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Radiative transport equation in rotated reference frames

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Abstract

A novel method for solving the linear radiative transport equation (RTE) in a three-dimensional homogeneous medium is proposed and illustrated with numerical examples. The method can be used with an arbitrary phase function $A(\hat{s}, \hat{s}')$ with the constraint that it depends only on the angle between the angular variables \hat{s} and \hat{s}' . This assumption corresponds to spherically symmetric (on average) random medium constituents. Boundary conditions are considered in the slab and half-space geometries. The approach developed in this paper is *spectral*. It allows for the expansion of the solution to the RTE in terms of analytical functions of angular and spatial variables to relatively high orders. The coefficients of this expansion must be computed numerically. However, the computational complexity of this task is much smaller than in the standard method of spherical harmonics. The solutions obtained are especially convenient for solving inverse problems associated with radiative transfer.

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1. Introduction

1.1. Background

The contemporary mesoscopic theoretical description of multiple scattering of waves in random media is most often based on the linear radiative transport equation (RTE) [1]. Unfortunately, the RTE is notoriously difficult to solve, even in the case of constant absorption and scattering coefficients. The known analytical solutions are few and of little practical importance. Yet, there is a growing need for accurate and computationally efficient solutions to the RTE in many fields of applied and fundamental science. For example, in optical tomography of biological tissues [2, 3], the use of the RTE is frequently required to accurately describe propagation of multiply scattered light. This is especially true in close proximity

to sources or boundaries [4], or in regions with high absorption and low scattering [5, 6]. Accordingly, significant effort has been devoted to developing and refining efficient approximate and numerical methods for solving the RTE. In particular, recently explored approaches have been based on the discrete ordinate method [7–9], cumulant expansion [10, 11], modifications of Ambarzumian’s method [12, 13] and different levels of the P_L approximation [14, 15]. Algorithms for inversion of the RTE have also been proposed [16–19].

The discrete ordinate method (see [20] for a detailed description) is, perhaps, the most common approach due to its simplicity and generality. An alternative to the discrete ordinate method is the method of spherical harmonics, often referred to as the P_L approximation, in cases with special symmetry. This approach has the advantage of expressing the angular dependence of the specific intensity in a basis of analytical functions³ rather than in the completely local basis of discrete ordinates. In particular, in the case of cylindrical symmetry (one-dimensional propagation), a very effective solution based on a continued fraction expansion can be obtained [21]. However, when no special symmetry is present in the problem, the method of spherical harmonics can be carried out in practice only to very low orders. In a recent paper [22], we have suggested a modification of the standard method of spherical harmonics. The modification is based on expanding the angular part of each Fourier component of the specific intensity in the basis of spherical functions defined in a reference frame whose z -axis is aligned with the direction of the Fourier wave vector \mathbf{k} . This approach resulted in significant mathematical simplifications and was referred to as *the modified method of spherical harmonics* in [22]. Here we find it more appropriate to call it *the method of rotated reference frames* (MRRF).

In [22], the derivation of the RTE Green’s function by the MRRF was only briefly sketched for the case of an infinite medium and numerical examples were limited to a few simple cases with spherical symmetry. Here we give the full mathematical details of the derivation and discuss the mathematical properties of the solutions obtained, derive plane-wave decomposition of Green’s function, and generalize the MRRF to the case of planar boundaries. We also provide extensive numerical examples for cases with no special symmetry. The paper is organized as follows. In section 1.2, we introduce the RTE and basic notations, and explain why the use of rotated reference frames is beneficial. In section 2 we define spherical functions in rotated reference frames. In section 3 we apply the MRRF to the derivation of Green’s function. In particular, Green’s function in the Fourier representation is given in section 3.1. Mathematical properties of the solutions are discussed in section 3.2. Different representations for Green’s function in real space are given in section 3.3. A plane-wave decomposition of Green’s function is derived in section 3.4. In section 3.5, we introduce evanescent modes of the homogeneous RTE. These modes are important mathematical constructs which can be used for solving the RTE in the presence of planar boundaries, as is shown in section 3.6. Section 4 contains numerical examples of applying the MRRF to calculating Green’s function in infinite space. Finally, section 5 contains a discussion.

The novel element of the MRRF is the use of a \mathbf{k} -dependent angular basis, not the use of a Fourier integral decomposition. The latter has been used to derive an analytic expression for Green’s function of the RTE in an infinite medium with isotropic scattering [23]. Note that this is the only case in which analytic solution to the three-dimensional RTE has been derived. The obtained solution, however, has proven to be of little use. First, it is given by a formally divergent integral which cannot be evaluated analytically and is difficult to

³ Here the term ‘analytical’ means ‘expressed in terms of well-characterized functions through explicit formulae’, not necessarily analytic in the Cauchy–Riemann sense.

compute numerically. Second, generalization of the method to non-isotropic scattering and bounded media is highly problematic. In the case of the MRRF, the Fourier integral plays only a secondary role. The main distinguishing feature of this approach is that the inverse Fourier transform is evaluated analytically. Thus, in the case of an infinite medium, this leads to expressions for the real-space Green's function given in section 3.3. In the case of planar interfaces, Green's function is given by a *two-dimensional* Fourier integral (as an expansion over evanescent plane wave modes, see sections 3.4–3.6). This integral cannot be evaluated analytically. However, two points must be made. First, the expansion is what is often needed for solving the inverse problem associated with transmission through an inhomogeneous slab [24]. The plane-wave decomposition of the RTE Green's function is of great interest and was recently studied with the use of the method of discrete ordinates [7, 8]. Second, such a decomposition can be obtained without the use of the MRRF only in the form of a one-dimensional integral with a complicated structure and then only in an infinite medium with isotropic scattering.

1.2. RTE and the conventional method of spherical harmonics

The RTE describes the propagation of the *specific intensity* $I(\mathbf{r}, \hat{\mathbf{s}})$, at the spatial point \mathbf{r} and flowing in the direction specified by the unit vector $\hat{\mathbf{s}}$, in a medium characterized by absorption and scattering coefficients μ_a and μ_s , and has the form

$$\hat{\mathbf{s}} \cdot \nabla I + (\mu_a + \mu_s)I = \mu_s AI + \varepsilon. \quad (1)$$

Here $\varepsilon = \varepsilon(\mathbf{r}, \hat{\mathbf{s}})$ is the source and A is the scattering operator defined by

$$AI(\mathbf{r}, \hat{\mathbf{s}}) = \int A(\hat{\mathbf{s}}, \hat{\mathbf{s}}')I(\mathbf{r}, \hat{\mathbf{s}}') d^2\hat{\mathbf{s}}'. \quad (2)$$

The phase function $A(\hat{\mathbf{s}}, \hat{\mathbf{s}}')$ is normalized according to the condition $\int A(\hat{\mathbf{s}}, \hat{\mathbf{s}}') d^2\hat{\mathbf{s}}' = 1$. We also assume that it depends only on the angle between $\hat{\mathbf{s}}$ and $\hat{\mathbf{s}}'$: $A(\hat{\mathbf{s}}, \hat{\mathbf{s}}') = f(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}')$. This fundamental assumption is often used and corresponds to scattering by spherically symmetric particles.

In the conventional method of spherical harmonics, all angle-dependent quantities are expanded in the basis of spherical harmonics defined in the laboratory frame [25]:

$$I(\mathbf{r}, \hat{\mathbf{s}}) = \sum_{lm} I_{lm}(\mathbf{r})Y_{lm}(\hat{\mathbf{s}}), \quad (3)$$

$$\varepsilon(\mathbf{r}, \hat{\mathbf{s}}) = \sum_{lm} \varepsilon_{lm}(\mathbf{r})Y_{lm}(\hat{\mathbf{s}}), \quad (4)$$

$$A(\hat{\mathbf{s}}, \hat{\mathbf{s}}') = \sum_{lm} A_l Y_{lm}(\hat{\mathbf{s}})Y_{lm}^*(\hat{\mathbf{s}}'). \quad (5)$$

In particular, truncating the above series at $l = 1$ leads to the well-known diffusion approximation to the RTE [25]. In the more general case, substituting expansions (3)–(5) into the RTE (1), multiplying the resulting equations by $Y_{l'm'}^*(\hat{\mathbf{s}})$ and integrating over $\hat{\mathbf{s}}$ leads to the following system of equations for $I_{lm}(\mathbf{r})$:

$$\sum_{l'm'} \left[R_{lm,l'm'}^{(x)} \frac{\partial I_{l'm'}}{\partial x} + R_{lm,l'm'}^{(y)} \frac{\partial I_{l'm'}}{\partial y} + R_{lm,l'm'}^{(z)} \frac{\partial I_{l'm'}}{\partial z} \right] + \sigma_l I_{lm} = \varepsilon_{lm}, \quad (6)$$

where $R^{(\alpha)} = \int s_\alpha Y_{lm}^*(\hat{\mathbf{s}})Y_{l'm'}(\hat{\mathbf{s}}) d^2\hat{\mathbf{s}}$ ($\alpha = x, y, z$) are matrices whose explicit form is given in [25] and

$$\sigma_l = \mu_a + \mu_s(1 - A_l). \quad (7)$$

This system of partial differential equations must be solved for $l = 0, 1, 2, \dots, l_{\max}$ and $m = -l, \dots, l$, where l_{\max} is the truncation order of the expansion (3)–(5).

In a classic text, Case and Zweifel wrote concerning the system of equations (6): ‘this rather awe-inspiring set of equations . . . has perhaps only academic interest’ ([25], p 219). We note that the root of the difficulty is not that the matrices $R^{(\alpha)}$ are dense (in fact, they only couple coefficients with $m' = m, l' = l \pm 1$ for $\alpha = z$ and $m' = m \pm 1, l' = l \pm 1$ for $\alpha = x, y$) or non-commuting (in fact, it is easy to verify that all $R^{(\alpha)}$ commute). The difficulty is that these matrices operate on the spatial derivatives of I_{lm} taken along different directions. Thus, by viewing the set of three matrices $R^{(\alpha)}$ as a three-dimensional vector of matrices \mathbf{R} , and using the Fourier representation for I_{lm} , we can rewrite the term in the square bracket of (6) as $i\mathbf{k} \cdot \mathbf{R}_{m,l,m'} I_{l,m'}(\mathbf{k})$. It can be seen that the matrix $\mathbf{k} \cdot \mathbf{R}$ depends explicitly on the direction and length of \mathbf{k} . (See similar formulation in [26].)

The method of rotated reference frames (MRRF), similar to the conventional method of spherical harmonics, does not lead to the separation of spatial and angular variables which is impossible for the RTE. However, by choosing a different \mathbf{k} -dependent angular basis, we replace the dot product $\mathbf{k} \cdot \mathbf{R}$ by an expression of the type kR , where $k = |\mathbf{k}|$ is a scalar and R is a single \mathbf{k} -independent block-diagonal matrix. It is shown below that, given generalized eigenvectors and eigenvalues of R which must be computed numerically, the solution can be obtained in terms of analytical functions of spatial and angular variables⁴.

2. Spherical functions in rotated frames

The ordinary spherical harmonics $Y_{lm}(\theta, \varphi)$ are functions of two polar angles in a fixed (laboratory) reference frame. Equivalently, we can view them as functions of a unit vector, $\hat{\mathbf{s}}$. In this case, θ and φ are the polar angles of $\hat{\mathbf{s}}$ in the laboratory frame. More generally, both the orientation of the reference frame and the direction of $\hat{\mathbf{s}}$ can vary. We will need to define spherical functions of a unit vector $\hat{\mathbf{s}}$ in a reference frame whose z -axis coincides with the direction of a given unit vector $\hat{\mathbf{k}}$. Obviously, there are infinitely many such reference frames. To define one uniquely, it is sufficient to consider a rotation of the laboratory frame with the following three Euler angles: $\alpha = \varphi_{\hat{\mathbf{k}}}, \beta = \theta_{\hat{\mathbf{k}}}$ and $\gamma = 0$, where $\theta_{\hat{\mathbf{k}}}$ and $\varphi_{\hat{\mathbf{k}}}$ are the polar angles of $\hat{\mathbf{k}}$ in the laboratory frame. The transformation from the laboratory frame (x, y, z) to the rotated frame (x', y', z') is illustrated in figure 1. We denote spherical functions of $\hat{\mathbf{s}}$ in the reference frame defined by the above transformation by $Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{k}})$. They can be expressed as linear combinations of the spherical functions defined in the original (laboratory) frame according to

$$Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{k}}) = Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{z}}') = \sum_{m'=-l}^l D_{m'm}^l(\varphi_{\hat{\mathbf{k}}}, \theta_{\hat{\mathbf{k}}}, 0) Y_{lm'}(\hat{\mathbf{s}}; \hat{\mathbf{z}}), \quad (8)$$

where

$$D_{mm'}^l(\alpha, \beta, \gamma) = \exp(-im\alpha) d_{mm'}^l(\beta) \exp(-im'\gamma) \quad (9)$$

are the Wigner D -functions; the explicit form of $d_{mm'}^l(\beta)$ is given, for example, in [27].

⁴ In principle, it should be also possible to use the fact that all matrices $R^{(\alpha)}$ in (6) commute and, hence, have the same set of eigenvectors, to solve (6) by diagonalizing just one \mathbf{k} -independent matrix and analytically inverting the Fourier transform, and thus avoid the use of rotated reference frames. This approach has some advantages and difficulties associated with it, and to the best of our knowledge, has not been explored so far. If successful, it should lead to the same solutions as described below.

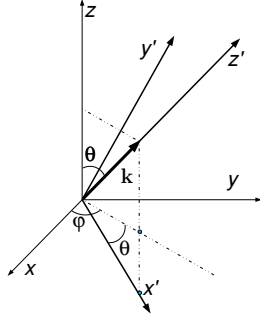


Figure 1. Illustration of the rotated reference frame.

It is important to note that the expansion of the scattering kernel into the spherical functions $Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{k}})$ is independent of the direction of $\hat{\mathbf{k}}$:

$$A(\hat{\mathbf{s}}, \hat{\mathbf{s}}') = \sum_{lm} A_l Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{k}}) Y_{lm}^*(\hat{\mathbf{s}}'; \hat{\mathbf{k}}). \quad (10)$$

Here the expansion coefficients A_l are independent of $\hat{\mathbf{k}}$ and are the same as in (5). This fact follows from the rotational invariance of the scalar product.

3. Theory

3.1. Green's function in the Fourier representation

By definition, Green's function $G(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}_0, \hat{\mathbf{s}}_0)$ satisfies RTE (1) with the source $\varepsilon = \delta(\mathbf{r} - \mathbf{r}_0)\delta(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0)$. We will refer to $\mathbf{r}_0, \hat{\mathbf{s}}_0$ and $\mathbf{r}, \hat{\mathbf{s}}$ as the location and direction of the source and detector, respectively. In infinite isotropic space, Green's function can be written in the following general form:

$$G(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}_0, \hat{\mathbf{s}}_0) = \sum_{lm, l'm'} \int \frac{d^3k}{(2\pi)^3} \exp[i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}_0)] Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{k}}) \langle lm | K(k) | l'm' \rangle Y_{l'm'}^*(\hat{\mathbf{s}}_0; \hat{\mathbf{k}}). \quad (11)$$

Here $K(k)$ is an unknown operator. The reciprocity of Green's function, $G(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}_0, \hat{\mathbf{s}}_0) = G(\mathbf{r}_0, -\hat{\mathbf{s}}_0; \mathbf{r}, -\hat{\mathbf{s}})$, together with the fact that G is real, implies the following symmetry property of K : $\langle l'm' | K | lm \rangle = (-1)^{l+l'} \langle lm | K | l'm' \rangle^*$. This can be also written as $\mathcal{P}K^\dagger\mathcal{P} = K$, where \mathcal{P} is the coordinate inversion operator with matrix elements $\langle lm | \mathcal{P} | l'm' \rangle = (-1)^l \delta_{ll'} \delta_{mm'}$ and \dagger denotes Hermitian conjugation. Thus, it can be seen that K is not a Hermitian operator.

Substituting (11) into (1) and using the orthogonality properties of the spherical functions, we arrive at the following operator equation for $K(k)$:

$$(ikR + \Sigma)K(k) = 1. \quad (12)$$

The matrices R and Σ are defined by

$$\begin{aligned} \langle lm | R | l'm' \rangle &= \int (\hat{\mathbf{s}} \cdot \hat{\mathbf{k}}) Y_{lm}^*(\hat{\mathbf{s}}; \hat{\mathbf{k}}) Y_{l'm'}(\hat{\mathbf{s}}; \hat{\mathbf{k}}) d^2\hat{\mathbf{s}} \\ &= \delta_{mm'} [b_{lm} \delta_{l'=l-1} + b_{l+1, m} \delta_{l'=l+1}], \end{aligned} \quad (13)$$

$$b_{lm} = \sqrt{(l^2 - m^2)/(4l^2 - 1)}, \quad (14)$$

$$\langle lm | \Sigma | l'm' \rangle = \sigma_l \delta_{ll'} \delta_{mm'}, \quad (15)$$

where σ_l is given by (7). The formal solution to (12) can be written as

$$K(k) = S(1 + ikW)^{-1}S, \quad (16)$$

where $S = 1/\sqrt{\Sigma}$ and $W = SRS$. Note that $\langle lm|S|l'm'\rangle = \delta_{ll'}\delta_{mm'}/\sqrt{\sigma_l}$ exists because $\sigma_l > 0$, which follows from the inequalities $A_l \leq 1$ and $\mu_a > 0$.⁵ Similarly to R , W is a real symmetric matrix. Therefore, we can use the spectral theorem to express $(1 + ikW)^{-1}$ in terms of the eigenvectors and eigenvalues of W , $|\psi_\mu\rangle$ and λ_μ , respectively. This immediately leads to the following expression for $K(k)$:

$$K(k) = \sum_{\mu} \frac{S|\psi_\mu\rangle\langle\psi_\mu|S}{1 + ik\lambda_\mu}. \quad (17)$$

Given the set of eigenvectors and eigenvalues, which can be found by numerical diagonalization of W , the above formula solves the problem in Fourier space. Since the components of $|\psi_\mu\rangle$ in the $|lm\rangle$ basis are purely real, it can be seen that K is symmetric.

3.2. Mathematical properties of the solution

3.2.1. Block structure of W . First, we note that W is block-diagonal: $\langle lm|W|l'm'\rangle = \delta_{mm'}\langle l|B(m)|l'\rangle$. Below, we will label different blocks $B(M)$ ($M = 0, \pm 1, \pm 2, \dots$) by the capital letter M . The matrix elements of $B(M)$ are given by

$$\langle l|B(M)|l'\rangle = \beta_l(M)\delta_{l'=l-1} + \beta_{l+1}(M)\delta_{l'=l+1}, \quad l, l' \geq |M|, \quad (18)$$

$$\beta_l(M) = b_{lM}/\sqrt{\sigma_l\sigma_{l-1}}. \quad (19)$$

Obviously, to find all eigenvalues and eigenvectors of W , it is sufficient to diagonalize each block separately. This task is further simplified because all blocks $B(M)$ are tridiagonal. We denote eigenvectors of a block $B(M)$ by $|\phi_n(M)\rangle$. Then the eigenvector of the full matrix W with the same eigenvalue is obtained according to

$$\langle lm|\psi_{Mn}\rangle = \delta_{mM}\langle l|\phi_n(M)\rangle. \quad (20)$$

The corresponding eigenvalue is denoted by λ_{Mn} , where we have introduced a composite index (M, n) . Note that $B(M) = B(-M)$.

3.2.2. Symmetry properties of the eigenvectors. The property $\mathcal{P}K^\dagger\mathcal{P} = K$ and equation (16) imply that $\mathcal{P}W\mathcal{P} = -W$. Thus, W is odd with respect to coordinate inversion. In particular, if $|\psi\rangle$ is an eigenvector of W with the eigenvalue λ , then $|\tilde{\psi}\rangle = \mathcal{P}|\psi\rangle$ is also an eigenvector of W but with an eigenvalue of the opposite sign, $\tilde{\lambda} = -\lambda$. The complete set of eigenvectors $\{|\psi_\mu\rangle : \mu \in \Omega\}$, where Ω is the set of all values of the index μ , can then be equivalently rewritten as $\{|\psi_\mu\rangle, |\tilde{\psi}_\mu\rangle : \mu \in \Omega^+\}$, where Ω^+ is the set of indices μ that correspond to positive eigenvalues λ_μ . The set of indices that correspond to negative eigenvalues can be denoted as Ω^- ; then $\Omega = \Omega^+ \cup \Omega^-$ and $\Omega^+ \cap \Omega^- = \{0\}$.

Using these properties, one can transform the summation over all values of μ in (17) to summation over $\mu \in \Omega^+$ (such sums will be denoted as \sum'_μ below). This fact facilitates the inverse Fourier transformation (see appendix A) and solution of the boundary-value problem discussed in section 3.6.

⁵ Purely scattering media with $\mu_a = 0$ can be considered separately.

3.2.3. *Continuous and discrete spectra.* Third, the eigenvalues λ_μ can belong either to the discrete or continuous spectrum. It is easy to see that the spectrum is continuous for $|\lambda| < 1/\mu_t$, where $\mu_t = \mu_a + \mu_s$, and discrete for $|\lambda| > 1/\mu_t$. Indeed, consider the three-point recurrence relation that follows from the equation $W|\psi\rangle = \lambda|\psi\rangle$:

$$\beta_l(m)\langle l-1, m|\psi\rangle + \beta_{l+1}(m)\langle l+1, m|\psi\rangle = \lambda\langle lm|\psi\rangle, \quad l \geq |m|. \quad (21)$$

In general, it has two types of solutions: polynomial and exponential. Consider the asymptotic properties of these solutions. In the limit $l \rightarrow \infty$ we have $A_l \rightarrow 0$, $\sigma_l \rightarrow \mu_t$, $b_{lm} \rightarrow 1/2$ and $\beta_l(m) \rightarrow 1/2\mu_t$. The recurrence relation then becomes

$$\langle l-1, m|\psi\rangle + \langle l+1, m|\psi\rangle = 2\mu_t\lambda\langle lm|\psi\rangle. \quad (22)$$

The polynomial solutions have the asymptotic form $\langle lm|\psi\rangle = p_l^m(\lambda\mu_t)$, where $p_l^m(x)$ are general orthogonal polynomials of degree l (not to be confused with the associated Legendre functions which solve the recurrence (21) in the particular case $\mu_s = 0$). In order for this solution to be an eigenvector of W , it must be bounded. Obviously, this requirement is equivalent to $|\lambda\mu_t| \leq 1$. Thus, for every $\lambda \in [-1/\mu_t, 1/\mu_t]$, there is a polynomial solution to the three-term recurrence relation that is an eigenvector of W .

For λ outside of the interval $[-1/\mu_t, 1/\mu_t]$, polynomial solutions are unbounded and, therefore, cannot be eigenvectors of W . We then consider exponential solutions which behave asymptotically as $\langle lm|\psi\rangle = (\pm 1)^l \exp(-pl)$ where p satisfies the equation $\cosh(p) = \pm\mu_t\lambda$. In order for this solution to be an eigenvector of W , p must be positive. But the above equation has positive roots only when $|\lambda| \geq 1/\mu_t$. Note that the exponentially decaying eigenvectors have a finite L^2 norm, and, hence, belong to the discrete spectrum. Further bounds on the discrete spectrum can be inferred from the Gershgorin theorem, which states that, for a fixed M , $|\lambda_{Mn}| \leq r_M = \max_{l \geq |M|} [\beta_l(M) + \beta_{l+1}(M)]$. It can be easily verified that $r_0 = 2/\sqrt{3}\mu_a$ and $r_M = 1/\mu_a$ for $|M| > 0$.

In numerical computations, the infinite-dimensional matrix W must be truncated and the continuous spectrum of W approximated by a discrete spectrum. In this paper we treat all eigenvalues as discrete. Thus, for example, the expression (17) contains only a sum over discrete modes, although, theoretically, summation over the continuous part of the spectrum must be expressed as an integral. Note that an expression involving only discrete spectra avails itself more readily to numerical implementation.

3.3. Green's function in real space

The dependence of solution (17) on \mathbf{k} is analytical. This allows us to obtain Green's function in the coordinate representation by Fourier transformation. We substitute (17) into the ansatz (11) and express the spherical functions $Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{k}})$ and $Y_{l'm'}(\hat{\mathbf{s}}_0; \hat{\mathbf{k}})$ in terms of spherical functions defined in the laboratory frame whose z -axis direction is given by a unit vector $\hat{\mathbf{z}}$ according to (8), (9). The direction of the x - and y -axes of the laboratory frame is arbitrary. This leads to the following expression:

$$G(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}_0, \hat{\mathbf{s}}_0) = \sum_{lm} \sum_{l'm'} Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{z}}) \langle lm|\chi(\mathbf{r} - \mathbf{r}_0; \hat{\mathbf{z}})|l'm'\rangle Y_{l'm'}^*(\hat{\mathbf{s}}_0; \hat{\mathbf{z}}), \quad (23)$$

where

$$\chi(\mathbf{r}; \hat{\mathbf{z}}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \exp(i\mathbf{k} \cdot \mathbf{r}) \mathcal{D}(\hat{\mathbf{k}}; \hat{\mathbf{z}}) K(k) \mathcal{D}^\dagger(\hat{\mathbf{k}}; \hat{\mathbf{z}}) \quad (24)$$

Here $\mathcal{D}(\hat{\mathbf{k}}; \hat{\mathbf{z}}) = \exp(-i\varphi_{\hat{\mathbf{k}}} J_z) \exp(-i\theta_{\hat{\mathbf{k}}} J_y)$ is the rotation operator whose matrix elements are given by the Wigner D -functions, $\langle lm|\mathcal{D}(\hat{\mathbf{k}}; \hat{\mathbf{z}})|l'm'\rangle = \delta_{ll'} D_{mm'}^l(\varphi_{\hat{\mathbf{k}}}, \theta_{\hat{\mathbf{k}}}, 0)$, $\varphi_{\hat{\mathbf{k}}}$ and $\theta_{\hat{\mathbf{k}}}$ are the

polar angles of \mathbf{k} in the laboratory frame, and \mathbf{J} is the angular momentum operator (with $\hbar = 1$). We note that operators \mathcal{D} are unitary and, hence, normal: $\mathcal{D}^{-1} = \mathcal{D}^\dagger$. However, \mathcal{D} does not commute with K . The fundamental simplification obtained by the MRRF is that \mathcal{D} is known analytically while K has a simple form given by (17). In particular, given numerical values of $|\psi_\mu\rangle$ and λ_μ , the dependence of $K(k)$ on k is also known analytically.

Below, we consider two different cases. In the first case, the direction of the laboratory frame z -axis coincides with the direction from the source to the detector, namely, $\hat{\mathbf{z}} = (\mathbf{r} - \mathbf{r}_0)/|\mathbf{r} - \mathbf{r}_0|$. This choice of the angular basis is convenient when the source and the detector are always placed on the same line, irrespective of the directions $\hat{\mathbf{s}}$ and $\hat{\mathbf{s}}_0$. In the second case, we choose $\hat{\mathbf{z}} = \hat{\mathbf{s}}_0$. This approach is useful when the source is scanned, e.g., over a two-dimensional plane, but its direction $\hat{\mathbf{s}}_0$ is fixed. This situation is typical for optical tomography in the slab geometry. The integral (24) for the two cases is evaluated in appendix A. The result is, in the first case:

$$\begin{aligned} \langle lm|\chi(\mathbf{r}; \hat{\mathbf{r}})|l'm'\rangle &= \frac{\delta_{mm'}}{2\pi\sqrt{\sigma_l\sigma_{l'}}} \sum_{M=-\bar{l}}^{\bar{l}} (-1)^M \sum_{j=0}^{\bar{l}} C_{l,M,l',-M}^{|l-l'|+2j,0} C_{l,m,l',-m}^{|l-l'|+2j,0} \\ &\times \sum'_\mu \frac{\langle lM|\psi_\mu\rangle\langle\psi_\mu|l'M\rangle}{\lambda_\mu^3} k_{|l-l'|+2j} \left(\frac{R}{\lambda_\mu} \right). \end{aligned} \quad (25)$$

Here $\bar{l} = \min(l, l')$, $k_n(x) = -i^n h_n^{(1)}(ix)$ is the modified spherical Bessel function of the first kind (defined without a factor of $\pi/2$), $C_{j_1 m_1 j_2 m_2}^{j_3 m_3}$ are the Clebsch–Gordan coefficients and \sum' denotes summation over only such indices μ that correspond to positive eigenvalues λ_μ . It can be seen that $\chi(\mathbf{r}; \hat{\mathbf{r}})$ is diagonal in m and m' , which corresponds to the invariance of Green's function with respect to a simultaneous rotation of the vectors $\hat{\mathbf{s}}$ and $\hat{\mathbf{s}}_0$ around the line connecting the source and the detector. Equation (25) can be further simplified by expressing the eigenvectors $|\psi_\mu\rangle$ in terms of the eigenvectors $|\phi_n(m)\rangle$ of the smaller blocks $B(m)$ as discussed in section 3.2.1. This result, as well as a number of special cases, were given in [22] and are not repeated here.

In the case $\hat{\mathbf{z}} = \hat{\mathbf{s}}_0$, expression (23) contains only matrix elements of $\chi(\mathbf{r}; \hat{\mathbf{s}}_0)$ with $m' = 0$. This follows from the fact that $Y_{l'm'}(\hat{\mathbf{s}}_0; \hat{\mathbf{s}}_0) = \delta_{m'0}\sqrt{(2l'+1)/4\pi}$. The corresponding expression for the matrix elements of $\chi(\mathbf{r}; \hat{\mathbf{s}}_0)$ is

$$\begin{aligned} \langle lm|\chi(\mathbf{r}; \hat{\mathbf{s}}_0)|l'0\rangle &= \frac{(-1)^l}{\sqrt{\pi(2l'+1)\sigma_l\sigma_{l'}}} \sum_{M=-\bar{l}}^{\bar{l}} \sum_{j=0}^{\bar{l}} Y_{|l-l'|+2j,m}^*(\hat{\mathbf{r}}; \hat{\mathbf{s}}_0) \\ &\times C_{l,M,|l-l'|+2j,0}^{l',M} C_{l,m,l',0}^{|l-l'|+2j,m} \sum'_\mu \frac{\langle lM|\psi_\mu\rangle\langle\psi_\mu|l'M\rangle}{\lambda_\mu^3} k_{|l-l'|+2j} \left(\frac{R}{\lambda_\mu} \right). \end{aligned} \quad (26)$$

Derivation of the above result is analogous to that for $\chi(\mathbf{r}; \hat{\mathbf{r}})$; see appendix A for details.

3.4. Plane-wave decomposition of Green's function

Having in mind further applications of the MRRF to solving boundary-value problems, we derive the plane-wave decomposition of Green's function. The latter is defined by the two-dimensional Fourier integral

$$\begin{aligned} G(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}_0, \hat{\mathbf{s}}_0) &= \sum_{lm} \sum_{l'm'} \int \frac{d^2q}{(2\pi)^2} \exp[i\mathbf{q} \cdot (\boldsymbol{\rho} - \boldsymbol{\rho}_0)] \\ &\times Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{z}}) \langle lm|\kappa(\mathbf{q}; z - z_0)|l'm'\rangle Y_{l'm'}^*(\hat{\mathbf{s}}_0; \hat{\mathbf{z}}). \end{aligned} \quad (27)$$

Here $\hat{\mathbf{z}}$ is a selected direction in space which coincides with the z -axis of the laboratory frame, $\boldsymbol{\rho}$ is a two-dimensional vector in the x - y plane ($\mathbf{r} = \boldsymbol{\rho} + z\hat{\mathbf{z}}$ and $\boldsymbol{\rho} \cdot \hat{\mathbf{z}} = 0$) and the direction of x - and y -axes is arbitrary. By comparing the above expression to (24), we find that

$$\kappa(\mathbf{q}; z) = \int_{-\infty}^{\infty} \frac{dk_z}{2\pi} \exp(ik_z z) \mathcal{D}(\mathbf{q} + \hat{\mathbf{z}}k_z; \hat{\mathbf{z}}) K\left(\sqrt{q^2 + k_z^2}\right) \mathcal{D}^\dagger(\mathbf{q} + \hat{\mathbf{z}}k_z; \hat{\mathbf{z}}). \quad (28)$$

Here $\mathcal{D}(\mathbf{q} + \hat{\mathbf{z}}k_z; \hat{\mathbf{z}})$ should be understood as a function of the polar angles of the vector $\mathbf{k} = \mathbf{q} + \hat{\mathbf{z}}k_z$ in the laboratory frame. The latter are defined by

$$\cos \theta = k_z / \sqrt{q^2 + k_z^2}, \quad \sin \theta = q / \sqrt{q^2 + k_z^2}. \quad (29)$$

Integral (28) can be evaluated analytically. The following expression for the matrix elements of $\kappa(\mathbf{q}; z)$ is derived in appendix B:

$$\begin{aligned} \langle lm | \kappa(\mathbf{q}; z) | l' m' \rangle &= \frac{\exp[-i(m - m')\varphi_{\hat{\mathbf{q}}}] [\text{sgn}(z)]^{l+l'+m+m'}}{\sqrt{\sigma_l \sigma_{l'}}} \sum_{m_1=-l}^l \sum_{m_2=-l'}^{l'} \sum_{\mu} \\ &\times d_{mm_1}^l [i\tau(q\lambda_\mu)] \langle lm_1 | \psi_\mu \rangle \frac{\exp[-Q_\mu(q)|z|]}{\lambda_\mu^2 Q_\mu(q)} \langle \psi_\mu | l' m_2 \rangle d_{m'm_2}^{l'} [i\tau(q\lambda_\mu)], \end{aligned} \quad (30)$$

where

$$Q_\mu(q) = \sqrt{q^2 + 1/\lambda_\mu^2}, \quad (31)$$

the complex angles $i\tau(x)$ are defined by the relations

$$\cos[i\tau(x)] = \sqrt{1 + x^2}, \quad \sin[i\tau(x)] = -ix, \quad (32)$$

and the angle $\varphi_{\hat{\mathbf{q}}}$ is the polar angle of the two-dimensional vector \mathbf{q} in the x - y plane. The Wigner d -functions $d_{mm'}^l(i\tau)$ in the above expression are algebraic functions of $\cos(i\tau)$ and $\sin(i\tau)$ (an explicit expression in terms of Jacobi polynomials is given in appendix B). An expression for $\kappa(\mathbf{q}; z)$ in terms of the block eigenvectors $\{\phi_n(M)\}$ which were introduced in section 3.2.1 is also given in appendix B. Here we note some of the symmetry properties of the matrices $\kappa(\mathbf{q}; z)$. Under inversion of the z -axis, we have $\kappa(\mathbf{q}, -z) = \mathcal{P}_z \kappa(\mathbf{q}, z) \mathcal{P}_z$, or, in component form,

$$\langle lm | \kappa(\mathbf{q}; -z) | l' m' \rangle = (-1)^{l+l'+m+m'} \langle lm | \kappa(\mathbf{q}; z) | l' m' \rangle. \quad (33)$$

Simultaneous inversion of the x - and y -axes (or, equivalently, rotation around the z -axis by the angle π) is expressed as $\kappa(-\mathbf{q}, z) = \mathcal{P}_{xy} \kappa(\mathbf{q}, z) \mathcal{P}_{xy}$, or, in component form,

$$\langle lm | \kappa(-\mathbf{q}; z) | l' m' \rangle = (-1)^{m+m'} \langle lm | \kappa(\mathbf{q}; z) | l' m' \rangle. \quad (34)$$

We also note some particular cases of expressions (27) and (30). First, consider the case $\hat{\mathbf{s}} = \hat{\mathbf{s}}_0 = \hat{\mathbf{z}}$. This corresponds to the source and detector being oriented perpendicular to the surface of a slab. We then use $Y_{lm}(\hat{\mathbf{z}}; \hat{\mathbf{z}}) = \delta_{m0} \sqrt{(2l+1)/4\pi}$ to obtain

$$G(\mathbf{r}, \hat{\mathbf{z}}; \mathbf{r}_0, \hat{\mathbf{z}}) = \sum_{l,l'=0}^{\infty} \frac{\sqrt{(2l+1)(2l'+1)}}{4\pi} \int \frac{d^2 q}{(2\pi)^2} \exp[i\mathbf{q} \cdot (\boldsymbol{\rho} - \boldsymbol{\rho}_0)] \langle l0 | \kappa(\mathbf{q}; z - z_0) | l'0 \rangle. \quad (35)$$

With the use of identity (A.12) given below, $\langle l0 | \kappa(\mathbf{q}; z) | l'0 \rangle$ can be expressed in terms of the associated Legendre functions of the first kind $P_l^m(x)$ as

$$\begin{aligned} \langle l0 | \kappa(\mathbf{q}; z) | l'0 \rangle &= \frac{[\text{sgn}(z)]^{l+l'}}{\sqrt{\sigma_l \sigma_{l'}}} \sum_{m_1=-l}^l \sum_{m_2=-l'}^{l'} \sqrt{\frac{(l-m_1)!(l'-m_2)!}{(l+m_1)!(l'+m_2)!}} \sum_{\mu} P_l^{m_1} [\lambda_\mu Q_\mu(q)] \\ &\times \langle lm_1 | \psi_\mu \rangle \frac{\exp[-Q_\mu(q)|z|]}{\lambda_\mu^2 Q_\mu(q)} \langle \psi_\mu | l' m_2 \rangle P_{l'}^{m_2} [\lambda_\mu Q_\mu(q)]. \end{aligned} \quad (36)$$

Next, consider the case $\mathbf{q} = 0$. The operator $\kappa(0; z)$ describes one-dimensional propagation due to a planar source. We use $d_{mm'}^l(0) = \delta_{mm'}$ to obtain

$$\langle lm|\kappa(0; z)|l'm'\rangle = \frac{\delta_{mm'}[\text{sgn}(z)]^{l+l'}}{\sqrt{\sigma_l\sigma_{l'}}} \sum_{\mu} \langle lm|\psi_{\mu}\rangle \frac{\exp(-|z|/\lambda_{\mu})}{\lambda_{\mu}} \langle \psi_{\mu}|l'm'\rangle. \quad (37)$$

3.5. Plane wave and evanescent modes for the RTE

Until now we considered solutions to the inhomogeneous RTE. However, the solution of boundary-value problems requires knowledge of the general solution to the homogeneous equation. We seek such a solution in the form $\exp(-\mathbf{k} \cdot \mathbf{r}) \sum_{lm} \langle lm|c\rangle Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{k}})$. Upon substitution of this ansatz into the RTE with $\varepsilon = 0$, we find that $|\mathbf{k}|$ must be the generalized eigenvalue (with the direction of \mathbf{k} being arbitrary) and $|c\rangle$ must be the generalized eigenvector of the equation $kR|c\rangle = \Sigma|c\rangle$, where the matrices R and Σ are defined by (13)–(15). Next we use (8) to express the spherical functions $Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{k}})$ in terms of the spherical functions $Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{z}})$ defined in a laboratory frame with the z -axis pointing in a selected direction. Then the general solutions to the homogeneous RTE (1) can be written as a superposition of the following modes:

$$I_{\hat{\mathbf{k}}, M, n}(\mathbf{r}, \hat{\mathbf{s}}) = \exp\left(\frac{-\hat{\mathbf{k}} \cdot \mathbf{r}}{\lambda_{Mn}}\right) \sum_{lm} Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{z}}) \frac{\exp(-im\varphi_{\hat{\mathbf{k}}})}{\sqrt{\sigma_l}} d_{mM}^l(\theta_{\hat{\mathbf{k}}}) \langle l|\phi_n(M)\rangle. \quad (38)$$

Here it is more convenient to use the notation for block eigenvectors $|\phi_n(M)\rangle$ which were introduced in section 3.2.1. The modes are labelled by the unit vector $\hat{\mathbf{k}}$ ($\hat{\mathbf{k}} \cdot \hat{\mathbf{k}} = 1$) whose polar angles in the laboratory frame are $\theta_{\hat{\mathbf{k}}}$ and $\varphi_{\hat{\mathbf{k}}}$ and by the composite index $\mu = (M, n)$. We note that it is sufficient to consider only modes with positive eigenvalues λ_{Mn} ($\mu \in \Omega^+$; see section 3.2.2) due to the obvious symmetry $I_{-\hat{\mathbf{k}}, -M, n}(-\mathbf{r}, \hat{\mathbf{s}}) = I_{\hat{\mathbf{k}}, M, n}(\mathbf{r}, \hat{\mathbf{s}})$.

However, the modes (38) with purely real vector $\hat{\mathbf{k}}$ cannot be used to construct a solution to a boundary-value problem in a half-space or in a slab. This is because each mode is exponentially growing in the direction $-\hat{\mathbf{k}}$. Therefore, it is necessary to define *evanescent* modes with complex-valued vectors $\hat{\mathbf{k}}$. These modes are oscillatory in the x - y plane and exponentially decaying (or growing) in the z -direction. Namely, let

$$\hat{\mathbf{k}} = -i\lambda_{Mn}\mathbf{q} \pm \hat{\mathbf{z}}\lambda_{Mn}Q_{Mn}(q), \quad (39)$$

where $\mathbf{q} \cdot \hat{\mathbf{z}} = 0$. The polar angles of $\hat{\mathbf{k}}$ are defined as follows: $\varphi_{\hat{\mathbf{k}}} = \varphi_{\hat{\mathbf{q}}}$, $\cos(\theta_{\hat{\mathbf{k}}}) = \hat{\mathbf{k}} \cdot \hat{\mathbf{z}} = \pm\lambda_{Mn}Q_{Mn}(q)$ and $\sin(\theta_{\hat{\mathbf{k}}}) = \hat{\mathbf{k}} \cdot \hat{\mathbf{q}} = -iq\lambda_{Mn}$. Thus, we can write $\theta_{\hat{\mathbf{k}}} = i\tau(q\lambda_{Mn})$, where the sine and cosine of the complex angle $i\tau(x)$ are given by (32). This gives rise to two kinds of evanescent modes:

$$I_{\mathbf{q}, M, n}^{(+)}(\mathbf{r}, \hat{\mathbf{s}}) = \exp[i\mathbf{q} \cdot \boldsymbol{\rho} - Q_{\mu}(q)z] \sum_{lm} Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{z}}) \frac{\exp(-im\varphi_{\hat{\mathbf{q}}})}{\sqrt{\sigma_l}} \times d_{mM}^l[i\tau(q\lambda_{Mn})] \langle l|\phi_n(M)\rangle, \quad (40)$$

$$I_{\mathbf{q}, M, n}^{(-)}(\mathbf{r}, \hat{\mathbf{s}}) = (-1)^M \exp[i\mathbf{q} \cdot \boldsymbol{\rho} + Q_{\mu}(q)z] \sum_{lm} Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{z}}) \frac{\exp(-im\varphi_{\hat{\mathbf{q}}})}{\sqrt{\sigma_l}} \times (-1)^{l+m} d_{m, -M}^l[i\tau(q\lambda_{Mn})] \langle l|\phi_n(M)\rangle. \quad (41)$$

Here we have used the symmetry properties of $d_{mM}^l(\theta)$ under the transformation $\theta \rightarrow \pi - \theta$ (which corresponds to change of sign of the factor $\cos(\theta)$); hence the additional phase factor $(-1)^{l+m}$ and the different sign of the index M in (41). The phase factor $(-1)^M$ is introduced for convenience.

The plane-wave decomposition (30) can be equivalently rewritten as an expansion in terms of evanescent waves:

$$G(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}_0, \hat{\mathbf{s}}_0) = \sum_{\mu}' \int \frac{d^2q}{(2\pi)^2} V_{\mathbf{q},\mu} I_{\mathbf{q},\mu}^{(\pm)}(\mathbf{r}, \hat{\mathbf{s}}) I_{-\mathbf{q},\mu}^{(\mp)}(\mathbf{r}_0, -\hat{\mathbf{s}}_0), \quad (42)$$

where

$$V_{\mathbf{q},\mu} = \frac{1}{\lambda_{\mu}^2 Q_{\mu}(q)} \quad (43)$$

and the upper signs must be selected if $z > z_0$ while the lower signs are selected if $z < z_0$. It can be easily verified that the expression (42) obeys the reciprocity condition.

Now we make the following observation. Evanescent waves propagating in different directions cannot, in principle, have identical angular dependence. In particular, by analysing only the angular dependence of specific intensity in the plane $z = 0$ (in infinite space), it is possible to tell if this intensity was produced by sources located to the left of the observation plane (in the region $z < 0$), or to the right. To demonstrate this point, we introduce vectors $|\eta_{\mu}(q)\rangle = |\eta_{Mn}(q)\rangle$ with components $\langle lm|\eta_{Mn}(q)\rangle = d_{mM}^l[i\tau(q\lambda_{Mn})]\langle l|\phi_n(M)\rangle$ and a set of vectors obtained from $|\eta_{\mu}(q)\rangle$ by coordinate inversion: $|\tilde{\eta}_{\mu}(q)\rangle = \mathcal{P}|\eta_{\mu}(q)\rangle$. The evanescent modes (40), (41) can be written as

$$I_{\mathbf{q},\mu}^{(+)}(\mathbf{r}, \hat{\mathbf{s}}) = \exp[i\mathbf{q} \cdot \boldsymbol{\rho} - Q_{\mu}(q)z] \sum_{lm} Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{z}}) \langle lm|\mathcal{A}(\hat{\mathbf{q}})|\eta_{\mu}(q)\rangle, \quad (44)$$

$$I_{\mathbf{q},\mu}^{(-)}(\mathbf{r}, \hat{\mathbf{s}}) = \exp[i\mathbf{q} \cdot \boldsymbol{\rho} + Q_{\mu}(q)z] \sum_{lm} Y_{lm}^*(\hat{\mathbf{s}}; \hat{\mathbf{z}}) \langle lm|\mathcal{A}^{\dagger}(-\hat{\mathbf{q}})|\tilde{\eta}_{\mu}(q)\rangle, \quad (45)$$

$$\langle lm|\mathcal{A}(\hat{\mathbf{q}})|l'm'\rangle = \delta_{ll'}\delta_{mm'} \exp(-im\varphi_{\hat{\mathbf{q}}})/\sqrt{\sigma_l}. \quad (46)$$

Here $\mathcal{A}(\hat{\mathbf{q}})$ is a diagonal matrix. Note that $\mathcal{A}(\hat{\mathbf{q}})$ depends only on the direction of the real vector \mathbf{q} , while $|\eta_{\mu}(q)\rangle$ depends only on its length. In the case $q = 0$ we have $|\eta_{\mu}(0)\rangle = |\psi_{\mu}\rangle$ and $|\tilde{\eta}_{\mu}(0)\rangle = |\psi_{\mu}\rangle$. Thus, the set $\{|\eta_{\mu}(0)\rangle, |\tilde{\eta}_{\mu}(0)\rangle\}$ forms an orthonormal basis in the Hilbert space spanned by the eigenvectors of W, \mathcal{H} . In the case $q \neq 0$, the vectors $\{|\eta_{\mu}(q)\rangle, |\tilde{\eta}_{\mu}(q)\rangle\}$ are no longer orthonormal. However, we believe on physical grounds that they still form a basis in \mathcal{H} .⁶ Then there exists a *dual basis* $\{|\zeta_{\mu}(q)\rangle, |\tilde{\zeta}_{\mu}(q)\rangle\}$ such that $\langle \zeta_{\mu}(q)|\eta_{\nu}(q)\rangle = \delta_{\mu\nu}$, $\langle \tilde{\zeta}_{\mu}(q)|\tilde{\eta}_{\nu}(q)\rangle = \delta_{\mu\nu}$ and $\langle \tilde{\zeta}_{\mu}(q)|\eta_{\nu}(q)\rangle = \langle \zeta_{\mu}(q)|\tilde{\eta}_{\nu}(q)\rangle = 0$.

Now assume that we have measured the specific intensity in the plane $z = 0$. Denote the two-dimensional Fourier transform of this function with respect to x and y by $I_0(\mathbf{q}, \hat{\mathbf{s}}) = \sum_{lm} I_{lm}(\mathbf{q}) Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{z}})$. The expansion coefficients $I_{lm}(\mathbf{q})$ are elements of a vector $|I(\mathbf{q})\rangle$. For every value of \mathbf{q} , we can form a vector $\mathcal{A}^{-1}(\hat{\mathbf{q}})|I(\mathbf{q})\rangle$, since $\mathcal{A}(\hat{\mathbf{q}})$ is invertible. If the sources are located to the left of the measurement plane, then $\langle \tilde{\zeta}_{\mu}(q)|\mathcal{A}^{-1}(\hat{\mathbf{q}})|I(\mathbf{q})\rangle = 0$ for every $\mu \in \Omega^+$. In other words, the projection of $\mathcal{A}^{-1}(\hat{\mathbf{q}})|I(\mathbf{q})\rangle$ onto the dual subspace spanned by $|\zeta_{\mu}(q)\rangle$ is equal to zero. Analogously, if the sources are located to the right of the observation plane, $\langle \zeta_{\mu}(q)|\mathcal{A}^{-1}(\hat{\mathbf{q}})|I(\mathbf{q})\rangle = 0$. Since the projection of a nonzero vector onto both subspaces cannot be simultaneously zero, the angular dependence of the specific intensity in the plane $z = 0$ carries information about the location of the source with respect to this plane. We emphasize that this analysis is only valid in the absence of boundaries.

⁶ We do not have a direct proof of this statement. However, in the opposite case, the boundary-value problem would not be uniquely solvable.

3.6. Boundary-value problem

Any solution to the RTE in a half-space or in a slab can be constructed as an expansion over modes (44), (45) with indices μ corresponding to only positive eigenvalues λ_μ . This fact is crucial for application of the MRRF to the boundary-value problem, which in radiative transport theory is formulated in the *half-range* of the angular variable. Now we demonstrate how it can be used to construct a solution to the boundary-value problem posed on one or two planar interfaces.

3.6.1. External source incident on a half-space. Consider the RTE in the half-space $z > 0$. In this section we assume that there are no *internal sources* in the medium, i.e., the RTE has a zero source term. The presence of external sources is expressed through an inhomogeneous boundary condition at the interface $z = 0$:

$$I_0(\boldsymbol{\rho}, \hat{\mathbf{s}}) = I_{\text{inc}}(\boldsymbol{\rho}, \hat{\mathbf{s}}), \quad \text{if } \hat{\mathbf{s}} \cdot \hat{\mathbf{z}} > 0. \quad (47)$$

Here $I_0(\boldsymbol{\rho}, \hat{\mathbf{s}})$ is the specific intensity evaluated at $z = 0$ and $I_{\text{inc}}(\boldsymbol{\rho}, \hat{\mathbf{s}})$ is the intensity incident from vacuum (the external source). The boundary condition (47) is formulated in the half-range of the angular variable.

The general solution to the RTE in the half-space $z > 0$ can be written as a superposition of outgoing evanescent waves of the form (44):

$$I(\mathbf{r}, \hat{\mathbf{s}}) = \int \frac{d^2q}{(2\pi)^2} \sum'_\mu F_{\mathbf{q},\mu}^{(+)} I_{\mathbf{q},\mu}^{(+)}(\mathbf{r}, \hat{\mathbf{s}}), \quad (48)$$

where the unknown coefficients $F_{\mathbf{q},\mu}^{(+)}$ must be found from the boundary condition (47). Now we use expansion (48) and expression (44) to calculate $I_0(\boldsymbol{\rho}, \hat{\mathbf{s}})$. Upon Fourier transformation of (47) with respect to $\boldsymbol{\rho}$, we arrive at the following equation:

$$\sum_{lm} \sum'_\mu Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{z}}) \langle lm | \mathcal{A}(\hat{\mathbf{q}}) | \eta_\mu(q) \rangle F_{\mathbf{q},\mu}^{(+)} = I_{\text{inc}}(\mathbf{q}, \hat{\mathbf{s}}), \quad \text{if } \hat{\mathbf{s}} \cdot \hat{\mathbf{z}} > 0. \quad (49)$$

Next, we multiply both sides of equation (49) by $Y_{l'm'}^*(\hat{\mathbf{s}}; \hat{\mathbf{z}})$ and integrate over all directions such that $\hat{\mathbf{s}} \cdot \hat{\mathbf{z}} > 0$. Note that integration in the right-hand side can be extended to all directions of $\hat{\mathbf{s}}$ since $I_{\text{inc}}(\mathbf{q}, \hat{\mathbf{s}})$ is identically zero for $\hat{\mathbf{s}} \cdot \hat{\mathbf{z}} < 0$. Thus, for a collimated narrow incident beam which crosses the boundary at $\boldsymbol{\rho} = \boldsymbol{\rho}_0$ in the direction $\hat{\mathbf{s}}_0$, we obtain

$$\sum'_\mu \langle lm | \mathcal{B} \mathcal{A}(\hat{\mathbf{q}}) | \eta_\mu(q) \rangle F_{\mathbf{q},\mu}^{(+)} = \exp(-i\mathbf{q} \cdot \boldsymbol{\rho}_0) Y_{lm}^*(\hat{\mathbf{s}}_0; \hat{\mathbf{z}}), \quad (50)$$

where matrix \mathcal{B} is given by

$$\begin{aligned} \langle lm | \mathcal{B} | l'm' \rangle &= \int_{\hat{\mathbf{s}} \cdot \hat{\mathbf{z}} > 0} Y_{lm}^*(\hat{\mathbf{s}}; \hat{\mathbf{z}}) Y_{l'm'}(\hat{\mathbf{s}}; \hat{\mathbf{z}}) d^2s \\ &= \frac{\delta_{mm'}}{2} \sqrt{\frac{(2l+1)(2l'+1)(l-m)!(l'-m)!}{(l+m)!(l'+m)!}} \int_0^1 P_l^m(x) P_{l'}^m(x) dx. \end{aligned} \quad (51)$$

For a fixed value of \mathbf{q} , (50) is a set of linear equations of infinite size. In practice, this set must be truncated so that $l \leq l_{\text{max}}$. Then the number of equations is $2N = (l_{\text{max}} + 1)^2$, where we have assumed for simplicity that l_{max} is odd. But the number of unknowns $F_{\mathbf{q},\mu}^{(+)}$ is only equal to N , since $\mu \in \Omega^+$. Therefore, (50) is formally overdetermined. However, not all equations in (50) are linearly independent. In fact, the rank of \mathcal{B} is exactly equal to half of its size, which is a consequence of half-range integration in (51). Therefore we come to the conclusion that (50) is a well-determined system of equations with respect to the N unknowns $F_{\mathbf{q},\mu}^{(+)}$.

Numerically, the problem of solving (50) can be solved in two different ways. A direct approach is to consider only equations in (50) which are linearly independent. This is achieved by only leaving equations in the system with l having the same parity as m , e.g., for a fixed m , $l = |m|, |m| + 2, |m| + 4, \dots$, with the restriction $l \leq l_{\max}$. Another approach is to seek the generalized Moore–Penrose pseudoinverse of (50). In this case eigenvectors of the truncated matrix \mathcal{B} must be found numerically. If the size of \mathcal{B} is even, half of its eigenvalues will be zero. Let $|\xi_v\rangle$ be the eigenvectors of \mathcal{B} with nonzero eigenvalues α_v . Then the system of equations (50) can be rewritten as

$$\alpha_v \sum_{\mu} \langle \xi_v | \mathcal{A}(\hat{\mathbf{q}}) | \eta_{\mu}(q) \rangle F_{\mathbf{q},\mu}^{(+)} = \exp(-i\mathbf{q} \cdot \boldsymbol{\rho}_0) \sum_{lm} \langle \xi_v | lm \rangle Y_{lm}^*(\hat{\mathbf{s}}_0; \hat{\mathbf{z}}). \quad (52)$$

We note that in the limit $l_{\max} \rightarrow \infty$, the eigenvectors of \mathcal{B} are known and are of simple form: $\langle lm | \xi_{\hat{\mathbf{s}}} \rangle = Y_{lm}^*(\hat{\mathbf{s}}; \hat{\mathbf{z}})$ with the eigenvalues being unity for $\hat{\mathbf{s}} \cdot \hat{\mathbf{z}} > 0$ and zero otherwise, i.e., \mathcal{B} is idempotent.

The system (52) can be simplified by the substitution $F_{\mathbf{q},\mu}^{(+)} = f_{\mathbf{q},\mu}^{(+)} \exp(-i\mathbf{q} \cdot \boldsymbol{\rho}_0)$. The coefficients $f_{\mathbf{q},\mu}^{(+)}$ are then independent of the source coordinate $\boldsymbol{\rho}_0$. Another simplification is achieved by noting that both \mathcal{A} and \mathcal{B} are diagonal in indices m and m' . In effect, the system (52) must be solved once for each value of $|\mathbf{q}|$; the dependence of the solution on the direction of \mathbf{q} is trivial. If, in addition, the incident beam is normal to the interface ($\hat{\mathbf{s}}_0 = \hat{\mathbf{z}}$), the solutions do not depend on $\hat{\mathbf{q}}$ at all.

The additional computational complexity associated with solving the boundary-value problem is then as follows. For every numerical value of the lengths of the vector \mathbf{q} which is used in the expansion (48), a system of linear equations of size $N = (l_{\max} + 1)^2$ must be solved (the cost of diagonalization of \mathcal{B} is negligibly small). Thus, consideration of boundary conditions adds significant computational complexity to the problem. This is a consequence of the fact that the rotation matrices $\exp[\tau(q\lambda_{\mu})J_y]$, unlike the matrix W , are not diagonal in m and m' . As a result, the system of equations (52) is not block diagonal and, in addition, q -dependent. However, the problem is easily solvable for $l_{\max} \leq 100$, which is, perhaps, more than is needed in any practical computation.

3.6.2. External source incident on a slab. The generalization of the mathematical apparatus developed in section 3.6.1 to the case of the RTE in a finite slab is straightforward. Consider RTE in the slab $0 < z < L$. The external source is assumed to be incident from the left. Then the boundary conditions read

$$I_0(\boldsymbol{\rho}, \hat{\mathbf{s}}) = I_{\text{inc}}(\boldsymbol{\rho}, \hat{\mathbf{s}}), \quad \text{if } \hat{\mathbf{s}} \cdot \hat{\mathbf{z}} > 0, \quad (53)$$

$$I_L(\boldsymbol{\rho}, \hat{\mathbf{s}}) = 0, \quad \text{if } \hat{\mathbf{s}} \cdot \hat{\mathbf{z}} < 0, \quad (54)$$

where I_0 and I_L are the specific intensities evaluated at the surfaces $z = 0$ and $z = L$, respectively. The general solution inside the slab has the form

$$I(\mathbf{r}, \hat{\mathbf{s}}) = \int \frac{d^2q}{(2\pi)^2} \sum_{\mu} [F_{\mathbf{q},\mu}^{(+)} I_{\mathbf{q},\mu}^{(+)}(\mathbf{r}, \hat{\mathbf{s}}) + F_{-\mathbf{q},\mu}^{(-)} I_{-\mathbf{q},\mu}^{(-)}(\mathbf{r}, -\hat{\mathbf{s}})], \quad (55)$$

where $F_{\mathbf{q},\mu}^{(+)}$ and $F_{\mathbf{q},\mu}^{(-)}$ are unknown coefficients. After some manipulations, we arrive at the following system of equations:

$$\sum_{\mu} \{ \langle lm | \mathcal{B} \mathcal{A}(\hat{\mathbf{q}}) | \eta_{\mu}(q) \rangle F_{\mathbf{q},\mu}^{(+)} + \exp[-Q_{\mu}(q)L] \langle l, -m | \mathcal{B} \mathcal{A}^{\dagger}(\hat{\mathbf{q}}) | \eta_{\mu}(q) \rangle F_{\mathbf{q},\mu}^{(-)} \} \\ = \exp(-i\mathbf{q} \cdot \boldsymbol{\rho}_0) Y_{lm}^*(\hat{\mathbf{s}}_0; \hat{\mathbf{z}}), \quad (56)$$

$$\sum_{\mu} \{ \exp[-Q_{\mu}(q)L] \langle lm | \mathcal{B} \mathcal{A}(\hat{\mathbf{q}}) | \tilde{\eta}_{\mu}(q) \rangle F_{\mathbf{q},\mu}^{(+)} + \langle l, -m | \mathcal{B} \mathcal{A}^{\dagger}(\hat{\mathbf{q}}) | \tilde{\eta}_{\mu}(q) \rangle F_{\mathbf{q},\mu}^{(-)} \} = 0. \quad (57)$$

This set of equations is the analogue of (50) for the case of a finite slab. In the limit $L \rightarrow \infty$ one has $F_{\mathbf{q},\mu}^{(-)} = 0$ and (56) coincides with (50). We note that for a fixed \mathbf{q} , (56), (57) is a set of $2N$ linearly independent equations for $2N$ unknowns. The methods briefly discussed in section 3.6.1 can be used to obtain the solution.

3.6.3. Internal source in a half-space. Next, we consider an internal source in the half-space $z > 0$. Here we assume that there are no external sources. However, if this is not so, the solution can be obtained by simple superposition.

Consider a point unidirectional source of the form $\varepsilon = \delta(\boldsymbol{\rho} - \boldsymbol{\rho}_0)\delta(z - z_0)\delta(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0)$, where $z_0 > 0$. The general solution in the region $0 < z < z_0$ is written as

$$I(\mathbf{r}, \hat{\mathbf{s}}) = \int \frac{d^2q}{(2\pi)^2} \sum_{\mu}' [V_{\mathbf{q},\mu} I_{\mathbf{q},\mu}^{(-)}(\mathbf{r}, \hat{\mathbf{s}}) I_{-\mathbf{q},\mu}^{(+)}(\mathbf{r}_0, -\hat{\mathbf{s}}_0) + F_{\mathbf{q},\mu}^{(+)} I_{\mathbf{q},\mu}^{(+)}(\mathbf{r}, \hat{\mathbf{s}})]. \quad (58)$$

The second term in the square brackets in the right-hand side of the above expression can be interpreted as the surface term in the Kirchhoff-type formula for Green's function (for the formulation of the Kirchhoff integral specific to the RTE see [25] or, for a more detailed derivation, [28]). The boundary condition at the interface $z = 0$ reads

$$I_0(\boldsymbol{\rho}, \hat{\mathbf{s}}) = 0, \quad \text{if } \hat{\mathbf{s}} \cdot \hat{\mathbf{z}} > 0. \quad (59)$$

The fact that the boundary condition is homogeneous reflects the fact that there are no external sources. The latter can be included by considering an inhomogeneous boundary condition of the type (47). By analogy with section 3.6.1, we immediately arrive at the following set of equations for the unknown coefficients $F_{\mathbf{q},\mu}^{(+)}$:

$$\sum_{\mu}' [\langle lm | \mathcal{B}\mathcal{A}(\hat{\mathbf{q}}) | \eta_{\mu}(q) \rangle F_{\mathbf{q},\mu}^{(+)} + V_{\mathbf{q},\mu} \langle l, -m | \mathcal{B}\mathcal{A}^{\dagger}(\hat{\mathbf{q}}) | \eta_{\mu}(q) \rangle I_{-\mathbf{q},\mu}^{(+)}(\mathbf{r}_0, -\hat{\mathbf{s}}_0)] = 0. \quad (60)$$

Similar to (50), this is a set of N linearly independent equations with respect to N unknowns.

4. Numerics

Now we illustrate the expressions obtained in section 3.3 for the RTE Green's function in an infinite medium with several numerical examples. We have computed Green's function by truncating the series in (23) at $l, l' \leq l_{\max}$ and using the reference frame in which the z -axis is aligned with the direction of the source, $\hat{\mathbf{s}}_0$. Correspondingly, the expression (26) was used to compute the matrix elements of χ . Note that in this expression the summation over M and j is finite; however, the summation over the modes $|\psi_{\mu}\rangle$ is infinite and must be truncated. We have found empirically that, for each block $B(M)$ of the matrix W , summation over $N = 500$ eigenmodes (which corresponds to 1000×1000 matrices $B(M)$) is sufficient for all cases shown below. Further increase of N does not change the result within double precision machine accuracy. The results start to deviate noticeably from those computed at $N = 500$ when N is taken to be smaller than ~ 100 , especially when l_{\max} is relatively large. Further, we have used the Henyey–Greenstein model for the phase function, so that $A_l = g^l$ where $0 < g < 1$ is a parameter. In all figures shown below we calculate the specific intensity $I(\mathbf{r}, \hat{\mathbf{s}})$ due to a point unidirectional source placed at the origin and illuminating in the z -direction. The distance from the source is measured in units of the transport free path, $\ell^* = 1/[\mu_a + (1 - g)\mu_s]$, which plays an important role in diffusion theory.

It should be noted that numerical implementation of the formulae derived in this paper requires a degree of caution because Green's function of the RTE is not square integrable with respect to both of its arguments, \mathbf{r} and $\hat{\mathbf{s}}$. Therefore, one cannot expect uniform point-wise convergence of the result with l_{\max} . Mathematically, this is manifested by the fact

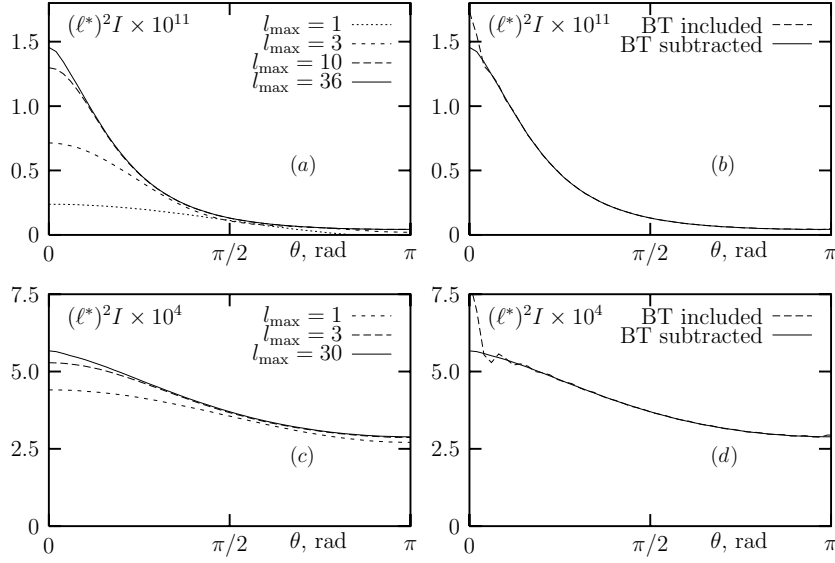


Figure 2. Angular dependence of the specific intensity for forward propagation at the distance z from the source. Left column (a), (c): convergence with parameter l_{\max} . Right column (b), (d): solid line shows the converged result obtained with subtraction of the ballistic term; dashed line: result obtained without subtraction of the ballistic term for the same l_{\max} . Top row (a), (b): $g = 0.5$, $\mu_a/\mu_s = 0.5$, $z = 20\ell^*$. Bottom row (c), (d): $g = 0.2$, $\mu_a/\mu_s = 0.01$ and $z = 10\ell^*$.

that the Bessel functions $k_l(x)$ that enter into (25), (26) diverge factorially for large orders: $k_l(x) \propto l!!(l \rightarrow \infty)$. This growth cannot be compensated either by the Clebsch–Gordan coefficients, or by the eigenvector components $\langle lm|\psi_\mu\rangle$ which decay, at best, exponentially (see discussion in section 3.2.3). Therefore, (23), (25), (26) must be viewed as expressions defining the *moments* of Green’s function and the latter as a generalized function or a distribution. Nevertheless, in most practical situations, the spatial and angular dependences of Green’s function can be approximated by smooth square-integrable functions by truncating (23) at certain values of l_{\max} that provide desirable angular resolution. Computations are further facilitated by analytical subtraction of the *ballistic component* of Green’s function:

$$G_b(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}_0, \hat{\mathbf{s}}_0) = \delta(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0)\delta(\hat{\mathbf{R}} - \hat{\mathbf{s}}_0)\frac{\exp(-\mu_t R)}{R^2}, \quad \mathbf{R} = \mathbf{r} - \mathbf{r}_0. \quad (61)$$

The corresponding ballistic contribution to χ_b is

$$\langle lm|\chi_b(R; \hat{\mathbf{s}}_0)|l'm'\rangle = \delta_{m0}\sqrt{(2l+1)(2l'+1)}\frac{\exp(-\mu_t R)}{4\pi R^2}. \quad (62)$$

However, it is impossible to remove the singularities *completely*, and the remainder of such a subtraction still remains non-square integrable.

The effect of subtraction of the ballistic term and convergence with l_{\max} for forward propagation is illustrated in figure 2. Here θ is the angle between the direction of observation, $\hat{\mathbf{s}}$, and the positive direction of the z -axis: $\cos\theta = \hat{\mathbf{s}} \cdot \hat{\mathbf{z}}$. In the left column (plots (a), (c)) we show the dependence of the specific intensity (with the ballistic term subtracted) on the maximum order of spherical functions l_{\max} . We assumed that convergence was reached when incrementing l_{\max} by 1 resulted in less than 0.1% relative change of the specific intensity in any direction. However, we emphasize again that this convergence is asymptotic. In the right column of images (b), (d), we compare the angular dependence of the specific intensity for the

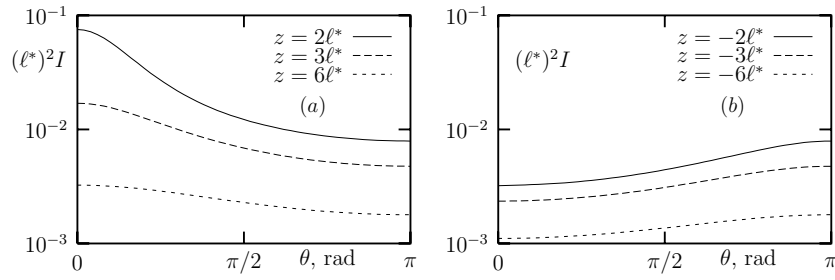


Figure 3. Angular dependence of the specific intensity for forward (a) and backward (b) propagation obtained at $l_{\max} = 21$, $g = 0.98$ and $\mu_a/\mu_s = 6 \cdot 10^{-5}$. The distance to the source z is assumed to be positive for forward propagation and negative for backward propagation.

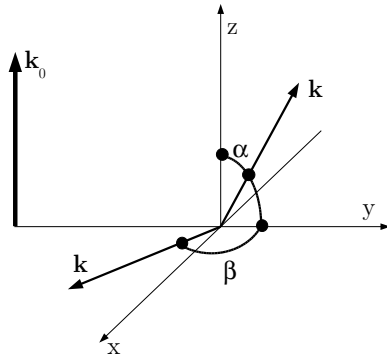


Figure 4. Illustration of angles α and β .

maximum value of l_{\max} which was used in the graph to the left with and without the ballistic term. Note that the subtracted ballistic term can be added back analytically to the solutions obtained. In all figures shown below, the ballistic term is subtracted.

Figure 3 illustrates the specific intensity for forward and backward propagation. Optical parameters were chosen to be close to those of typical biological tissues in the near infrared spectral region (see figure caption for details). The point of observation is placed at $\mathbf{r} = (0, 0, z)$, where z is positive for forward propagation and negative for backward propagation, and θ is defined in both cases as the angle between the vector $\hat{\mathbf{s}}$ and the positive direction of the z -axis. It can be seen from the figure that the specific intensity in the backward direction is significantly smaller compared to that in the forward direction, even at relatively large source–detector separations ($|z| = 6l^*$). It can be also seen that the angular distribution of the specific intensity in the forward direction is more sharply peaked than that in the backward direction. This can be explained by noting that backward propagation involves more scattering events than forward propagation of the same distance.

Now we turn to the off-axis case. Here the source is still placed at the origin and illuminates in the positive z direction, while the point of observation is placed at a point $\mathbf{r} = (0, y, 0)$. Below, we show two type of graphs. In the first case, the vector $\hat{\mathbf{s}}$ is in the y - z plane, and its orientation is characterized by the angle α with respect to the positive direction of the z -axis. In the second case, $\hat{\mathbf{s}}$ is in the x - y plane (perpendicular to $\hat{\mathbf{s}}_0$) and is characterized by the angle β with respect to the positive direction of the y -axis. The angles α and β (not to be confused with the Euler angles) are illustrated in figure 4. Note that α varies from 0 to 2π while β is restricted to the interval $[0, \pi]$ due to the obvious symmetry.

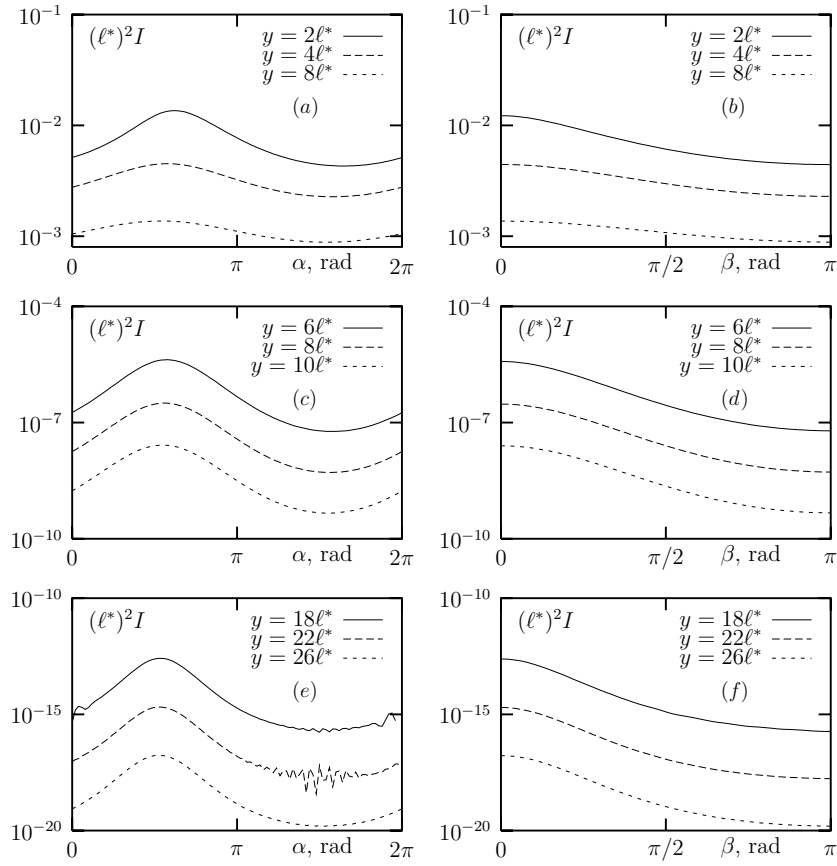


Figure 5. Angular distribution of specific intensity for off-axis propagation. Parameters: $g = 0.98$ and $\mu_a/\mu_s = 6 \cdot 10^{-5}$ (a), (b), $\mu_a/\mu_s = 0.03$ (c), (d), $\mu_a/\mu_s = 0.2$ (e), (f).

In figure 5 we illustrate the specific intensity for highly forward-peaked scattering ($g = 0.98$) and the following three different ratios of μ_a/μ_s : $6 \cdot 10^{-5}$, 0.03 and 0.2. Note that the corresponding ratios of μ_a/μ'_s , where $\mu'_s = (1 - g)\mu_s$ is the reduced scattering coefficient, are 0.003, 1.5 and 10, respectively. In the first case, the transport mean free path is mainly determined by scattering, while in the third case it is determined by absorption. The left column of images (a), (c), (e) illustrates the angular dependence of the specific intensity as a function of the angle α (vector \hat{s} is in the y - z plane). The oscillations visible in figure 5(e) is due to the non-square integrability discussed above. However, the values of the specific intensity at the region where the oscillations are visible are 2 to 3 orders of magnitude smaller than those at the peak.

It is interesting to analyse the position of the maximum of the curves in figures 5(a), (c), (e), α_0 . As the distance between the source and the detector increases, α_0 approaches $\pi/2$. This corresponds to a vector \hat{s} coinciding with the direction from the source to detector. However, for relatively small source–detector separations, α_0 is larger than $\pi/2$. The dependence of α_0 on the source–detector separation is illustrated in figure 6(a) for physiological parameters. The dependence of α_0 on the source–detector separation can be understood at the qualitative level. Indeed, at large separations, the angular distribution of the specific intensity is expected to be independent of the source orientation, with the maximum attained when \hat{s} is aligned

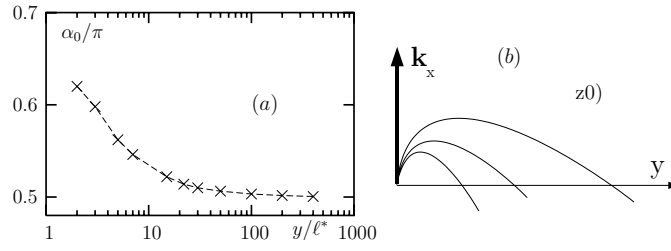


Figure 6. (a) Dependence of the position of maximum α_0 on the distance to the source, y , for physiological parameters: $g = 0.98$ and $\mu_a/\mu_s = 6 \cdot 10^{-5}$. (b) Schematic illustration of typical 'photon trajectories' that correspond to maxima in graphs 5(a), (c), (e).

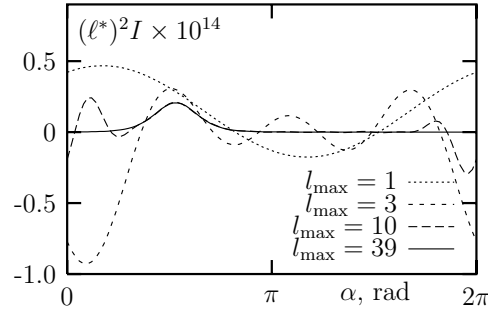


Figure 7. Convergence of the specific intensity with l_{\max} for $g = 0.98$, $\mu_a/\mu_s = 0.2$ and $y = 22\ell^*$.

with the direction from the source to the detector. This corresponds to $\alpha_0 = \pi/2$. At smaller separations, the 'photons' arrive at the detector locations along some 'typical' (most probable) trajectories which are schematically illustrated in figure 6(b). We assume here that α_0 is determined by the angle at which the most probable trajectory crosses the y -axis.

In figures 5(b), (d), (f), the specific intensity is shown as a function of the angle β (vector \hat{s} is in the x - y plane). In this case, the maximum of the curves always corresponds to $\beta = 0$, which could be also inferred from the symmetry. We note that $I_{xy}(\beta = 0) = I_{yz}(\alpha = \pi/2)$, where the lower subscripts indicate the plane in which contains the vector \hat{s} .

The curves shown in figure 5 have a dynamic range of approximately 10^3 . A dynamic range of this magnitude was obtained due to the use of large values of l_{\max} . For smaller values of l_{\max} , the result can be grossly inaccurate and even negative. For example, in figure 7 we illustrate convergence with l_{\max} to one of the curves shown in figure 5(e). An accurate value of specific intensity at $\alpha \approx \pi/2$ ($\approx 10^{-3}$ relative error) was obtained at $l_{\max} = 39$. Note that at $l_{\max} = 10$, the computed specific intensity is still grossly inaccurate.

5. Discussion

The theoretical approach developed in this paper is, essentially, a spectral approach. Spectral methods have been studied extensively for the one-dimensional RTE [29]. However, in the 3D case these methods become very difficult to use. The substantially novel element of this paper is that we derive a usable spectral method for the full three-dimensional RTE with an arbitrary phase function and planar boundaries. The analytical part of the solution is of considerable complexity. However, this complexity is traded for the relative simplicity of the numerical

part. In fact, we believe that we have reduced the numerical part of the computations to the absolute minimum which is allowed by the mathematical nature of the problem.

This paper is limited to consideration of spatially independent optical coefficients and phase functions. However, we note that Green's function for a macroscopically homogeneous medium is of special interest, since it is used in linearized image reconstruction in optical tomography [24] and, more generally, in nonlinear image reconstruction based on the inversion of a functional series or the Newton–Kantorovich method [30]. Assuming the presence of only absorptive inhomogeneities in the medium, the linearized kernel of the integral equation of diffusion tomography has the form (in the slab imaging geometry) [24]

$$\Gamma(\rho_1, \rho_2; \mathbf{r}) = \int G(\rho_1, z=0, \hat{\mathbf{s}}_1 = \hat{\mathbf{z}}; \mathbf{r}, \hat{\mathbf{s}}) G(\mathbf{r}, \hat{\mathbf{s}}; \rho_2, z=L, \hat{\mathbf{s}}_2 = \hat{\mathbf{z}}) d^2s, \quad (63)$$

where ρ_1 and ρ_2 are the transverse coordinates of the source and detector, respectively, located on opposite surfaces of the slab, and G is the slab Green's function with constant absorption and scattering coefficients. One of the advantages of solutions obtained in this paper, compared to those based on discrete ordinates, is that the angular integral in the above formula can be evaluated analytically [31].

Acknowledgment

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Appendix A. Calculation of the integral (24)

In this appendix we evaluate the integral (24) for different choices of $\hat{\mathbf{z}}$. Written in component form, this integral reads

$$\begin{aligned} \langle lm | \chi(\mathbf{r}; \hat{\mathbf{z}}) | l' m' \rangle &= \frac{1}{\sqrt{\sigma_l \sigma_{l'}}} \sum_{m_1=-l}^l \sum_{m_2=-l'}^{l'} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \exp(i\mathbf{k} \cdot \mathbf{r}) \exp[-i(m - m')\varphi_{\mathbf{k}}] \\ &\times d_{mm_1}^l(\theta_{\mathbf{k}}) d_{m'm_2}^{l'}(\theta_{\mathbf{k}}) \sum_{\mu} \frac{\langle lm_1 | \psi_{\mu} \rangle \langle \psi_{\mu} | l' m_2 \rangle}{1 + ik\lambda_{\mu}}. \end{aligned} \quad (A.1)$$

We start with the case $\hat{\mathbf{z}} = \hat{\mathbf{r}}$. Then we have $\mathbf{k} \cdot \hat{\mathbf{r}} = kr \cos \theta_{\mathbf{k}}$. We also note that $\langle lm_1 | \psi_{\mu} \rangle \langle \psi_{\mu} | l' m_2 \rangle \propto \delta_{m_1 m_2}$, so that the summation over m_1 and m_2 can be replaced by summation over a single index M which runs from $-\bar{l}$ to \bar{l} , where $\bar{l} = \min(l, l')$. Then (A.1) can be rewritten as

$$\langle lm | \chi(\mathbf{r}; \hat{\mathbf{r}}) | l' m' \rangle = \frac{1}{\sqrt{\sigma_l \sigma_{l'}}} \sum_{M=-\bar{l}}^{\bar{l}} \int_0^{\infty} \frac{k^2 dk}{(2\pi)^2} \sum_{\mu} \frac{\langle lM | \psi_{\mu} \rangle \langle \psi_{\mu} | l' M \rangle}{1 + ik\lambda_{\mu}} I, \quad (A.2)$$

where I is the angular part of the integral (the list of formal arguments of I is omitted):

$$I = \int \frac{\sin \theta_{\mathbf{k}} d\theta_{\mathbf{k}} d\varphi_{\mathbf{k}}}{2\pi} \exp[i(m' - m)\varphi_{\mathbf{k}}] \exp(ikr \cos \theta_{\mathbf{k}}) d_{mM}^l(\theta_{\mathbf{k}}) d_{m'M}^{l'}(\theta_{\mathbf{k}}). \quad (A.3)$$

The integral over $\varphi_{\mathbf{k}}$ is evaluated immediately with the result $2\pi \delta_{mm'}$. Integration over $\theta_{\mathbf{k}}$ requires expanding the exponent in the integrand as

$$\exp(ikr \cos \theta_{\mathbf{k}}) = \sum_{L=0}^{\infty} i^L (2L+1) j_L(kr) d_{00}^L(\theta_{\mathbf{k}}), \quad (A.4)$$

where $j_L(x)$ are the spherical Bessel functions of the first kind, and using the following formula (see [27], section 4.11.2, formula 8, and the symmetry properties of d -functions given in section 4.11, formula 1 of the same reference):

$$\int_0^\pi d_{mM}^l(\theta) d_{mM}^{l'}(\theta) d_{00}^L(\theta) \sin \theta \, d\theta = \frac{2(-1)^{m-M}}{2L+1} C_{l,m,l',-m}^{L,0} C_{l,M,l',-M}^{L,0}, \quad (\text{A.5})$$

where $C_{j_1 m_1 j_2 m_2}^{j_3 m_3}$ are the Clebsch–Gordan coefficients. Taking into account that $C_{l,m,l',-m}^{L,0}$ is nonzero only for $|l-l'| \leq L \leq l+l'$, we obtain

$$I = 2\delta_{mm'}(-1)^{m-M} \sum_{L=|l-l'|}^{l+l'} i^L j_L(kr) C_{l,m,l',-m}^{L,0} C_{l,M,l',-M}^{L,0}. \quad (\text{A.6})$$

Next, we substitute this result into (A.5) and, after some rearrangement, arrive at

$$\begin{aligned} \langle lm | \chi(\mathbf{r}; \hat{\mathbf{r}}) | l' m' \rangle &= \frac{2\delta_{mm'}(-1)^m}{\sqrt{\sigma_l \sigma_{l'}}} \sum_{M=-\bar{l}}^{\bar{l}} (-1)^M \sum_{L=|l-l'|}^{l+l'} i^L C_{l,m,l',-m}^{L,0} C_{l,M,l',-M}^{L,0} \\ &\times \sum_{\mu} \langle lM | \psi_{\mu} \rangle \langle \psi_{\mu} | l'M \rangle \int_0^\infty \frac{k^2 \, dk}{(2\pi)^2} \frac{j_L(kr)}{1 + ik\lambda_{\mu}}. \end{aligned} \quad (\text{A.7})$$

To evaluate the radial integral, we exploit the symmetry properties of the above expression. First, we note that $C_{l,M,l',-M}^{L,0} = (-1)^{l+l'+L} C_{l,-M,l',M}^{L,0}$, while $\langle lM | \psi_{\mu} \rangle$ does not depend on the sign of M . Thus, the addition of terms with positive and negative values of M in the above formula (for $M \neq 0$) gives zero unless $l+l'+L$ is even. Likewise, in the case $M = 0$, $C_{l,0,l',0}^{L,0} = 0$ unless the above sum of indices is even. Correspondingly, the only nonzero contributions to the sum over L corresponds to $L = |l-l'| + 2j$, where the index j runs from 0 to \bar{l} . Next, we use the symmetry property of the eigenvectors discussed in section 3.2.2. This property allows one to limit summation over the eigenvector indices μ to only the values corresponding to positive eigenvalues λ_{μ} while simultaneously replacing the factor $1/(1+ik\lambda_{\mu})$ by $1/(1+ik\lambda_{\mu}) + (-1)^{l+l'}/(1-ik\lambda_{\mu})$. Thus, we obtain

$$\begin{aligned} \langle lm | \chi(\mathbf{r}; \hat{\mathbf{r}}) | l' m' \rangle &= \frac{2\delta_{mm'}(-1)^m}{\sqrt{\sigma_l \sigma_{l'}}} \sum_{M=-\bar{l}}^{\bar{l}} (-1)^M \sum_{j=0}^{\bar{l}} i^{|l-l'|+2j} C_{l,m,l',-m}^{|l-l'|+2j,0} C_{l,M,l',-M}^{|l-l'|+2j,0} \\ &\times \sum_{\mu} \langle lM | \psi_{\mu} \rangle \langle \psi_{\mu} | l'M \rangle J, \end{aligned} \quad (\text{A.8})$$

where J is the radial integral given by

$$J = \int_0^\infty \frac{k^2 \, dk}{(2\pi)^2} j_{|l-l'|+2j}(kr) \frac{1 + (-1)^{l+l'} - ik\lambda_{\mu}[1 - (-1)^{l+l'}]}{1 + k^2\lambda_{\mu}^2}. \quad (\text{A.9})$$

The parity of the Bessel functions in the above integral is the same as that of $l+l'$. Therefore, the integrand is an even function of k for all values of the indices, and the integral can be extended to $-\infty$ and calculated by residues. The result is

$$J = \pi i^{-(|l-l'|+2j)} \lambda_{\mu}^{-3} k_{|l-l'|+2j}(r/\lambda_{\mu}). \quad (\text{A.10})$$

Upon substitution of this result into (A.8), we obtain the formula (25).

In the case $\hat{\mathbf{z}} = \hat{\mathbf{s}}_0$ the dot product $\mathbf{k} \cdot \mathbf{r}$ cannot be written as $kr \cos \theta_{\mathbf{k}}$. Therefore, the exponent in the angular integral I is expanded as

$$\exp(i\mathbf{k} \cdot \mathbf{r}) = 4\pi \sum_{LM'} i^L j_L(kr) Y_{LM'}(\hat{\mathbf{k}}; \hat{\mathbf{s}}_0) Y_{LM'}^*(\hat{\mathbf{r}}; \hat{\mathbf{s}}_0). \quad (\text{A.11})$$

We further take advantage of the identity

$$Y_{LM'}(\theta_{\mathbf{k}}, \varphi_{\mathbf{k}}) = (-1)^{M'} \sqrt{4\pi/(2L+1)} d_{0M'}^L(\theta_{\mathbf{k}}) \exp(iM'\varphi_{\mathbf{k}}) \quad (\text{A.12})$$

to transform the angular integration to the general form (A.6). Note that azimuthal integration results in a factor of $\delta_{M'm}$ and thus removes summation over M' . The final result for I is

$$I = \frac{2(-1)^l \sqrt{4\pi}}{\sqrt{2l'+1}} \sum_{L=|l-l'|}^{l+l'} i^L j_L(kr) Y_{Lm}^*(\hat{\mathbf{r}}; \hat{\mathbf{s}}_0) C_{l,M,L,0}^{l',M} C_{l,m,l',0}^{L,m}, \quad (\text{A.13})$$

where we have also used $C_{L,M,l'-M}^{L,0} = (-1)^{l-M} \sqrt{(2L+1)/(2l'+1)} C_{l,M,L,0}^{l',M}$. The radial integration, and the symmetry considerations explained above, remain without change. Substitution of (A.13) into (A.2) and subsequent radial integration leads to the formula (26).

Appendix B. Calculation of the integral (28)

Integral (28), written in terms of components, reads

$$\langle lm|\kappa(\mathbf{q}; z)|l'm'\rangle = \frac{\exp[-i(m-m')]}{\sqrt{\sigma_l \sigma_{l'}}} \sum_{M=-l}^l \sum_n \frac{\langle l|\phi_n(M)\rangle \langle \phi_n(M)|l'\rangle}{\lambda_{nM}^2} I. \quad (\text{B.1})$$

Here I is the integral over k_z :

$$I = \int_{-\infty}^{\infty} \frac{dk_z}{2\pi} \exp(ik_z z) d_{mM}^l(\theta) d_{m'M}^{l'}(\theta) \frac{1 + (-1)^{l+l'} - i\lambda_{Mn} \sqrt{q^2 + k_z^2} [1 - (-1)^{l+l'}]}{k_z^2 + q^2 + 1/\lambda_{Mn}^2}, \quad (\text{B.2})$$

where we have used the notations introduced in section 3.2.1 for block eigenvectors $|\phi_n(M)\rangle$. The angle θ is defined by (29) in section 3.4. The Wigner d -functions can be written in terms of $\cos \theta$ as

$$d_{mM}^l(\theta) = \xi_{mM} Z_{mM}^l \left(\frac{1 - \cos \theta}{2} \right)^{\frac{|m-M|}{2}} \left(\frac{1 + \cos \theta}{2} \right)^{\frac{|m+M|}{2}} P_s^{(u,v)}(\cos \theta), \quad (\text{B.3})$$

where $\xi_{mM} = 1$ if $m \leq M$ and $\xi = (-1)^{m+M}$ if $m > M$,

$$Z_{mM}^l = \sqrt{\frac{(l - |m - M|/2 - |m + M|/2)! (l + |m + M|/2 - |m + M|/2)!}{(l + |m - M|/2 - |m + M|/2)! (l - |m + M|/2 - |m + M|/2)!}}, \quad (\text{B.4})$$

and $P_s^{(u,v)}(x)$ in expression (B.3) are Jacobi polynomials with $s = l - |m - M|/2 - |m + M|/2$, $u = |m - M|$ and $v = |m + M|$.

The integrand in (B.2) is not, in general, an analytic function of k_z . However, the expression for Green's function contains a summation over M . It can be shown explicitly that the combination

$$d_{mM}^l(\theta) d_{m'M}^{l'}(\theta) + d_{m-M}^l(\theta) d_{m'-M}^{l'}(\theta) \quad (\text{B.5})$$

contains only even powers of the factor $\sqrt{k_z^2 + q^2}$ if $l + l'$ is even and only odd powers of the same factor if $l + l'$ is odd (a general proof of this statement is available but omitted). Taking into account the factor $\sqrt{q^2 + k_z^2} [1 - (-1)^{l+l'}]$ in the right-hand side of (B.2), we arrive at the conclusion that the integrand becomes analytic after addition of terms with positive and negative values of M . Note that the eigenvectors and eigenvalues do not depend on the sign of M and the above consideration applies to the case $M = 0$. Consequently, one can evaluate (B.2) by residues choosing a branch of the complex-valued function $\sqrt{k_z^2 + q^2}$ arbitrarily.

The integrand of (B.2) has simple poles at $k_z = \pm i\sqrt{q^2 + 1/\lambda_{Mn}^2}$. Taking into account these poles leads to the following expression:

$$I = \frac{[\text{sgn}(z)]^{l+l'+m+m'} \lambda_{Mn} \exp[-\sqrt{1 + (q\lambda_{Mn})^2} |z|/\lambda_{Mn}]}{\sqrt{1 + (q\lambda_{Mn})^2}} d_{mM}^l[i\tau(q\lambda_{Mn})] d_{m'M}^{l'}[i\tau(q\lambda_{Mn})]. \quad (\text{B.6})$$

Substitution of (B.6) into (B.1) leads to an expression which is equivalent to (28).

We note that the integrand of (B.2) has another set of poles. Namely, these are poles of the functions $d_{mM}^l[\theta(k_z)]$ at $k_z = \pm iq$. These poles are of a purely geometrical nature. We have calculated analytically the contributions of these poles to Green's function to the few lowest orders in l, l' , and found that they cancel each other. However, we do not have a general proof of such cancellation to all orders. On the other hand, it is clear that if these poles could contribute to the plane-wave decomposition of Green's function, the result would not satisfy the RTE since the matrix W is bounded and has no infinite eigenvalues. To confirm the validity of the obtained analytical expression, we have computed I numerically by the fourth-order Simpson rule for a model set of parameters. Then we used this result to compute Green's function for the particular case $\hat{s} = \hat{s}_0 = \hat{z}$. The result coincided with the one predicted by formula (35) with machine accuracy in double precision.

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