{1}{2\pi\mathrm{i}} \int_L I_{ll'}(k,s) \exp(sct) ds, \tag{36}$$

where $\gamma^0_{ll'}(k,t)$ is adopted from Eq. (21) and L denotes a line along the imaginary axis in the complex s plane; see Fig. 2. The function $I_{ll'}(k,s)$ has one real-valued pole at $s_0 = k\cot(k/\mu_s) - \mu_t$, where $-\mu_t \leqslant s_0 \leqslant -\mu_a$, which is only existent when $|k| \leqslant \mu_s\pi/2$. Furthermore the denominator of $I_{ll'}(k,s)$ has additionally two branch points at $s = -\mu_t \pm \mathrm{i}k$ so it is necessary to introduce a branch cut parallel to the imaginary axis with parametrization $s(\eta) = -\mu_t + \mathrm{i}k\eta$, where $|\eta| \leqslant 1$.

Thus, by using the residue theorem the contour integral in relation (36) can be written as

$$\frac{1}{2\pi\mathrm{i}} \int_L I_{ll'}(k,s)\exp(sct)ds = \mathrm{Res}\{I_{ll'}(k,s)\exp(sct), s = s_0\} + \frac{1}{2\pi\mathrm{i}} \int_B I_{ll'}(k,s)\exp(sct)ds, \tag{37}$$

so that the time-dependent matrix elements can be obtained as

$$\chi_{ll'}^{0}(k,t)=\gamma_{ll'}^{0}(k,t)+\frac{\mu_s}{2\pi}(-1)^{l+l'}\sqrt{(2l+1)(2l'+1)}\exp(-\mu_t ct)\int_{-1}^{1}\left[\frac{Q_l(\eta+\mathrm{i}0)Q_{l'}(\eta+\mathrm{i}0)}{k-z_1(\eta)}-\frac{Q_l(\eta-\mathrm{i}0)Q_{l'}(\eta-\mathrm{i}0)}{k-z_2(\eta)}\right]\exp(\mathrm{i}k\eta ct)d\eta$$
$$-\sqrt{(2l+1)(2l'+1)}\exp(-\mu_t ct)\frac{Q_l[\mathrm{i}\cot(k/\mu_s)]Q_{l'}[\mathrm{i}\cot(k/\mu_s)]}{\sin^2(k/\mu_s)}\exp[k\cot(k/\mu_s)ct]\Theta\left(\mu_s\frac{\pi}{2}-|k|\right), \quad (38)$$

where $Q_l(\eta\pm \mathrm{i}0)=Q_l(\eta)\mp \mathrm{i}\pi/2P_l(\eta)$ and $z_{1/2}(\eta)=\mu_s\{\mp\pi-\mathrm{i}\ln[(1+\eta)/(1-\eta)]\}/2$. The function $\Theta(x)$ is the unit step function. We additionally note that the spherical symmetric particle density $\Phi(r,t)$ caused by the isotropic point source $S(\mathbf{r},t)=\delta(r)\delta(t)/(4\pi r^2)$ corresponds in Fourier space with the element $\Phi(k,t)=c\chi_{00}^{0}(k,t)$. Thus, the application of the inverse Fourier transform for spherically symmetric functions

$$\Phi(r,t)=\frac{1}{2\pi^2}\int_0^\infty \Phi(k,t)j_0(kr)k^2dk \quad (39)$$

leads to the time-domain particle density for values $t>r/c$:

$$\Phi(r,t)=c\frac{\delta(r-ct)}{4\pi r^2}\exp(-\mu_t ct)+\frac{\mu_s}{4\pi rt}\exp(-\mu_t ct)\ln\frac{ct+r}{ct-r}$$
$$+\frac{c\mu_s^2}{16\pi^2 r}\exp(-\mu_t ct)\int_0^1\left|\frac{1-\eta}{1+\eta}\right|^{\mu_s(r-\eta ct)/2}\left[\left(\pi^3-3\pi\ln^2\frac{1-\eta}{1+\eta}\right)\cos\left(\mu_s\pi\frac{r-\eta ct}{2}\right)\right.$$
$$\left.+\ln\frac{1-\eta}{1+\eta}\left(3\pi^2-\ln^2\frac{1-\eta}{1+\eta}\right)\sin\left(\mu_s\pi\frac{r-\eta ct}{2}\right)\right]\Theta(r-\eta ct)d\eta$$
$$+\frac{c}{2\pi^2\mu_s^2 r}\exp(-\mu_t ct)\int_0^{\pi/2\mu_s}\frac{\exp[k\cot(k/\mu_s)ct]}{\sin^2(k/\mu_s)}\sin(kr)k^3dk. \quad (40)$$

Note that a very similar expression for the density caused by a isotropic point source has already been derived in the work of Ref. [27].

III. NUMERICAL RESULTS

The derived Green's function is validated against the Monte Carlo method [6], which converges in the limit of an infinitely large number of simulated particles to the exact solution of the RTE. For the following comparison, the Henyey-Greenstein phase function with anisotropy parameter $g=0.9$ is used. The optical properties of the scattering medium are assumed to be $\mu_a=0.1\,\mathrm{mm}^{-1}$, $\mu_s=10\,\mathrm{mm}^{-1}$, and $c=3\times10^8$ m/s. In the Monte Carlo simulations the angular resolution for the detected particles was $\Delta\theta=\pm\pi/90, \Delta\varphi=\pm\pi/45$, whereas the spatial resolution was ±0.25 mm.

Due to convenience the point unidirectional source is placed at the origin of the coordinate system of Fig. 1 so that $\mathbf{r}_0=0$. The corresponding unit vectors $\hat{\mathbf{s}}$ and $\hat{\mathbf{s}}_0$ are denoted in

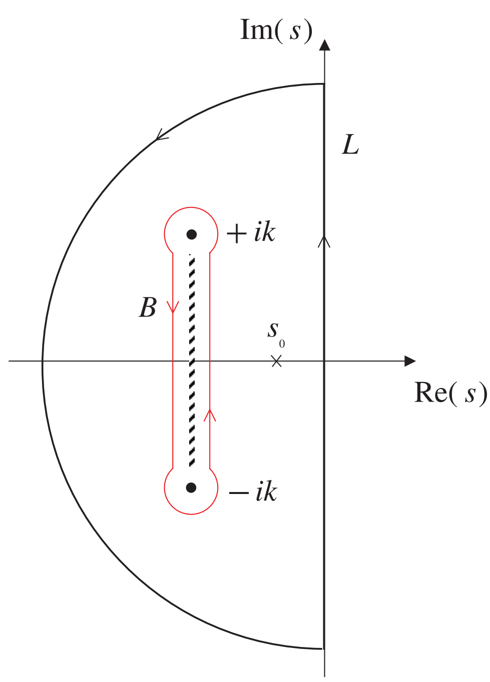

FIG. 2. (Color online) Complex s plane with corresponding curves for evaluation of the contour integral.

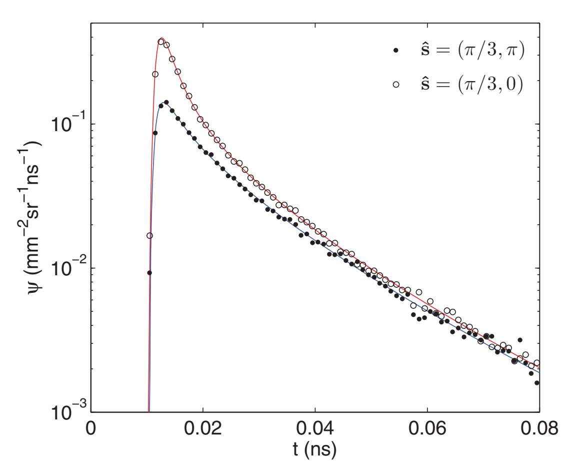

FIG. 3. (Color online) Time-resolved Green's function of the RTE caused by a point unidirectional source with direction $\hat{\mathbf{s}}_0=(\pi/4,0)$ evaluated for two different directions $\hat{\mathbf{s}}$. The detection of the specific intensity takes place at the point $(r,\theta_r,\varphi_r)=(3\,\mathrm{mm},0,0)$.

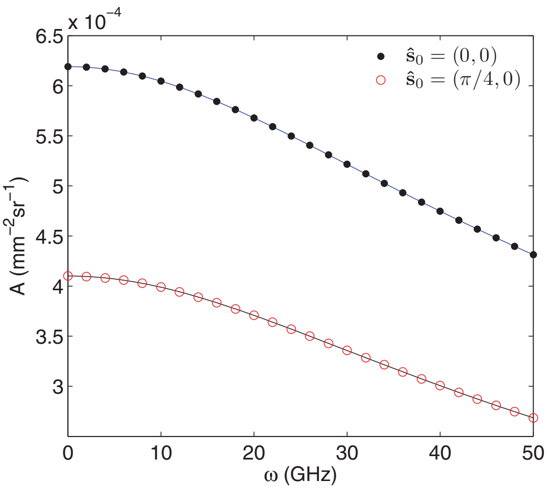

FIG. 4. (Color online) Amplitude as a function of the angular modulation frequency evaluated for two different source directions $\hat{\mathbf{s}}_0$.

the form

$$\hat{\mathbf{s}} := (\theta,\varphi) = \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix}. \tag{41}$$

For the first comparison the time-domain Green's function is calculated with formula (14) and simulated with the Monte Carlo method [7] for two different directions $\hat{\mathbf{s}}$ of propagation. We note that the simulation time needed to obtain the Monte Carlo results was more than 100 days using a single state of the art processor. The resulting specific intensity is shown in Fig. 3. The derived analytical Green's function (solid curves) agrees in both cases with the Monte Carlo method (symbols).

Next the Green's function is considered as function of the angular modulation frequency ω using Eq. (29). In order to verify the derived formula we performed a discrete-time Fourier transform (DTFT) of the time-domain Green's function. For fixed vectors of the source direction, the direction of propagation, and the position vector, one obtains the function

$$\psi(\omega) = \sum_{n=-\infty}^{\infty} T\psi(nT)e^{-\mathrm{i}\omega nT}, \tag{42}$$

where T is the sampling interval. The corresponding amplitude $A(\omega) = |\psi(\omega)|$ and phase $\phi(\omega) = -\arg\{\psi(\omega)\}$ are evaluated for $\hat{\mathbf{s}} = (\pi/3,0)$ at the point $(r,\theta_r,\varphi_r) = (5\,\mathrm{mm},0,0)$ and shown in Figs. 4 and 5, respectively, for two source directions $\hat{\mathbf{s}}_0$. The symbols correspond with formula (29) whereas the solid curves are the results of the DTFT. It can be seen that the amplitude and phase obtained from Eq. (29) agree well with the results obtained from the DTFT.

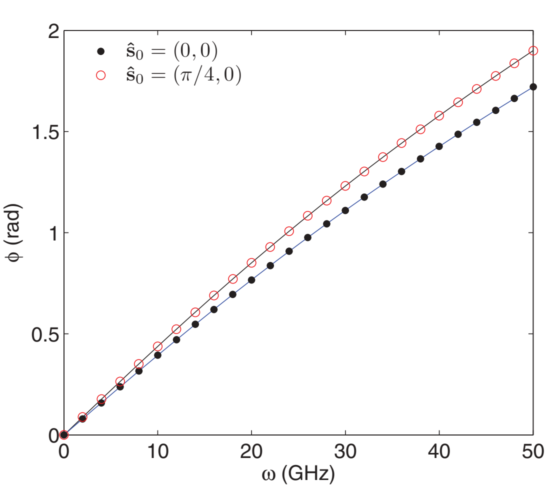

FIG. 5. (Color online) Argument of the complex amplitude as a function of the angular modulation frequency evaluated for two different source directions $\hat{\mathbf{s}}_0$.

IV. CONCLUSIONS

In this study the general Green's function for an anisotropically scattering unbounded medium illuminated by a point unidirectional source was derived. The dependence on all variables is found analytically apart from the radial distance between source and detector. This quantity is given by a spherical Hankel transform which has to be carried out numerically. The derived formulas have been successfully validated with Monte Carlo simulations.

In addition, the corresponding Green's function for an harmonically modulated source was derived and successfully validated using the solution for a δ source in time and performing the discrete-time Fourier transform. Furthermore, a special solution for the general Green's function of an isotropically scattering unbounded medium was presented.

Besides the direct application of the derived Green's function, it also represents the particular solution to the RTE which is needed for solving boundary value problems. Finally, we note that the solution is also usable for the validation of numerical methods, such as the Monte Carlo method.

APPENDIX: EVALUATION OF THE FOURIER INTEGRAL

This Appendix contains one possibility for performing the inverse Fourier transform according to Eq. (2). The matrix elements of Green's function in Fourier space (13) depends only on the length k of the wave vector $\mathbf{k}$. Therefore the inverse transform regarding the angular variables requires knowledge of the integral

$$\int Y^{*}_{l'M}(\hat{\mathbf{s}}_0;\hat{\mathbf{k}})Y_{lM}(\hat{\mathbf{s}};\hat{\mathbf{k}})\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{R})d^2s_{\mathbf{k}}. \tag{A1}$$

In the following we make use of the rotational invariance and determine at first the specific intensity in the positive z direction leading to $\hat{\mathbf{R}} = \hat{\mathbf{z}}$. The Fourier kernel becomes now independent of the azimuthal angle and can be written in terms of the Wigner d function as

$$\exp(\mathrm{i}kR\cos\theta_{\mathbf{k}}) = \sum_{L=0}^{\infty} \mathrm{i}^L(2L+1)j_L(kR)d^L_{00}(\theta_{\mathbf{k}}). \tag{A2}$$

The product of the SH in Eq. (A1) is considered in the explicit form

$$Y^*_{l'M}(\hat{\mathbf{s}}_0;\hat{\mathbf{k}})Y_{lM}(\hat{\mathbf{s}};\hat{\mathbf{k}}) = \sum_{m=-l}^{l}\sum_{n=-l'}^{l'} d^l_{mM}(\theta_{\mathbf{k}})\exp(-\mathrm{i}m\varphi_{\mathbf{k}}) \times Y_{lm}(\hat{\mathbf{s}})d^{l'}_{nM}(\theta_{\mathbf{k}})\exp(\mathrm{i}n\varphi_{\mathbf{k}})Y^*_{l'n}(\hat{\mathbf{s}}_0). \quad \text{(A3)}$$

The integration of Eq. (A3) over the azimuthal angle can be immediately performed resulting in

$$\int_0^{2\pi} Y^*_{l'M}(\hat{\mathbf{s}}_0;\hat{\mathbf{k}})Y_{lM}(\hat{\mathbf{s}};\hat{\mathbf{k}})d\varphi_{\mathbf{k}} = 2\pi\sum_{m=-\bar{l}}^{\bar{l}} d^l_{mM}(\theta_{\mathbf{k}})Y_{lm}(\hat{\mathbf{s}})d^{l'}_{mM}(\theta_{\mathbf{k}})Y^*_{l'm}(\hat{\mathbf{s}}_0), \quad \text{(A4)}$$

where $\bar{l} = \min(l,l')$. The result of the integration regarding the polar angle yields

$$\int_0^{\pi} d^l_{mM}(\theta_{\mathbf{k}})d^{l'}_{mM}(\theta_{\mathbf{k}})d^L_{00}(\theta_{\mathbf{k}})\sin\theta_{\mathbf{k}}d\theta_{\mathbf{k}} = (-1)^{m+M}\frac{2}{2L+1}C^{L,0}_{l,m,l',-m}C^{L,0}_{l,M,l',-M}. \quad \text{(A5)}$$

Note that the above integral is only nonzero for values which satisfy the triangular condition $|l-l'| \leqslant L \leqslant l+l'$. At this stage the inverse Fourier transform regarding the angular variables is completed under the assumption that $\hat{\mathbf{R}} = \hat{\mathbf{z}}$. However, the obtained result can be directly expanded to the general case $\hat{\mathbf{R}} \neq \hat{\mathbf{z}}$ via rotation of the whole system into the direction of an arbitrary unit vector $\hat{\mathbf{R}}$. In other words it is possible to rotate virtually the whole system until the unit vectors $\hat{\mathbf{R}}$ and $\hat{\mathbf{z}}$ become parallel. Then, we also must rotate the unit vectors of the direction $\hat{\mathbf{s}}$ and the source $\hat{\mathbf{s}}_0$ in the same way to reconstitute the original situation. This task can be accomplished by rotating the SH in Eq. (A4) about the azimuthal and polar angles of $\hat{\mathbf{R}}$. Taking into account all results and discussions above, we arrive at the following useful integral transform pair for rotated SH:

$$\int Y^*_{l'M}(\hat{\mathbf{s}}_0;\hat{\mathbf{k}})Y_{lM}(\hat{\mathbf{s}};\hat{\mathbf{k}})\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{R})d^2s_{\mathbf{k}} = 4\pi(-1)^M\sum_{m=-\bar{l}}^{\bar{l}}(-1)^m Y^*_{l'm}(\hat{\mathbf{s}}_0;\hat{\mathbf{R}})Y_{lm}(\hat{\mathbf{s}};\hat{\mathbf{R}}) \times \sum_{L=|l-l'|}^{l+l'}\mathrm{i}^L j_L(kR)C^{L,0}_{l,m,l',-m}C^{L,0}_{l,M,l',-M}. \quad \text{(A6)}$$

Multiplying the obtained result with $c\chi^M_{ll'}(k,t)/(2\pi)^3$ and performing the integration regarding the radial coordinate k leads to the real space Green's function from Eq. (14).

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