Journal of Quantitative Spectroscopy & Radiative Transfer 97 (2006) 228–251

Journal of Quantitative Spectroscopy & Radiative Transfer

www.elsevier.com/locate/jqsrt

Vector Green's function algorithm for radiative transfer in plane-parallel atmosphere

Yi Qin*, Michael A. Box

School of Physics, University of New South Wales, Australia

Received 17 January 2005; accepted 14 April 2005

Abstract

Green's function is a widely used approach for boundary value problems. In problems related to radiative transfer, Green's function has been found to be useful in land, ocean and atmosphere remote sensing. It is also a key element in higher order perturbation theory. This paper presents an explicit expression of the Green's function, in terms of the source and radiation field variables, for a plane-parallel atmosphere with either vacuum boundaries or a reflecting (BRDF) surface. Full polarization state is considered but the algorithm has been developed in such way that it can be easily reduced to solve scalar radiative transfer problems, which makes it possible to implement a single set of code for computing both the scalar and the vector Green's function.

Keywords: Radiative transfer; Green's function; Polarization

1. Introduction

The Green's function, which originated from the work on potential theory by Mr. George Green [1], has been widely used to solve boundary value problems [2]. The concept of Green's function has been introduced into linear transport (including radiative transfer and neutron transport) theory by Case and Zweifel [3] and Bell and Glasstone [4]. In particular, Case and

*Corresponding author. Environmental Remote Sensing Group, CSIRO Land and Water, GPO Box 1666, Canberra ACT 2601, Australia. Tel.: +61 2 62465735, fax: +61 2 62465800.

E-mail address: yi.qin@csiro.au (Y. Qin).

0022-4073/$ - see front matter
doi:10.1016/j.jqsrt.2005.04.009

Zweifel [3] developed an explicit expression for the Green's function for infinite, homogeneous, and isotropically scattering media with vanishing boundary conditions at infinity, which after being generalized to anisotropically scattering media has been used successfully to compute efficiently the particular solution of the discrete-ordinate method (DOM) [5–9].

Before proceeding to further review of works related to Green's function and its applications, we briefly discuss the concept of the Green's function and its relation with the normal radiative transfer solution computed, for example, by DOM [10,6,11].

The radiative transfer equation can be equivalently expressed in terms of the radiative transfer operator as (cf. [4]):

$$\mathbf{L}\mathbf{I}(\tau,\mu,\phi)=\mathbf{Q}(\tau,\mu,\phi), \tag{1}$$

where $\mathbf{I}$ is a 4-vector of the Stokes parameters, I, Q, U and V; $\mathbf{Q}$ is the source function, which should be given in flux rather than intensity; (τ,μ,ϕ) are respectively the optical depth, cosine of the zenith angle and the azimuth angle. The vector radiative transfer operator, $\mathbf{L}$, can be written (for plane-parallel geometry or infinite medium) as:

$$\mathbf{L}=\mu\frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{E}_4-\mathbf{E}_4+\frac{\tilde{\omega}_0(\tau)}{4\pi}\int_{-1}^{1}\mathrm{d}\mu'\int_0^{2\pi}\mathrm{d}\phi'\mathbf{M}(\tau,\mu,\phi;\mu',\phi')\circ\,, \tag{2}$$

where $\mathbf{E}_4$ is the 4×4 identity matrix; $\tilde{\omega}_0$ is the single scattering albedo; $\mathbf{M}$ is the scattering matrix whose detail does not affect our discussion in this section and will be discussed in the next section. The symbol, "$\circ$", in the last term denotes the object on which the integral operator acts, and when $\mathbf{I}$ is inserted into the integration, its arguments (μ,ϕ) should be replaced by (μ',ϕ'). We specify that the τ axis points downwards and $\mu=\pm1$ point to the zenith and the nadir respectively.

In the case that $\mathbf{Q}$ takes the special form of

$$\mathbf{Q}(\tau,\mu,\phi)=\delta(\tau-\tau_0)\delta(\mu-\mu_0)\delta(\phi-\phi_0)\mathbf{E}_4, \tag{3}$$

we denote the solution of Eq. (1) as $\mathbf{G}$, i.e.,

$$\mathbf{L}\mathbf{G}(\tau,\mu,\phi;\tau_0,\mu_0,\phi_0)=\delta(\tau-\tau_0)\delta(\mu-\mu_0)\delta(\phi-\phi_0)\mathbf{E}_4. \tag{4}$$

It is apparent that $\mathbf{G}$ must be a 4×4 matrix function, and Eq. (3) represents a generalized beam source that illuminates in a mono-direction from a given vertical location, and extends horizontally indefinitely.

Eq. (4) is often used as the definition of the Green's function. Multiply both sides of Eq. (4) from the right with $\mathbf{Q}(\tau_0,\mu_0,\phi_0)$, integrate over τ_0, μ_0 and ϕ_0 over the whole valid range, and note that every term of the $\mathbf{L}$ operator can be moved outside the integrations. We obtain:

$$L\left(\iiint\mathrm{d}\tau_0\,\mathrm{d}\mu_0\,\mathrm{d}\phi_0\mathbf{G}(\tau,\mu,\phi;\tau_0,\mu_0,\phi_0)\mathbf{Q}(\tau_0,\mu_0,\phi_0)\right)=\mathbf{Q}(\tau,\mu,\phi). \tag{5}$$

Comparing Eq. (5) with Eq. (1) suggests that

$$\mathbf{I}(\tau,\mu,\phi)\equiv\iiint\mathrm{d}\tau'\,\mathrm{d}\mu'\,\mathrm{d}\phi'\mathbf{G}(\tau,\mu,\phi;\tau',\mu',\phi')\mathbf{Q}(\tau',\mu',\phi'), \tag{6}$$

which shows that the radiation field generated by an arbitrary source can be computed from the Green's function. Eq. (6) can be used as an alternative definition of the Green's function. It can be shown, by reversing the arguments leading to Eq. (5), that Eq. (4) must hold if Eq. (6) is true.

We note that the Green's function can be uniquely determined only after the domain of the problem and the associated boundary conditions have been specified. The radiation field as computed by Eq. (6) is also a function of the domain and boundary condition of the Green's function being used. For example, with the infinite medium Green's function (IMGF) the result of Eq. (6) will be the radiation field that satisfies the vanishing boundary condition at infinity. In addition to the IMGF, the (scalar) finite medium Green's function (FMGF) has also been found to be very useful in some applications, as discussed in following paragraphs.

In surface remote sensing, the so called atmosphere—BRDF (Bi-directional Reflectance Distribution Function) coupling has been a challenging task in the past. By means of the FMGF, Lyapustin and Knyazikhin [12,13] showed that the radiance observed from space can be explicitly expressed in terms of the surface BRDF, which generalizes the expression for Lambertian surfaces [14]. This formulation allows for re-computing the radiance for updated surface parameters without re-solving the atmosphere radiative transfer equation. Therefore, it allows for quick trial-evaluation loops. Landgraf et al. [15] also used FMGF in surface remote sensing in connection with perturbation theory [16,17]. However, although the concept of the Green's function is used in these works, the explicit expression for the FMGF is not provided. In Lyapustin and Knyazikhin [12] it is briefly mentioned that a standard radiative transfer code is used to compute the Green's function, while in Landgraf et al. [15] the method is not discussed.

In the computation of higher order radiative perturbation [16,18,19], the Green's function is a key step which requires us to compute the FMGF. We may use a standard radiative transfer code (assuming it supports beam sources of arbitrary position and direction) to accumulate a numerical Green's function by solving the radiative transfer equation for a set of beam sources of different angles and positions. However, this approach is, at least, inefficient even after extending the DOM for fast multi-source solutions [20,8]. Furthermore, a numerical Green's function does not allow for analytical calculations on the source variables. Such ability could be critical, for example, in higher order perturbation computation where, by employing the explicit FMGF expression, we have demonstrated very significant CPU-time reduction [21].

Green's function was used by Benedetti et al. [22] to investigate the influence of cloud and aerosol vertical (extinction coefficient) variation on remotely sensed reflected sunlight. An explicit expression for the FMGF was developed in this work using matrix exponential together with a doubling-adding approach. However, this complicated expression was derived for a single layer only, and the radiance (or equivalently the source) is restricted to be at the two boundaries of the layer. The work by Benedetti et al. [22] therefore provides a special case of the FMGF but (unfortunately) it is not what we were searching for, and the approach used by them probably is also difficult to be generalized for arbitrary radiance (or source) position in multi-layered media.

Applications of the Green's function concept are explored by several other authors as well, for example in cloud remote sensing [23,24], in surface BRDF modeling [25], and the application of the IMGF in neutron transport problems [26,27]. These works however also did not provide an explicit expression for the FMGF.

The purpose of this paper is to present an explicit expression for the finite medium Green's function, in terms of the source and radiance position and direction, for a vertically varying and anisotropically scattering atmosphere with two boundary types including a reflective (BRDF) surface. Our development will consider the full polarization state, but it has been done in such way that the formulation for the scalar (intensity only) case can be written out systematically. We note that the main purpose of this paper is not to present an alternative algorithm for solving normal forward radiative transfer problems, such as the DOM [10,6,14,11], which considers the source as fixed (direction and position) rather than as variable. However the Green's function algorithm, as will be seen, does have deep roots in DOM.

In the next section, the Green's function for an infinite medium is re-developed, making the paper more self-contained. The finite medium Green's function for vacuum surface and BRDF surface are then presented in Sections 3 and 3.2 respectively. We summarize finally in Section 4. A number of appendices are included to provide better support for the main paper.

2. Infinite medium Green's function

This section derives the expression for the IMGF, in terms of the source variables, (τ_0, μ_0, ϕ_0), and radiation field variables, (τ, μ, ϕ). The contents of this section are not new but are included to be more self-contained.

2.1. The problem of the infinite medium Green's function

In the case of an infinite, homogeneous and arbitrarily scattering atmosphere, plane-parallel geometry can be used but the origin of the optical depth may be set arbitrarily. We rewrite the radiative transfer equation for the Green's function, Eq. (4), in the more common form of an integral-differential equation as

$$\begin{aligned}\mu\frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{G}(\tau,\mu,\phi;\tau_0,\mu_0,\phi_0) &= \mathbf{G}(\tau,\mu,\phi;\tau_0,\mu_0,\phi_0)\\ &-\frac{\tilde{\omega}_0}{4\pi}\int_{-1}^{1}\mathrm{d}\mu'\int_0^{2\pi}\mathrm{d}\phi'\mathbf{M}(\mu,\phi;\mu',\phi')\mathbf{G}(\tau,\mu',\phi';\tau_0,\mu_0,\phi_0),\end{aligned} \tag{7}$$

where $\tilde{\omega}_0$ and $\mathbf{M}$ do not depend on τ. In Eq. (7) the source term, Eq. (3), is not included: it is imposed (equivalently) through the so called "jump condition" [3]:

$$\lim_{\tau\to\tau_0-}\mathbf{G}(\tau,\mu,\phi;\tau_0,\mu_0,\phi_0)-\lim_{\tau\to\tau_0+}\mathbf{G}(\tau,\mu,\phi;\tau_0,\mu_0,\phi_0)=\frac{\delta(\mu-\mu_0)\delta(\phi-\phi_0)}{\mu}\mathbf{E}_4 \tag{8}$$

which is easily understood according to the energy conservation law. We see that $\mathbf{G}$ is discontinuous at $\tau=\tau_0$. In Eq. (8) $1/\mu$ is added to the right-hand side because the source is unit flux, or $1/\mu$ unit intensity. In addition to the jump condition, the following vanishing boundary condition should also be satisfied

$$\lim_{\tau-\tau_0\to\pm\infty}\mathbf{G}(\tau,\mu,\phi;\tau_0,\mu_0,\phi_0)=\mathbf{0} \tag{9}$$

which should always be physically true under the current setting except in the case of ideally vacuum medium, a condition which can be handled easily and is excluded from this work.

So far the scattering property of the medium has not been specified. In this work we restrict the scattering phase matrix to be of the following pattern [see Section A.3 for detailed discussions about the **M** and **P** matrices]:

$$\mathbf{P}(\zeta) = \begin{pmatrix} a_1(\zeta) & b_1(\zeta) & 0 & 0 \\ b_1(\zeta) & a_2(\zeta) & 0 & 0 \\ 0 & 0 & a_3(\zeta) & b_2(\zeta) \\ 0 & 0 & -b_2(\zeta) & a_4(\zeta) \end{pmatrix}, \tag{10}$$

which represents scattering by ensembles of randomly oriented particles with a plane of symmetry [28].

2.2. Azimuth angle expansion

We now use the normal DOM approach to reduce the radiative transfer equation and boundary conditions to a set of sub-problems, by expanding the phase matrix and Green's function in Fourier series. The matrix, **M**, can be expanded as [5,6] (see also Section A.3):

$$\mathbf{M}(\mu, \phi; \mu', \phi') = \sum_{m=0}^{2N-1} \sum_{\alpha=1}^{2} \mathbf{Z}_\alpha^m(\phi - \phi')\mathbf{A}^m(\mu, \mu')\mathbf{D}_\alpha, \tag{11}$$

where $\mathbf{Z}_1^m(\phi)$ and $\mathbf{Z}_2^m(\phi)$, as defined in Eqs. (A.45)–(A.46), are 4×4 diagonal matrices composed by $\cos(m\phi)$ and $\sin(m\phi)$, $\mathbf{D}_1$ and $\mathbf{D}_2$ are 4×4 constant diagonal matrices defined in Eq. (A.44). The matrix **A** is defined as [5,6] (see also Section A.3):

$$\mathbf{A}^m(\mu, \mu') = \sum_{l=m}^{2N-1} \mathbf{P}_l^m(\mu)\mathbf{B}_l^m\mathbf{P}_l^m(\mu'), \tag{12}$$

where $\mathbf{P}_l^m(\mu)$, defined in Eq. (A.49), is composed by several orthogonal polynomials, and $\mathbf{B}_l^m$, defined in Eq. (A.50), is the expansion of the phase matrix.

The Green's function is also expanded as

$$\mathbf{G}(\tau, \mu, \phi; \tau_0, \mu_0, \phi_0) = \sum_{m=0}^{2N-1} \sum_{\alpha=1}^{2} \mathbf{Z}_\alpha^m(\phi - \phi_0)\mathbf{G}_\alpha^m(\tau, \mu; \tau_0, \mu_0). \tag{13}$$

Insert Eqs. (11)–(13) into Eqs. (7)–(9), we obtain for $m = 0, 1, \ldots, 2N-1$ and $\alpha = 1, 2$ the following set of sub-problems (see Section A.4):

$$\mu \frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{G}_\alpha^m(\tau, \mu; \tau_0, \mu_0) = \mathbf{G}_\alpha^m(\tau, \mu; \tau_0, \mu_0) - \frac{\tilde{\omega}}{2}\int_{-1}^{1} \mathrm{d}\mu' \sum_{l=m}^{2N-1} \mathbf{P}_l^m(\mu)\mathbf{B}_l^m\mathbf{P}_l^m(\mu')\mathbf{G}_\alpha^m(\tau, \mu'; \tau_0, \mu_0) \tag{14}$$

with correspondingly the boundary conditions:

$$\lim_{\tau \to \tau_{0-}} \mathbf{G}_\alpha^m(\tau, \mu; \tau_0, \mu_0) - \lim_{\tau \to \tau_{0+}} \mathbf{G}_\alpha^m(\tau, \mu; \tau_0, \mu_0) = \frac{\delta(\mu - \mu_0)}{2\pi\mu}\mathbf{D}_\alpha \tag{15}$$

$$\lim_{\tau - \tau_0 \to \pm\infty} \mathbf{G}_\alpha^m(\tau, \mu; \tau_0, \mu_0) = \mathbf{0} \tag{16}$$

Each of these sub-problems can be solved independently, and we will only deal with Eqs. (14)–(16) thereafter. For simplicity, we will omit m from now on. The subscript, α, may also be omitted.

2.3. Elemental solutions

To solve Eq. (14) numerically, we represent the Green's function approximately as a matrix function:

$$\{\mathbf{G}(\tau, \mu_i; \tau_0, \mu_j)\}_{i,j=\pm 1,\ldots,\pm N_s}, \tag{17}$$

where μ_i's are the Gaussian quadrature points of order $2N_s$, and $\mu_{-i} \equiv -\mu_i$. Replacing the integration in Eq. (14) with Gaussian quadrature we obtain:

$$\mu_i \frac{\mathrm{d}\mathbf{G}(\tau, \mu_i; \tau_0, \mu_0)}{\mathrm{d}\tau} = \mathbf{G}(\tau, \mu_i; \tau_0, \mu_0) - \sum_{j=\pm 1}^{\pm N_s} \left(\frac{\tilde{\omega}}{2} w_j \sum_{l=m}^{2N-1} \mathbf{P}_l^m(\mu_i) \mathbf{B}_l^m \mathbf{P}_l^m(\mu_j) \mathbf{G}(\tau, \mu_j; \tau_0, \mu_0) \right)$$
$$i = \pm 1, \pm 2, \ldots, \pm N_s, \tag{18}$$

where w_j are the Gaussian quadrature weights corresponding to μ_j, and $w_{-j} \equiv w_j$. We seek the following form of solution to Eq. (18):

$$\mathbf{G}(\tau, -\mu_i; \tau_0, \mu_0) = \mathbf{D}\boldsymbol{\varphi}_j(-\mu_i) \mathrm{e}^{-\boldsymbol{\lambda}_j(\tau-\tau_0)}, \tag{19}$$

$$\mathbf{G}(\tau, +\mu_i; \tau_0, \mu_0) = \boldsymbol{\varphi}_j(+\mu_i) \mathrm{e}^{-\boldsymbol{\lambda}_j(\tau-\tau_0)}, \tag{20}$$

where $\boldsymbol{\varphi}_j(\pm\mu_i)$ are 4×4 matrices, $\boldsymbol{\lambda}_j$ are 4×4 diagonal matrices, and $\mathbf{D}$ is 4×4 constant diagonal matrix defined in Eq. (A.44). Inserting respectively Eq. (19) and Eq. (20) into Eq. (18), and noting Eqs. (A.51)–(A.52), leads to:

$$\boldsymbol{\varphi}_j(-\mu_i)\boldsymbol{\lambda}_j = \sum_{k=1}^{N_s} [-\mathbf{X}_{ik}\boldsymbol{\varphi}_j(-\mu_k) - \mathbf{Y}_{ik}\boldsymbol{\varphi}_j(+\mu_k)], \tag{21}$$

$$\boldsymbol{\varphi}_j(+\mu_i)\boldsymbol{\lambda}_j = \sum_{k=1}^{N_s} [\mathbf{Y}_{ik}\boldsymbol{\varphi}_j(-\mu_k) + \mathbf{X}_{ik}\boldsymbol{\varphi}_j(+\mu_k)], \tag{22}$$

where $\mathbf{X}_{ik}$ and $\mathbf{Y}_{ik}$ are 4×4 matrices defined by:

$$\mathbf{X}_{ik} = \mu_i^{-1} \left[\frac{\tilde{\omega}}{2} w_k \sum_{l=m}^{2N-1} \mathbf{P}_l^m(\mu_i) \mathbf{B}_l^m \mathbf{P}_l^m(\mu_k) - \delta_{ik} \mathbf{E}_4 \right], \tag{23}$$

$$\mathbf{Y}_{ik} = \mu_i^{-1} \left[\frac{\tilde{\omega}}{2} w_k \sum_{l=m}^{2N-1} (-1)^{l-m} \mathbf{P}_l^m(\mu_i) \mathbf{B}_l^m \mathbf{D} \mathbf{P}_l^m(\mu_k) \right]. \tag{24}$$

Write Eqs. (21)–(22) in more compact form:

$$\begin{bmatrix} {}_-\boldsymbol{\varphi}_j \\ {}_+\boldsymbol{\varphi}_j \end{bmatrix} \boldsymbol{\lambda}_j = \begin{bmatrix} -\mathbf{X} & -\mathbf{Y} \\ \mathbf{Y} & \mathbf{X} \end{bmatrix} \begin{bmatrix} {}_-\boldsymbol{\varphi}_j \\ {}_+\boldsymbol{\varphi}_j \end{bmatrix}, \tag{25}$$

where ${}_{\pm}\boldsymbol{\varphi}_j$ are $4N_s \times 4$ matrices and $\mathbf{X}$ and $\mathbf{Y}$ are $4N_s \times 4N_s$ matrices:

$$ {}_{\pm}\boldsymbol{\varphi}_j \equiv \{\boldsymbol{\varphi}_j(\mu_{\pm k})\}_{k=1,\ldots,N_s}, \tag{26} $$

$$ \mathbf{X} = \{\mathbf{X}_{ik}\}_{i,k=1,\ldots,N_s}, \quad \mathbf{Y} = \{\mathbf{Y}_{ik}\}_{i,k=1,\ldots,N_s}. \tag{27} $$

Eq. (25) is a general real matrix eigenvalue problem of order $8N_s$, which can be solved using any standard numerical library, e.g., LAPACK [29]. However, by adding (subtracting) the first row of Eq. (25) to (from) the second row we find:

$$ ({}_{+}\boldsymbol{\varphi}_j - {}_{-}\boldsymbol{\varphi}_j)\boldsymbol{\lambda}_j = (\mathbf{X}+\mathbf{Y})({}_{+}\boldsymbol{\varphi}_j + {}_{-}\boldsymbol{\varphi}_j), \tag{28} $$

$$ ({}_{+}\boldsymbol{\varphi}_j + {}_{-}\boldsymbol{\varphi}_j)\boldsymbol{\lambda}_j^2 = (\mathbf{X}-\mathbf{Y})(\mathbf{X}+\mathbf{Y})({}_{+}\boldsymbol{\varphi}_j + {}_{-}\boldsymbol{\varphi}_j). \tag{29} $$

Eq. (29) is an eigenvalue problem of order $4N_s$, half that of Eq. (25)—an efficient technique used first by Asano [30] for scalar radiative transfer problems. Once Eq. (29) is solved, ${}_{\pm}\boldsymbol{\varphi}_j$ can be found using Eq. (28).

Eq. (29) shows that the eigenvalues, $\boldsymbol{\lambda}_j$, must be in pairs of opposite sign. It is well known that in the case of scalar radiative transfer the eigenvalues and eigenvectors are always real valued. In the case of vector radiative transfer, it is reported by Siewert [5,6] and observed by us that some of the eigenvalues and corresponding eigenvectors could be complex valued, and those complex-valued eigenvalues and eigenvectors must be in conjugate pairs. Generally for a real valued matrix, if an eigenvalue (eigenvector) is complex valued, its conjugate must also be an eigenvalue (eigenvector) of the matrix.

To simplify notation, we put all the eigenvectors into a single matrix:

$$ \begin{bmatrix} {}_{-}\boldsymbol{\varphi}_{-1} \cdots {}_{-}\boldsymbol{\varphi}_{-N_s} & {}_{-}\boldsymbol{\varphi}_{1} \cdots {}_{-}\boldsymbol{\varphi}_{N_s} \\ {}_{+}\boldsymbol{\varphi}_{-1} \cdots {}_{+}\boldsymbol{\varphi}_{-N_s} & {}_{+}\boldsymbol{\varphi}_{1} \cdots {}_{+}\boldsymbol{\varphi}_{N_s} \end{bmatrix} \equiv \begin{bmatrix} {}_{-}\boldsymbol{\Phi}_{-} & {}_{-}\boldsymbol{\Phi}_{+} \\ {}_{+}\boldsymbol{\Phi}_{-} & {}_{+}\boldsymbol{\Phi}_{+} \end{bmatrix}, \tag{30} $$

which forms a $8N_s \times 8N_s$ matrix with four sub-matrices, ${}_{\pm}\boldsymbol{\Phi}_{\pm}$. The rows of ${}_{\pm}\boldsymbol{\Phi}_{\pm}$ correspond to μ_i's with their sign indicated by the left subscript, and the columns correspond to λ_j's with their sign indicated by the right subscript. If the left or right subscript is omitted, it means the whole $8N_s$ rows or columns. We will also frequently use the transpose, denoted by a superscript, T, of the eigenvector matrix. In that case, because the rows will be corresponding to the λ_j's and the columns to the μ_i's, the meaning of the left and right subscripts of ${}_{\pm}\boldsymbol{\Phi}_{\pm}$ should also be exchanged.

By multiplying both sides of Eq. (25) by -1 we can see that, if $({}_{-}\boldsymbol{\varphi}_j^{\mathrm{T}}, {}_{+}\boldsymbol{\varphi}_j^{\mathrm{T}})^{\mathrm{T}}$ is an eigenvector corresponding to $\boldsymbol{\lambda}_j$, then $({}_{+}\boldsymbol{\varphi}_j^{\mathrm{T}}, {}_{-}\boldsymbol{\varphi}_j^{\mathrm{T}})^{\mathrm{T}}$ must be an eigenvector corresponding to $-\boldsymbol{\lambda}_j$, therefore,

$$ \begin{aligned} {}_{\pm}\boldsymbol{\Phi}_{\pm} &\equiv {}_{\mp}\boldsymbol{\Phi}_{\mp}, \\ {}_{\pm}\boldsymbol{\Phi}_{\mp} &\equiv {}_{\mp}\boldsymbol{\Phi}_{\pm}. \end{aligned} \tag{31} $$

Other frequently used interchangeable notations are summarized below:

$$\mu_{\pm j} \equiv \pm\mu_j, \tag{32}$$

$$w_{\pm j} \equiv w_j, \tag{33}$$

$$\boldsymbol{\lambda}_{\pm j} \equiv \pm\boldsymbol{\lambda}_j. \tag{34}$$

2.4. The infinite medium Green's function

The following orthogonality property of the eigenvectors has been shown by Siewert [5,6] and re-developed in Section A.5:

$$\int_{-1}^{1} \boldsymbol{\psi}_k^{\mathrm{T}}(\mu)\mu\boldsymbol{\varphi}_j(\mu)\,\mathrm{d}\mu = \mathbf{N}_j\delta_{jk}, \quad j = \pm 1, \ldots, \pm N_s, \tag{35}$$

where $\mathbf{N}_j$ is a 4×4 diagonal matrix, and $\boldsymbol{\psi}_k$ are the eigenvectors for the problem defined by Eq. (25) but with $\mathbf{B}_l^m$ in Eqs. (23)–(24) replaced by $(\mathbf{B}_l^m)^{\mathrm{T}}$. It has also been shown in Section A.5 that $\boldsymbol{\psi}_k(\mu) = \mathfrak{R}\boldsymbol{\varphi}_k(\mu)$ where $\mathfrak{R} = \mathrm{diag}(1, 1, 1, -1)$, and the eigenvalues corresponding to $\boldsymbol{\psi}_k$ are the same as those of the original problem. Replacing the integration of Eq. (35) with Gaussian quadrature, the orthogonality can be written:

$$\boldsymbol{\Psi}^{\mathrm{T}}\boldsymbol{\mu}\mathbf{w}\boldsymbol{\Phi} = \mathbf{N}, \tag{36}$$

where

$$\boldsymbol{\mu} = \mathrm{diag}(\boldsymbol{\mu}_-, \boldsymbol{\mu}_+), \quad \boldsymbol{\mu}_\pm = \mathrm{diag}(\mu_{\pm j}\mathbf{E}_4,\ j = 1, \ldots, N_s), \tag{37}$$

$$\mathbf{w} = \mathrm{diag}(\mathbf{w}_-, \mathbf{w}_+), \quad \mathbf{w}_\pm = \mathrm{diag}(w_{\pm j}\mathbf{E}_4,\ j = 1, \ldots, N_s), \tag{38}$$

$$\mathbf{N} = \mathrm{diag}(\mathbf{N}_-, \mathbf{N}_+), \quad \mathbf{N}_\pm = \mathrm{diag}(\mathbf{N}_{\pm j},\ j = 1, \ldots, N_s). \tag{39}$$

From Eq. (36) it is straightforward to show that:

$$\boldsymbol{\Phi}^{-1} = \mathbf{N}^{-1}\boldsymbol{\Psi}^{\mathrm{T}}\boldsymbol{\mu}\mathbf{w}, \tag{40}$$

$$(\boldsymbol{\Psi}^{\mathrm{T}})^{-1} = \boldsymbol{\mu}\mathbf{w}\boldsymbol{\Phi}\mathbf{N}^{-1}, \tag{41}$$

$$\mathbf{N}_- = -\mathbf{N}_+. \tag{42}$$

We now use the orthogonality property to develop the infinite medium Green's function. In Section 2.3 it was shown that $2N_s$ pairs of $(\boldsymbol{\lambda}_j, \boldsymbol{\varphi}_j)$ can be found from Eq. (25), and each of them forms an elemental solution, i.e., Eqs. (19)–(20). All the elemental solutions satisfy Eq. (18), and so do any of their linear combinations, i.e.,

$$\sum_j \boldsymbol{\Omega}(\mu)\boldsymbol{\varphi}_j(\mu)\mathrm{e}^{\boldsymbol{\lambda}_j(\tau_0-\tau)}\mathbf{C}_j, \tag{43}$$

where $\mathbf{C}_j$ are unknown 4×4 coefficient matrices, and

$$\mathbf{\Omega}(\mu) = \begin{cases} \mathbf{D}, & \mu<0, \\ \mathbf{E}_4, & \mu>0, \end{cases} \tag{44}$$

where by using $\mathbf{\Omega}(\mu)$ the elemental solution defined in Eqs. (19)–(20) can be written uniformly. In the remainder of this section we will determine the proper linear combination of the elemental solutions so that the conditions, Eqs. (15)–(16), are satisfied.

The exponential component of Eqs. (19)–(20) indicates that to satisfy the vanishing boundary condition, Eq. (16), $\mathrm{Re}(\boldsymbol{\lambda}_j)(\tau - \tau_0)$ must be negative, which suggests that the solutions for $\tau<\tau_0$ and $\tau>\tau_0$ should be defined separately. Because of the angular discretization as shown in Eq. (17), the jump condition, Eq. (15), will generate a system of $8N_s$ equations corresponding to $2N_s$ zenith angles. As a result, $8N_s$ unknowns, or $2N_s$ terms of the linear combination can be determined. The above analysis suggests the following solutions:

$$\mathbf{G}_-^{\infty}(\mu) = -\sum_{j=-1}^{-N_s} \mathbf{\Omega}(\mu)\boldsymbol{\varphi}_j(\mu)\mathrm{e}^{\boldsymbol{\lambda}_j(\tau_0-\tau)}\mathbf{C}_j \quad \text{for } \tau<\tau_0, \tag{45}$$

$$\mathbf{G}_+^{\infty}(\mu) = \sum_{j=1}^{N_s} \mathbf{\Omega}(\mu)\boldsymbol{\varphi}_j(\mu)\mathrm{e}^{\boldsymbol{\lambda}_j(\tau_0-\tau)}\mathbf{C}_j \quad \text{for } \tau>\tau_0, \tag{46}$$

which parallel those of the scalar radiative transfer equation [3, Section 5.2]. Note that we have attached the superscript, ∞, to $\mathbf{G}$ to indicate the infinite medium. Inserting Eqs. (45)–(46) into Eq. (15) leads to

$$\sum_{j=\pm 1}^{\pm N_s} \mu\boldsymbol{\varphi}_j(\mu)\mathbf{C}_j = -\frac{1}{2\pi}\delta(\mu - \mu_0)\mathbf{\Omega}(\mu)\mathbf{D}_\alpha. \tag{47}$$

By using Eq. (35) we obtain

$$\mathbf{C}_j = -\frac{1}{2\pi}\mathbf{N}_j^{-1}{}_j\mathbf{\Psi}^{\mathrm{T}}(\mu_0)\mathbf{\Omega}(\mu_0)\mathbf{D}_\alpha. \tag{48}$$

Inserting Eq. (48) back into Eqs. (45)–(46), the infinite medium Green's function is obtained as

$$\mathbf{G}_\pm^{\infty}(\tau, \mu; \tau_0, \mu_0) = \mathbf{\Omega}(\mu)\sum_{j=1}^{N_s} \boldsymbol{\varphi}_{\pm j}(\mu)\mathrm{e}^{\boldsymbol{\lambda}_{\pm j}(\tau_0-\tau)}(-2\pi\mathbf{N}_+)^{-1}{}_{\pm j}\mathbf{\Psi}^{\mathrm{T}}(\mu_0)\mathbf{\Omega}(\mu_0)\mathbf{D}_\alpha, \tag{49}$$

where the subscript, "$\pm$", correspond to $\tau>\tau_0$ and $\tau<\tau_0$ respectively. In the case $\tau = \tau_0$, $\mathbf{G}^{\infty}$ is not defined. We use the reciprocity principle to complete the definition. We specify, when $\tau = \tau_0$, $\mathbf{G}_+^{\infty}$ is for $\mu_0<0$ and $\mathbf{G}_-^{\infty}$ for $\mu_0<0$. Written in more compact form, we have:

$$\mathbf{G}_{\pm\alpha}^{\infty}(\tau, \mu; \tau_0, \mu_0) = \mathbf{\Omega}(\mu)\hat{\mathbf{G}}_\pm^{\infty}(\tau, \mu; \tau_0, \mu_0)\mathbf{\Omega}(\mu_0)\mathbf{D}_\alpha, \tag{50}$$

$$\hat{\mathbf{G}}_\pm^{\infty}(\tau, \mu; \tau_0, \mu_0) = \mathbf{\Phi}_\pm(\mu)\tilde{\mathbf{\Lambda}}_\pm(\tau, \tau_0)_\pm\mathbf{\Psi}^{\mathrm{T}}(\mu_0), \tag{51}$$

$$\tilde{\mathbf{\Lambda}}_\pm(\tau, \tau_0) = -\frac{1}{2\pi}\mathrm{e}^{\boldsymbol{\lambda}_\pm(\tau_0-\tau)}\mathbf{N}_+^{-1}, \tag{52}$$

where

$$\boldsymbol{\lambda} = \mathrm{diag}(\boldsymbol{\lambda}_-, \boldsymbol{\lambda}_+), \quad \boldsymbol{\lambda}_\pm = \mathrm{diag}(\boldsymbol{\lambda}_{\pm j},\ j = 1, \ldots, N_s). \tag{53}$$

By using the jump condition we have imposed a beam source of unit flux. Therefore the solution shown in Eq. (50) contains the complete (diffusely and directly transmitted) radiation field. In some cases it might be desirable to remove the direct component, denoting it as $\mathbf{G}^{\infty}_{\pm\mathrm{dir}}$, which can be derived by assuming $\tilde{\omega}_0 = 0$. In such case, $\mathbf{X} = -\boldsymbol{\mu}_+^{-1}$ and $\mathbf{Y} = \mathbf{0}$, which means that $\boldsymbol{\lambda} = \boldsymbol{\mu}^{-1}$, ${}_+\boldsymbol{\Phi}_+ = \mathbf{0}$, ${}_+\boldsymbol{\Phi}_- = c\mathbf{E}$ (the identity matrix times a non-zero constant), and $\mathbf{N} = -\mathbf{w}\boldsymbol{\mu}$ from Eq. (36). It is found from Eq. (50) that

$$\mathbf{G}^{\infty}_{\pm\mathrm{dir}}(\tau, \mu_i; \tau_0, \mu_j) = \frac{\delta_{ij} w_i^{-1}}{2\pi\mu_i} H\left(-\frac{\tau_0 - \tau}{\mu_i}\right) \mathrm{e}^{(\tau_0 - \tau)\mathbf{E}_4/\mu_i}, \tag{54}$$

where H is the Heaviside step function. It may be noted that, had Beer's law been used to compute the directly transmitted component, we would see $\delta(\mu_i - \mu_j)$ in the place of $\delta_{ij} w_i^{-1}$. This difference can be understood as the result of discretizing $\delta(\mu_i - \mu_j)$ so that the definition of the Dirac delta function,

$$\int_{-1}^{1} \delta(\mu - \mu_j)\, \mathrm{d}\mu \approx \sum_{i=\pm 1}^{\pm N_s} w_i (\delta_{ij} w_j^{-1}) = 1 \tag{55}$$

is maintained. The (implicit) replacement of $\delta(\mu_i - \mu_j)$ with $\delta_{ij} w_i^{-1}$ is in fact essential so that the direct component will be computed correctly when using the Green's function matrix to compute, for example, Eq. (57), by means of Gaussian quadrature.

Before ending this section, we show that if a source can be expanded as

$$\mathbf{Q}(\tau, \mu, \phi; \tau_0, \mu_0, \phi_0) = \sum_{m=0}^{2N-1} \sum_{\alpha=1}^{2} \mathbf{Z}^m_\alpha(\phi - \phi_0) \mathbf{Q}^m_\alpha(\tau, \mu; \tau_0, \mu_0) \tag{56}$$

by virtue of Eqs. (6), (13) and (50), the radiation field generated by this source in the infinite medium will have the same expansion as Eq. (56) but with the coefficient defined as

$$\mathbf{I}^m_\alpha(\tau, \mu) = 2\pi \int \mathrm{d}\tau_0 \int_{-1}^{1} \mathrm{d}\mu_0 \boldsymbol{\Omega}(\mu) \hat{\mathbf{G}}^{m,\infty}_\alpha(\tau, \mu; \tau_0, \mu_0) \boldsymbol{\Omega}(\mu_0) \mathbf{Q}^m_\alpha(\tau_0, \mu_0). \tag{57}$$

This equation will be used in the next section to construct the FMGF.

3. The finite medium Green's function

In this section, we derive the FMGR for vacuum (free) boundaries (FMGF-VB). We assume the atmosphere is composed of a stack of plane-parallel layers, each of which is homogeneous and has finite optical thickness. The layers are numbered from top to bottom as layer $1, 2, \ldots, N_p$. Therefore, the optical thickness in layer p is $\tau^{p-1} < \tau \leqslant \tau^p$. We assume the optical thickness at the top of the atmosphere is $\tau^0 = 0$, and at the bottom of the atmosphere $\tau^N = \tau_a$. For such geometry, the following boundary and continuity conditions should be satisfied:

$$\mathbf{G}^1_\alpha(0, \mu; \tau_0, \mu_0) = \mathbf{0} \quad \mu < 0, \tag{58}$$

$$\mathbf{G}_\alpha^{p-1}(\tau^{p-1},\mu;\tau_0,\mu_0)=\mathbf{G}_\alpha^{p}(\tau^{p-1},\mu;\tau_0,\mu_0)\quad p=2,\ldots,N_p, \tag{59}$$

$$\mathbf{G}_\alpha^{N_p}(\tau^{N_p},\mu;\tau_0,\mu_0)=\mathbf{0}\quad \mu>0, \tag{60}$$

where $\mathbf{G}_\alpha^p$ denotes the expansion of the FMGF for layer p, similar to Eq. (13), with m omitted for simplicity.

3.1. Constructing finite medium Green's function

The Placzek lemma [4, Section 2.5] states that, for a given source, the radiative transfer problem in a finite homogeneous layer is equivalent to the problem in an infinite medium with the same scattering properties as the finite layer, for three sources: the original source, and two pseudo-sources which are imposed on the boundaries of the finite layer and illuminate outwards. The pseudo-sources have angular distributions such that the boundary and continuity conditions are satisfied. The pseudo-sources evidently have the same effect as the integral constants in the DOM (cf. [5,6]). The objective of this section is to determine the pseudo-sources from the boundary and continuity conditions.

According to the Placzek lemma, we denote the pseudo-sources imposed on the upper and lower boundaries of layer p respectively as $\delta(\tau-\tau^{p-1})\mathbf{S}_t^p(\mu)$ where $\mu>0$, and $\delta(\tau-\tau^p)\mathbf{S}_b^p(\mu)$ where $\mu<0$. Using Eq. (57), we can write the combined radiation field for layer p as

$$\begin{aligned}\mathbf{G}_\alpha^p(\tau,\mu;\tau_0,\mu_0)=\;&\delta_{p,p_0}\boldsymbol{\Omega}(\mu)\hat{\mathbf{G}}^{p,\infty}(\tau,\mu;\tau_0,\mu_0)\boldsymbol{\Omega}(\mu_0)\mathbf{D}_\alpha+2\pi\int_0^1\mathrm{d}\mu'\boldsymbol{\Omega}(\mu)\hat{\mathbf{G}}_+^{p,\infty}(\tau,\mu;\tau^{p-1},\mu')\\&\times\boldsymbol{\Omega}(\mu')\mathbf{S}_{t,\alpha}^p(\mu';\tau_0,\mu_0)+2\pi\int_{-1}^0\mathrm{d}\mu'\boldsymbol{\Omega}(\mu)\hat{\mathbf{G}}_-^{p,\infty}(\tau,\mu;\tau^p,\mu')\\&\times\boldsymbol{\Omega}(\mu')\mathbf{S}_{b,\alpha}^p(\mu';\tau_0,\mu_0),\end{aligned} \tag{61}$$

where the first term is the radiation field generated by the original source. Because each layer is treated independently, the original source is effective only when it is inside this layer, i.e., $p=p_0$ where p_0 denotes the source layer ($\tau^{p_0-1}<\tau_0\leqslant\tau^{p_0}$). The second term is the radiation field generated by the upper boundary pseudo-source, $\delta(\tau-\tau^{p-1})\mathbf{S}_t^p(\mu)$, recalling the choice of the proper IMGF expression as explained following Eq. (49). The last term is the radiation field generated by the lower boundary pseudo-source, $\delta(\tau-\tau^p)\mathbf{S}_b^p(\mu)$.

3.2. Solving the pseudo-source problem

In the above subsection, we have constructed the Green's function for each layer, with unknown the pseudo-sources. In this subsection we derive the pseudo-sources in accordance with the boundary and continuity conditions. Firstly, we use Gaussian quadrature to replace the integrations in Eq. (61), and by using Eqs. (37)–(38) and Eq. (50), we rewrite Eq. (61) in compact form as

$$\mathbf{G}_\alpha^p(\tau,\mu;\tau_0,\mu_0)=\delta_{p,p_0}\boldsymbol{\Omega}(\mu)\hat{\mathbf{G}}^{p,\infty}(\tau,\mu;\tau_0,\mu_0)\boldsymbol{\Omega}(\mu_0)\mathbf{D}_\alpha+\boldsymbol{\Omega}(\mu)\boldsymbol{\Gamma}^p(\tau,\mu)\mathbf{S}_\alpha^p(\tau_0,\mu_0), \tag{62}$$

where

$$\mathbf{\Gamma}^p(\tau,\mu) = [\mathbf{\Phi}_+^p \quad \mathbf{\Phi}_-^p] \begin{bmatrix} \mathbf{\Lambda}_+^p(\tau,\tau^{p-1}) & \mathbf{0} \\ \mathbf{0} & \mathbf{\Lambda}_-^p(\tau,\tau^p) \end{bmatrix}, \tag{63}$$

$$\mathbf{S}_\alpha^p(\tau_0,\mu_0) = \begin{bmatrix} -(\mathbf{N}_+^p)^{-1}{}_+\mathbf{\Psi}_+^{p^{\mathrm{T}}}\mathbf{\Omega}_+\boldsymbol{\mu}\mathbf{w}\mathbf{S}_{t,\alpha}^p(\tau_0,\mu_0) \\ -(\mathbf{N}_+^p)^{-1}{}_-\mathbf{\Psi}_-^{p^{\mathrm{T}}}\mathbf{\Omega}_-\boldsymbol{\mu}\mathbf{w}\mathbf{S}_{b,\alpha}^p(\tau_0,\mu_0) \end{bmatrix}, \tag{64}$$

where

$$\mathbf{\Lambda}_\pm^p(\tau,\tau') = \mathrm{e}^{\boldsymbol{\lambda}_\pm^p(\tau'-\tau)}. \tag{65}$$

By applying the boundary conditions to Eq. (62) we can obtain two systems of linear equations corresponding to $\alpha = 1$ and 2 respectively and with the same coefficient matrix. For $\alpha = 1$, the 3rd and 4th right-hand side (RHS) columns vanish due to $\mathbf{D}_1$, as do the 1st and 2nd RHS columns for $\alpha = 2$ due to $\mathbf{D}_2$. We note that the (common) coefficient matrix is not singular (otherwise no solution can be found for either α, which is physically untrue), therefore $\mathbf{S}_1^p$ and $\mathbf{S}_2^p$ must vanish at those columns corresponding to the vanishing RHS columns. This suggests that $\mathbf{S}_1^p$ and $\mathbf{S}_2^p$ can be combined as $\mathbf{S}^p$ and we can write $\mathbf{S}_\alpha^p = \mathbf{S}^p\mathbf{D}_a$. With $\mathbf{S}^p$ defined as such, the two linear systems can also be combined and written as:

$$-\mathbf{\Gamma}^1(0,\mu_-)\mathbf{S}^1 = \delta_{1,p_0}\hat{\mathbf{G}}_-^{1,\infty}(0,\mu_-;\tau_0,\mu_0)\mathbf{\Omega}(\mu_0), \tag{66}$$

$$\begin{aligned}\mathbf{\Gamma}^{p-1}(\tau^{p-1},\mu)\mathbf{S}^{p-1} - \mathbf{\Gamma}^p(\tau^{p-1},\mu)\mathbf{S}^p &= \delta_{p,p_0}\hat{\mathbf{G}}_-^{p,\infty}(\tau^{p-1},\mu;\tau_0,\mu_0)\mathbf{\Omega}(\mu_0) \\ &\quad - \delta_{p-1,p_0}\hat{\mathbf{G}}_+^{p-1,\infty}(\tau^{p-1},\mu;\tau_0,\mu_0)\mathbf{\Omega}(\mu_0) \quad p = 2,\ldots,N_p,\end{aligned} \tag{67}$$

$$\mathbf{\Gamma}^{N_p}(\tau^{N_p},\mu_+)\mathbf{S}^{N_p} = -\delta_{N_p,p_0}\hat{\mathbf{G}}_+^{N_p,\infty}(\tau^{N_p},\mu_+;\tau_0,\mu_0)\mathbf{\Omega}(\mu_0), \tag{68}$$

where $\mu_\pm$, when appearing in $\mathbf{\Gamma}^p(\tau,\mu)$, means that only the rows for $\mu>0$ or $\mu<0$ are included.

We further define

$$\mathbf{\Gamma}_0^{p_0}(\tau_0,\mu_0) = \begin{bmatrix} \mathbf{\Lambda}_-^{p_0}(\tau^{p_0-1},\tau_0) & \mathbf{0} \\ \mathbf{0} & \mathbf{\Lambda}_+^{p_0}(\tau^{p_0},\tau_0) \end{bmatrix} \begin{bmatrix} {}_-\mathbf{\Psi}^{p_0\mathrm{T}}(\mu_0) \\ {}_+\mathbf{\Psi}^{p_0\mathrm{T}}(\mu_0) \end{bmatrix} \tag{69}$$

and

$$\mathbf{T}^{p,\infty} = \delta_{p,p_0} \begin{bmatrix} \mathbf{0} & H(\tau-\tau_0)\mathbf{\Xi}^p\mathbf{\Lambda}_+(\tau^{p-1},\tau^p) \\ H(\tau_0-\tau)\mathbf{\Xi}^p\mathbf{\Lambda}_+(\tau^{p-1},\tau^p) & \mathbf{0} \end{bmatrix}, \tag{70}$$

where

$$\mathbf{\Xi}^p = (-2\pi\mathbf{N}_+^p)^{-1} \tag{71}$$

and $H(x)$ is the Heaviside step function which equals 1 when $x>0$ and zero when $x<0$. $H(x)$ is not defined for $x = 0$, which corresponds to the special case of $\tau = \tau_0$. We have provided a supplementary definition of $\mathbf{G}_{\pm}^{\infty}$ for $\tau = \tau_0$ following Eq. (49). For simplicity, we will not discuss this special case further. Using Eqs. (69)–(71), the IMGF can be rewritten as

$$\hat{\mathbf{G}}^{p,\infty}(\tau,\mu;\tau_0,\mu_0) = \mathbf{\Gamma}^p(\tau,\mu)\mathbf{T}^{p,\infty}\mathbf{\Gamma}_0^{p_0}(\tau_0,\mu_0). \tag{72}$$

After inserting Eq. (72) back into Eqs. (66)–(68) we note that the right-hand side (RHS) contains a common factor, $\mathbf{\Gamma}_0^{p_0}(\tau_0,\mu_0)\mathbf{\Omega}(\mu_0)$, which can be removed by moving it to the left and denoting

$$\mathbf{T}^{p,p_0} = \mathbf{S}^p(\mathbf{\Gamma}_0^{p_0}(\tau_0,\mu_0)\mathbf{\Omega}(\mu_0))^{-1}. \tag{73}$$

We then obtain:

$$-\mathbf{\Gamma}^1(0,-\mu)\mathbf{T}^{1,p_0} = \delta_{1,p_0}\lfloor_{-}\mathbf{\Phi}_{-}^{p_0}\mathbf{\Xi}^{p_0} \quad \mathbf{0}\rfloor, \tag{74}$$

$$\mathbf{\Gamma}^{p-1}(\tau^{p-1},\mu)\mathbf{T}^{p-1,p_0} - \mathbf{\Gamma}^p(\tau^{p-1},\mu)\mathbf{T}^{p,p_0} = \delta_{p,p_0}[\mathbf{\Phi}_{-}^{p_0}\mathbf{\Xi}^{p_0} \quad \mathbf{0}] - \delta_{p-1,p_0}[\mathbf{0} \quad \mathbf{\Phi}_{+}^{p_0}\mathbf{\Xi}^{p_0}],$$
$$p = 2,3,\ldots,N \tag{75}$$

$$\mathbf{\Gamma}^{N_p}(\tau^{N_p},+\mu)\mathbf{T}^{N_p,p_0} = -\delta_{N_p,p_0}[\mathbf{0} \quad {}_{+}\mathbf{\Phi}_{+}^{p_0}\mathbf{\Xi}^{p_0}]. \tag{76}$$

It is apparent that $\mathbf{T}^{p,p_0}$ only depends on the layer numbers, p and p_0. We have therefore obtained a source-independent system of equations, with a block-band coefficient matrix. The system can be solved using a standard routine. For example, LAPACK [29] provides a subroutine to solve a general real band system by factorizing the coefficient matrix. By doing so, the solution for many RHS vectors (corresponding to source layers) can be found very efficiently using back-substitution.

3.3. The uniform expression of the FMGF-VB

Having obtained the pseudo-source kernels, $\mathbf{T}^{p,p_0}$, and recalling Eq. (62), Eq. (73) and $\mathbf{S}_{\alpha}^p = \mathbf{S}^p\mathbf{D}_a$, the Green's function for vacuum lower boundary (IMGF-VB) can be written as

$$\mathbf{G}_{\alpha}^p(\tau,\mu;\tau_0,\mu_0) = \mathbf{\Omega}(\mu)\hat{\mathbf{G}}^p(\tau,\mu;\tau_0,\mu_0)\mathbf{\Omega}(\mu_0)\mathbf{D}_{\alpha}, \tag{77}$$

where

$$\hat{\mathbf{G}}_{\alpha}^p(\tau,\mu;\tau_0,\mu_0) = \mathbf{\Gamma}^p(\tau,\mu)\tilde{\mathbf{T}}^{p,p_0}\mathbf{\Gamma}_0^{p_0}(\tau_0,\mu_0), \tag{78}$$

where $\mathbf{\Gamma}^p(\tau,\mu)$ and $\mathbf{\Gamma}_0^{p_0}(\tau_0,\mu_0)$ are defined in Eq. (63) and Eq. (69), and the kernel $\tilde{\mathbf{T}}^{p,p_0}$ has combined the IMGF and the pseudo-source kernels:

$$\tilde{\mathbf{T}}^{p,p_0} = \mathbf{T}^{p,\infty} + \mathbf{T}^{p,p_0}. \tag{79}$$

When $p \neq p_0$, i.e., the source is not in layer p, $\tilde{\mathbf{T}}^{p,p_0}$ is independent of τ_0 and τ. When $p = p_0$, $\tilde{\mathbf{T}}^{p,p_0}$ changes at $\tau = \tau_0$ due to the IMGF kernel, which reflects the fact that the radiation field is discontinuous when the beam source joins in through the jump condition, Eqs. (8) and (15).

The major steps to obtain the FMGF include an eigenvalue problem as defined in Eqs. (25) and (29), and a linear system defined in Eqs. (74)–(76). Both are found to be numerically stable. However, we note that $\mathbf{T}^{p,\infty}$ as defined in Eq. (70) has a growing exponential term which could cause overflow if the source layer is very thick, combined with very large eigenvalues, which occurs when a quadrature point is very close to 0.0 (or 90°) and the layer is strongly absorbing. Simple solutions exist if it does become a problem: for example, splitting the source layer into thinner sub-layers before starting to solve the problem, or computing the IMGF part in Eqs. (77)–(78) separately using Eqs. (50)–(51).

A permanent solution that we consider to introduce in the future uses the layer splitting method, but the splitting will be carried out after the eigenvalue problem and the pseudo-source problem have been completed, when the maximum sub-layer thickness can be determined precisely. The kernel for the new layers can then be computed from the old kernels, which involves (at most) two multiplications of a (full) matrix with a diagonal matrix for each new layer. This method does not change the formulations obtained, while the extra computation is considered to be small.

4. The finite medium Green's function for reflective surface

In this section, we use Eqs. (77)–(78) to construct the Green's function for a medium with a reflective surface. The reflective surface is described by a general BRDF represented by a 4×4 matrix function, with the assumption that it can be expand as

$$\mathbf{R}(\mu, \phi; \mu', \phi') = \sum_{m=0}^{N_m} \sum_{\alpha=1}^{2} \mathbf{Z}_\alpha^m(\phi - \phi')\boldsymbol{\Omega}(\mu)\mathbf{R}^m(\mu, \mu')\boldsymbol{\Omega}(\mu')\mathbf{D}_\alpha, \tag{80}$$

where (μ', ϕ') denotes the incidence direction and (μ, ϕ) the reflection direction. This expansion implies that the two diagonal 2×2 blocks must be symmetric about $\phi - \phi' = 0$, and the anti-diagonal blocks must be antisymmetric about $\phi - \phi' = 0$. Also note that with $\mu > 0$ and $\mu' < 0$, the elements of the $\mathbf{R}^m$ matrix can be computed using:

$$\begin{aligned} R_{ij}^m(\mu, \mu') &= \frac{1}{2\pi}\Omega_j \int_0^{2\pi} \mathrm{d}\phi' R_{ij}(\mu, \phi; \mu', \phi') z_{ij}^m(\phi - \phi'), \\ &= \Omega_j \sum_{k=1}^{N_a} w_k R_{ij}(\mu; \mu'; \Delta\phi_k) z_{ij}^m(\Delta\phi_k) \quad i,j = 1,2,3,4, \end{aligned} \tag{81}$$

where $\Omega_j = 1$ for $j = 1,2$ or $\Omega_j = -1$ for $j = 3,4$, and $z_{ij}^m(\phi) = \cos m\phi$ for the two diagonal 2×2 blocks, $z_{ij}^m(\phi) = \sin m\phi$ for the left bottom block, while $z_{ij}^m(\phi) = -\sin m\phi$ for the right top block. The $\Delta\phi_k$'s are the Gaussian quadrature points linearly re-scaled from (0, 1) to (0, π). The reflected radiance is expressed as

$$\mathbf{I}_r(\tau_a, \mu, \phi; \tau_0, \mu_0, \phi_0) = \frac{1}{\pi} \int_0^{2\pi} \mathrm{d}\phi' \int_{-1}^{0} \mathrm{d}\mu' \mathbf{R}(\mu, \phi; \mu', \phi')|\mu'| \mathbf{G}_s(\tau_a, \mu', \phi'; \tau_0, \mu_0, \phi_0), \tag{82}$$

where τ_a is the optical depth at the bottom of the atmosphere and $\mathbf{G}_s$ is the radiation field after the surface has been introduced, which is yet to be determined. We expand $\mathbf{G}_s$ as

$$\mathbf{G}_s(\tau, \mu, \phi; \tau_0, \mu_0, \phi_0) = \sum_{m=0}^{N_m} \sum_{\alpha=1}^{2} \mathbf{z}_\alpha^m(\phi - \phi_0)\mathbf{G}_{s,\alpha}^m(\tau, \mu; \tau_0, \mu_0) \tag{83}$$

and by inserting Eq. (80) and Eq. (83) into Eq. (82) we obtain

$$\mathbf{I}_r(\tau_a,\mu,\phi;\tau_0,\mu_0,\phi_0) = 2\sum_{m=0}^{2N-1}\sum_{\alpha=1}^{2}\mathbf{Z}_\alpha^m(\phi-\phi_0)\boldsymbol{\Omega}(\mu)\mathbf{R}^m(\mu,\boldsymbol{\mu}_-) \times\boldsymbol{\Omega}(\boldsymbol{\mu}_-)\mathbf{w}_+\boldsymbol{\mu}_+\mathbf{G}_{s,\alpha}^m(\tau_a,\boldsymbol{\mu}_-;\tau_0,\mu_0), \tag{84}$$

where we have replaced the integration over μ' with Gaussian quadrature. The variables $\mathbf{w}_+$ and $\boldsymbol{\mu}_+$ are diagonal matrices defined in Eqs. (37)–(38), and the "vector argument", $\boldsymbol{\mu}_-$, is interpreted generally as

$$\mathbf{F}(\boldsymbol{\mu}_\pm) = \{\mathbf{F}(\mu_{\pm j})\}_{j=1,\ldots,N_s}, \tag{85}$$

where $\mathbf{F}(\mu_{\pm j})$ are 4×4 matrices which may or may not be diagonal. The radiative transfer problem of a reflective surface can be viewed as a problem of vacuum boundaries with two sources: the original source and a source equivalent to the reflected radiance, therefore

$$\mathbf{G}_s(\tau,\mu,\phi;\tau_0,\mu_0,\phi_0) = \mathbf{G}(\tau,\mu,\phi;\tau_0,\mu_0,\phi_0) + \int_0^{2\pi}\mathrm{d}\phi'\int_0^1\mathrm{d}\mu'\mathbf{G}(\tau,\mu,\phi;\tau_a,\mu',\phi') \times|\mu'|\mathbf{I}_r(\tau_a,\mu',\phi';\tau_0,\mu_0,\phi_0), \tag{86}$$

where the first term on the RHS represents the radiation generated by the original source, which is just the Green's function for vacuum boundaries. The second term is the radiation field generated by the reflected radiation. Inserting Eq. (84) into Eq. (86) we obtain:

$$\mathbf{G}_{s,\alpha}^m(\tau,\mu;\tau_0,\mu_0) = \boldsymbol{\Omega}(\mu)\hat{\mathbf{G}}^m(\tau,\mu;\tau_0,\mu_0)\boldsymbol{\Omega}(\mu_0)\mathbf{D}_\alpha + \boldsymbol{\Omega}(\mu)\hat{\mathbf{G}}^m(\tau,\mu;\tau_a,\boldsymbol{\mu}_+)\tilde{\mathbf{R}}^m \times\boldsymbol{\Omega}(\boldsymbol{\mu}_-)\mathbf{G}_{s,\alpha}^m(\tau_a,\boldsymbol{\mu}_-;\tau_0,\mu_0), \tag{87}$$

where we have replaced the integration over μ' with Gaussian quadrature, and

$$\tilde{\mathbf{R}}^m = 4\pi\mathbf{w}_+\boldsymbol{\mu}_+\mathbf{R}^m(\boldsymbol{\mu}_+,\boldsymbol{\mu}_-)\mathbf{w}_+\boldsymbol{\mu}_+. \tag{88}$$

We solve Eq. (87) for $\mathbf{G}_{s,\alpha}^m(\tau_a,\boldsymbol{\mu}_-;\tau_0,\mu_0)$, and insert it back to Eq. (87) to obtain the final result as

$$\mathbf{G}_{s,\alpha}^m(\tau,\mu;\tau_0,\mu_0) = \boldsymbol{\Omega}(\mu)\hat{\mathbf{G}}_s^m(\tau,\mu;\tau_0,\mu_0)\boldsymbol{\Omega}(\mu_0)\mathbf{D}_\alpha \tag{89}$$

where

$$\hat{\mathbf{G}}_s^m(\tau,\mu;\tau_0,\mu_0) = \hat{\mathbf{G}}^m(\tau,\mu;\tau_0,\mu_0) + \hat{\mathbf{G}}^m(\tau,\mu;\tau_a,\boldsymbol{\mu}_+)\tilde{\mathbf{R}}^m[\mathbf{E}-\hat{\mathbf{G}}^m(\tau_a,\boldsymbol{\mu}_-;\tau_a,\boldsymbol{\mu}_+)\tilde{\mathbf{R}}^m]^{-1} \times\hat{\mathbf{G}}^m(\tau_a,\boldsymbol{\mu}_-;\tau_0,\mu_0), \tag{90}$$

where $\mathbf{E}$ is the $4N_s\times 4N_s$ identity matrix. Writing Eq. (90) in a form consistent with Eq. (78), we have

$$\hat{\mathbf{G}}_s^{p,p_0}(\tau_0,\mu_0;\tau,\mu) = \boldsymbol{\Gamma}^p(\tau,\mu)\tilde{\mathbf{T}}_s^{p,p_0}(\mathbf{A}_s;\tau,\tau_0)\boldsymbol{\Gamma}_0^{p_0}(\tau_0,\mu_0), \tag{91}$$

where we have reattached the layer numbers, p and p_0, and omitted m, and

$$\tilde{\mathbf{T}}_s^{p,p_0} = \tilde{\mathbf{T}}^{p,p_0} + \tilde{\mathbf{T}}^{p,N_p}\tilde{\mathbf{T}}_{ms}^{N_p,N_p}\tilde{\mathbf{T}}^{N_p,p_0}, \tag{92}$$

where

$$\tilde{\mathbf{T}}_{ms}^{N_p,N_p}(\mathbf{R}) = \mathbf{\Gamma}_0^{N_p}(\tau_a, \boldsymbol{\mu}_+)\tilde{\mathbf{R}}[\mathbf{E} - \mathbf{\Gamma}^{N_p}(\tau_a, \boldsymbol{\mu}_-)\tilde{\mathbf{T}}^{N_p,N_p}\mathbf{\Gamma}_0^{N_p}(\tau_a, \boldsymbol{\mu}_+)\tilde{\mathbf{R}}]^{-1}\mathbf{\Gamma}^{N_p}(\tau_a, \boldsymbol{\mu}_-), \tag{93}$$

where N_p is the total number of atmospheric layers. We see that the Green's function with a reflective surface is similar to that for vacuum boundaries, except that the kernel matrix, $\tilde{\mathbf{T}}_s^{p,p_0}$, also depends on the surface BRDF matrix.

5. Summary

An explicit expression for the Green's function for plane-parallel geometry, with vacuum or BRDF surface has been developed, which considers the full polarization state but the development can be easily reduced to consider the intensity only. The algorithm has been implemented using Fortran 95, which will be discussed in a separate paper.

The benefit of developing such an explicit expression for the Green's function is two fold: firstly an analytical expression allows for analytical computations when the Green's function is employed, which is impossible if the GF is represented numerically; secondly, computing the Green's function is much more efficient. In contrast, using a standard radiative transfer code to "accumulate" a numerical GF could be very expensive, especially when the mesh of the source optical thickness has to be dense.

We would like to point out that, although the Green's function can be used to compute the radiation field generated by virtually any source, such an approach may not necessarily be the most efficient way for normal forward radiative transfer problems, where specialized algorithm such as DOM should be used. On the other hand, the Green's function approach becomes useful in, for example, inversion problems where the radiation field needs be computed repeatedly for changing surface BRDF, changing surface/deep space temperature or emissivity, or changing atmosphere temperature profile. The work by Benedetti et al. [22] showed another example where we have a changing profile of extinction coefficient. In all such examples, the Green's function approach makes it possible to reveal explicitly the dependence of the radiation field on the changing parameters.

Appendix A

A.1. Generalized spherical function

The generalized spherical function was initially introduced by Gelfand and Sapiro [31] for representation of rotation groups, and used by Siewert [6] in radiative transfer computation with polarization. For $l \geqslant \sup(|m|, |n|)$, the generalized spherical function is defined as

$$P_l^{m,n}(\mu) = A_{m,n}^l(1-\mu)^{-(n-m)/2}(1+\mu)^{-(n+m)/2}\frac{\mathrm{d}^{l-n}}{\mathrm{d}\mu^{l-n}}[(1-\mu)^{l-m}(1+\mu)^{l+m}], \tag{A.1}$$

where

$$A_{m,n}^l(\mu) = \frac{(-1)^{l-m}i^{n-m}}{2^l(l-m)!}\left[\frac{(l-m)!(l+n)!}{(l+m)!(l-n)!}\right]^{1/2}. \tag{A.2}$$

When $m=0$, $P_l^{m,n}$ reduces to

$$P_l^{0,n}(\mu) = i^n \left[\frac{(l-n)!}{(l+n)!}\right]^{1/2} P_l^n(\mu), \tag{A.3}$$

where P_l^n is the associated Legendre polynomial defined as

$$P_l^n(\mu) = \frac{1}{2^l l!}(1-\mu^2)^{n/2} \frac{\mathrm{d}^{l+n}}{\mathrm{d}\mu^{l+n}}(\mu^2-1)^l. \tag{A.4}$$

The generalized spherical function has the following orthogonality property:

$$(-1)^{m-n} \int_{-1}^{1} P_j^{m,n}(\mu) P_k^{m,n}(\mu)\,\mathrm{d}\mu = \left(\frac{2}{2k+1}\right)\delta_{jk} \tag{A.5}$$

and recursive relations

$$e_{m,n}^l P_{l+1}^{m,n}(\mu) = (2l+1)\mu P_l^{m,n}(\mu) - f_{m,n}^l P_{l-1}^{m,n}(\mu) - \frac{mn(2l+1)}{l(l+1)} P_l^{m,n}(\mu), \tag{A.6}$$

$$\alpha_{m+1} P_l^{m+1,n} = \frac{1}{2}(1+\mu)\alpha_n P_l^{m,n-1} + \frac{1}{2}(1-\mu)\alpha_{n+1} P_l^{m,n+1} - in\sqrt{1-\mu^2} P_l^{m,n}, \tag{A.7}$$

$$\alpha_m P_l^{m-1,n} = \frac{1}{2}(1-\mu)\alpha_n P_l^{m,n-1} + \frac{1}{2}(1+\mu)\alpha_{n+1} P_l^{m,n+1} + in\sqrt{1-\mu^2} P_l^{m,n}, \tag{A.8}$$

where

$$e_{m,n}^l = \frac{1}{l+1}[(l+m+1)(l-m+1)(l+n+1)(l-n+1)]^{1/2}, \tag{A.9}$$

$$f_{m,n}^l = \frac{1}{l}[(l+m)(l-m)(l+n)(l-n)]^{1/2}, \tag{A.10}$$

$$\alpha_n = \sqrt{(l+n)(l-n+1)}. \tag{A.11}$$

The generalized spherical function has the following addition theorem which will be used in phase matrix expansion:

$$\mathrm{e}^{-im\phi_2} P_l^{m,n}(\cos\theta)\mathrm{e}^{-in\phi_1} = \sum_{k=-l}^{l} \mathrm{e}^{-ik\phi} P_l^{m,k}(\cos\theta') P_l^{k,n}(\cos\theta''), \tag{A.12}$$

where

$$\cos\theta = \cos\theta'\cos\theta'' + \sin\theta'\sin\theta''\cos\phi, \tag{A.13}$$

$$\tan\phi_1 = \frac{\sin\phi\sin\theta''}{\cos\theta'\sin\theta''\cos\phi + \sin\theta'\cos\theta''}, \tag{A.14}$$

$$\tan\phi_2 = \frac{\sin\phi\sin\theta'}{\sin\theta'\cos\theta''\cos\phi + \cos\theta'\sin\theta''}. \tag{A.15}$$

A.2. R_l^m and T_l^m functions

The R_l^m and T_l^m functions are defined in terms of $P_l^{m,n}$ as:

$$R_l^m(\mu) = -\frac{1}{2} i^m \left[\frac{(l+m)!}{(l-m)!}\right]^{1/2} [P_l^{m,2}(\mu) + P_l^{m,-2}(\mu)], \tag{A.16}$$

$$T_l^m(\mu) = -\frac{1}{2} i^m \left[\frac{(l+m)!}{(l-m)!}\right]^{1/2} [P_l^{m,2}(\mu) - P_l^{m,-2}(\mu)]. \tag{A.17}$$

These two functions are computed using the following recursions:

For $m = 0$:

$$T_l^0(\mu) = 0 \quad \text{for all } l \geqslant 0, \tag{A.18}$$

$$R_0^0(\mu) = R_1^0(\mu) = 0, \tag{A.19}$$

$$R_2^0(\mu) = \frac{\sqrt{6}}{4}(1-\mu^2), \tag{A.20}$$

$$R_{l+1}^0(\mu) = (x_l^0)^{-1}[(2l+1)\mu R_l^0(\mu) - y_l^0 R_{l-1}^0(\mu)], \tag{A.21}$$

where x_l^m and y_l^m are defined in Eqs. (A.31)–(A.32).

For $m = 1$ and $l \leqslant 2$:

$$R_1^1(\mu) = 0, \tag{A.22}$$

$$T_1^1(\mu) = 0, \tag{A.23}$$

$$R_2^1(\mu) = -\frac{1}{2}\mu\sqrt{6}(1-\mu^2)^{1/2}, \tag{A.24}$$

$$T_2^1(\mu) = -\frac{1}{2}\sqrt{6}(1-\mu^2)^{1/2}. \tag{A.25}$$

For $m \geqslant 2$ and $l = m$:

$$R_m^m(\mu) = K_m(1+\mu^2)(1-\mu^2)^{m/2-1}, \tag{A.26}$$

$$T_m^m(\mu) = K_m(2\mu)(1-\mu^2)^{m/2-1}, \tag{A.27}$$

where

$$K_m = \frac{(2m)!}{2^m}[(m-2)!(m+2)!]^{-1/2}. \tag{A.28}$$

For all others:

$$R_{l+1}^m(\mu) = (x_l^m)^{-1}[(2l+1)\mu R_l^m(\mu) - y_l^m R_{l-1}^1(\mu) - z_l^m T_l^m(\mu)], \tag{A.29}$$

$$T_{l+1}^m(\mu) = (x_l^m)^{-1}[(2l+1)\mu T_l^m(\mu) - y_l^m T_{l-1}^m(\mu) - z_l^m R_l^m(\mu)], \tag{A.30}$$

where

$$x_l^m = \frac{l-m+1}{l+1}[(l+3)(l-1)]^{1/2}, \tag{A.31}$$

$$y_l^m = (1-\delta_{ml})\frac{l+m}{l}(l^2-4)^{1/2}, \tag{A.32}$$

$$z_l^m = \frac{2m(2l+1)}{l(l+1)}. \tag{A.33}$$

A.3. Scattering phase matrix and expansion

The scattering matrix of the radiative transfer equation, **M** in Eq. (2/7), is defined as

$$\mathbf{M}(\mu,\phi;\mu',\phi') = \mathbf{L}(\pi - i_2)\mathbf{P}(\mu,\phi;\mu',\phi')\mathbf{L}(-i_1), \tag{A.34}$$

where i_1 and i_2 are respectively the angle between the incidence meridian plane and the scattering plane (containing both the incident and scattering light), and the angle between the scattering meridian plane and the scattering plane, and

$$\mathbf{L}(\pi - i) = \mathbf{L}(-i) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(2i) & -\sin(2i) & 0 \\ 0 & \sin(2i) & \cos(2i) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{A.35}$$

and

$$\mathbf{P}(\zeta) = \begin{pmatrix} a_1(\zeta) & b_1(\zeta) & 0 & 0 \\ b_1(\zeta) & a_2(\zeta) & 0 & 0 \\ 0 & 0 & a_3(\zeta) & b_2(\zeta) \\ 0 & 0 & -b_2(\zeta) & a_4(\zeta) \end{pmatrix}, \tag{A.36}$$

which represents scattering by ensembles of randomly oriented particles with a plane of symmetry [28]. **P** is normalized as:

$$\int_{-1}^{1} a_1(\zeta)\,\mathrm{d}\zeta = 2 \tag{A.37}$$

and the elements can be expanded as

$$a_1(\zeta) = \sum_{l=0}^{2N-1} \beta_l P_l(\zeta), \quad \beta_0 = 1, \tag{A.38}$$

$$a_2(\zeta) = \sum_{l=2}^{2N-1} \left(\frac{(l-2)!}{(l+2)!}\right)^{1/2} [\alpha_l R_l^2(\zeta) + \xi_l T_l^2(\zeta)], \tag{A.39}$$

$$a_3(\zeta) = \sum_{l=2}^{2N-1} \left(\frac{(l-2)!}{(l+2)!}\right)^{1/2} [\xi_l R_l^2(\zeta) + \alpha_l T_l^2(\zeta)], \tag{A.40}$$

$$a_4(\zeta) = \sum_{l=0}^{2N-1} \delta_l P_l(\zeta), \tag{A.41}$$

$$b_1(\zeta) = \sum_{l=2}^{2N-1} \left(\frac{(l-2)!}{(l+2)!}\right)^{1/2} \gamma_l P_l^2(\zeta), \tag{A.42}$$

$$b_2(\zeta) = -\sum_{l=2}^{2N-1} \left(\frac{(l-2)!}{(l+2)!}\right)^{1/2} \varepsilon_l P_l^2(\zeta), \tag{A.43}$$

where $P_l(\zeta)$ is the Legendre polynomial, $P_l^m(\zeta)$ is the associated Legendre polynomial, and $R_l^m(\zeta)$ and $T_l^m(\zeta)$ are defined in Section A.2.

By defining

$$\mathbf{D}_1 = \mathrm{diag}(1,1,0,0), \quad \mathbf{D}_2 = \mathrm{diag}(0,0,1,1), \quad \mathbf{D} = \mathrm{diag}(1,1,-1,-1) \tag{A.44}$$

and

$$\mathbf{Z}_1^m(\phi) = (2-\delta_{0m})\mathrm{diag}(\cos m\phi, \cos m\phi, \sin m\phi, \sin m\phi), \tag{A.45}$$

$$\mathbf{Z}_2^m(\phi) = (2-\delta_{0m})\mathrm{diag}(-\sin m\phi, -\sin m\phi, \cos m\phi, \cos m\phi), \tag{A.46}$$

it has been shown by Siewert [5,6,32,33] that the phase matrix can be written as

$$\mathbf{M}(\mu,\phi;\mu',\phi') = \sum_{m=0}^{2N-1} \sum_{\alpha=1}^{2} \mathbf{Z}_\alpha^m(\phi-\phi')\mathbf{A}^m(\mu,\mu')\mathbf{D}_\alpha, \tag{A.47}$$

where

$$\mathbf{A}^m(\mu,\mu') = \sum_{l=m}^{2N-1} \mathbf{P}_l^m(\mu)\mathbf{B}_l^m\mathbf{P}_l^m(\mu'), \tag{A.48}$$

where

$$\mathbf{P}_l^m(\mu) = \begin{pmatrix} P_l^m(\mu) & 0 & 0 & 0 \\ 0 & R_l^m(\mu) & -T_l^m(\mu) & 0 \\ 0 & -T_l^m(\mu) & R_l^m(\mu) & 0 \\ 0 & 0 & 0 & P_l^m(\mu) \end{pmatrix} \tag{A.49}$$

and $\mathbf{B}_l^m = (l-m)!/(l+m)!\mathbf{B}_l$ and $\mathbf{B}_l$ is defined by

$$\mathbf{B}_l = \begin{pmatrix} \beta_l & \gamma_l & 0 & 0 \\ \gamma_l & \alpha_l & 0 & 0 \\ 0 & 0 & \xi_l & -\varepsilon_l \\ 0 & 0 & \varepsilon_l & \delta_l \end{pmatrix}, \tag{A.50}$$

where $\mathbf{B}_l$ is the expansion of the phase matrix computed using Eqs. (A.38)–(A.43).

We write down the following relations regarding $\mathbf{P}_l^m$ and $\mathbf{B}_l^m$ which are useful in the main text, these relations can be deduced from the definition of $\mathbf{P}_l^m$ and $\mathbf{B}_l^m$:

$$\mathbf{P}_l^m(-\mu) = (-1)^{l-m}\mathbf{D}\mathbf{P}_l^m(\mu)\mathbf{D}, \tag{A.51}$$

$$\mathbf{D}\mathbf{B}_l^m\mathbf{D} = \mathbf{B}_l^m, \quad \mathbf{D}\mathbf{B}_l^m = \mathbf{B}_l^m\mathbf{D}. \tag{A.52}$$

A.4. Azimuth expansion and reduction

This section computes the following expression which is encountered several times in the main text:

$$\int_0^{2\pi} \mathrm{d}\phi'\mathbf{A}(\phi,\phi')\mathbf{B}(\phi',\phi_0), \tag{A.53}$$

where $\mathbf{A}(\phi,\phi')$ and $\mathbf{B}(\phi',\phi_0)$ are 4×4 matrix functions that can be expanded as:

$$\mathbf{A}(\phi,\phi') = \sum_{m=0}^{2N-1}\sum_{\alpha=1}^{2}\mathbf{Z}_\alpha^m(\phi-\phi')\mathbf{A}^m\mathbf{D}_\alpha, \tag{A.54}$$

$$\mathbf{B}(\phi',\phi_0) = \sum_{n=0}^{2N-1}\sum_{\beta=1}^{2}\mathbf{Z}_\beta^n(\phi'-\phi_0)\mathbf{B}_\beta^n, \tag{A.55}$$

where $\mathbf{Z}_\alpha^m(\phi)$ and $\mathbf{D}_\alpha$ are diagonal matrices defined in Section A.3.

Because $\mathbf{Z}_\alpha^0(\phi) = \mathbf{D}_\alpha$, Eq. (A.54) suggests that only the two 2×2 diagonal blocks of $\mathbf{A}^0$ are active, and the anti-diagonal blocks of $\mathbf{A}^0$ can be set to arbitrary values. We also note that:

$$\mathbf{Z}_1^m(\phi-\phi') = \mathbf{Z}_1^m(\phi-\phi_0)\cos m(\phi'-\phi_0) - \mathbf{Z}_2^m(\phi-\phi_0)\sin m(\phi'-\phi_0), \tag{A.56}$$

$$\mathbf{Z}_2^m(\phi-\phi') = \mathbf{Z}_2^m(\phi-\phi_0)\cos m(\phi'-\phi_0) + \mathbf{Z}_1^m(\phi-\phi_0)\sin m(\phi'-\phi_0). \tag{A.57}$$

The above relations lead to

$$\int_0^{2\pi} \mathrm{d}\phi'\mathbf{A}(\phi,\phi')\mathbf{B}(\phi',\phi_0) = 2\pi\sum_{m=0}^{2N-1}\sum_{\alpha=1}^{2}\mathbf{Z}_\alpha^m(\phi-\phi_0)\mathbf{A}^m\mathbf{B}_\alpha^m. \tag{A.58}$$

A.5. Orthogonality of eigenvectors

This section derives the orthogonality property of the eigenvectors defined by Eq. (25). Inserting Eqs. (19)–(20) into Eq. (14), and using the definition of $\mathbf{X}$ and $\mathbf{Y}$, Eqs. (23)–(24), we have:

$$-\mu\boldsymbol{\varphi}_j(-\mu)\boldsymbol{\lambda}_j = \int_0^1 \mathrm{d}\mu'\tilde{\mathbf{Y}}(\mu,\mu')\boldsymbol{\varphi}_j(\mu') + \int_0^1 \mathrm{d}\mu'\tilde{\mathbf{X}}(\mu,\mu')\boldsymbol{\varphi}_j(-\mu'), \tag{A.59}$$

$$\mu\boldsymbol{\varphi}_j(\mu)\boldsymbol{\lambda}_j = \int_0^1 \mathrm{d}\mu'\tilde{\mathbf{X}}(\mu,\mu')\boldsymbol{\varphi}_j(\mu') + \int_0^1 \mathrm{d}\mu'\tilde{\mathbf{Y}}(\mu,\mu')\boldsymbol{\varphi}_j(-\mu'), \tag{A.60}$$

where $\tilde{\mathbf{X}}(\mu,\mu') = \mu\mathbf{X}(\mu,\mu')$, $\tilde{\mathbf{Y}}(\mu,\mu') = \mu\mathbf{Y}(\mu,\mu')$. We note that in Eqs. (A.59)–(A.60) μ is always positive. Merging Eq. (A.59) and Eq. (A.60) we have

$$\begin{pmatrix} -\mu\mathbf{E}_4 & \mathbf{0} \\ \mathbf{0} & \mu\mathbf{E}_4 \end{pmatrix}\begin{pmatrix} \boldsymbol{\varphi}_j(-\mu) \\ \boldsymbol{\varphi}_j(\mu) \end{pmatrix}\boldsymbol{\lambda}_j = \int_0^1 \mathrm{d}\mu'\mathbf{H}(\mu,\mu')\begin{pmatrix} \boldsymbol{\varphi}_j(-\mu') \\ \boldsymbol{\varphi}_j(\mu') \end{pmatrix}, \tag{A.61}$$

where

$$\mathbf{H}(\mu,\mu') = \begin{bmatrix} \tilde{\mathbf{X}}(\mu,\mu') & \tilde{\mathbf{Y}}(\mu,\mu') \\ \tilde{\mathbf{Y}}(\mu,\mu') & \tilde{\mathbf{X}}(\mu,\mu') \end{bmatrix}. \tag{A.62}$$

Multiplying both sides with $[\boldsymbol{\psi}_k^{\mathrm{T}}(-\mu)\;\; \boldsymbol{\psi}_k^{\mathrm{T}}(\mu)]$ and integrating over μ from 0 to 1, gives

$$\mathbf{N}_{kj}\boldsymbol{\lambda}_j = \int_0^1 \mathrm{d}\mu\begin{pmatrix} \boldsymbol{\psi}_k(-\mu) \\ \boldsymbol{\psi}_k(\mu) \end{pmatrix}^{\mathrm{T}} \int_0^1 \mathrm{d}\mu'\mathbf{H}(\mu,\mu')\begin{pmatrix} \boldsymbol{\varphi}_j(-\mu') \\ \boldsymbol{\varphi}_j(\mu') \end{pmatrix}, \tag{A.63}$$

where $\mathbf{N}_{kj}$ are 4×4 matrices defined as

$$\mathbf{N}_{kj} = \int_0^1 \mathrm{d}\mu\begin{pmatrix} \boldsymbol{\psi}_k(-\mu) \\ \boldsymbol{\psi}_k(\mu) \end{pmatrix}^{\mathrm{T}}\begin{pmatrix} -\mu\mathbf{E}_4 & \mathbf{0} \\ \mathbf{0} & \mu\mathbf{E}_4 \end{pmatrix}\begin{pmatrix} \boldsymbol{\varphi}_j(-\mu) \\ \boldsymbol{\varphi}_j(\mu) \end{pmatrix}. \tag{A.64}$$

We now replace $\mathbf{B}_l^m$ in Eqs. (23)–(24) with $(\mathbf{B}_l^m)^{\mathrm{T}}$, and denote the corresponding matrices $\tilde{\mathbf{X}}$, $\tilde{\mathbf{Y}}$ and $\mathbf{H}$ etc. as $\tilde{\mathbf{X}}^+$, $\tilde{\mathbf{Y}}^+$ and $\mathbf{H}^+$ etc. Because

$$(\mathbf{B}_l^m)^{\mathrm{T}} = \Re\mathbf{B}_l^m\Re, \tag{A.65}$$

$$\mathbf{P}_l^m(\mu) = \Re\mathbf{P}_l^m(\mu)\Re, \tag{A.66}$$

where $\Re = \mathrm{diag}(1,1,1,-1)$, we can find from Eq. (23)

$$\mathbf{X}_{ik}^+ = \Re\mathbf{X}_{ik}\Re, \tag{A.67}$$

$$\mathbf{Y}_{ik}^+ = \Re\mathbf{Y}_{ik}\Re, \tag{A.68}$$

which shows that the new problem has the same eigenvalues, and the corresponding eigenvectors, denoted as $\boldsymbol{\psi}_k$, are related to $\boldsymbol{\varphi}_k$ by

$$\boldsymbol{\psi}_k(\mu) = \Re\boldsymbol{\varphi}_k(\mu). \tag{A.69}$$

Similar to Eq. (A.61), we can obtain for the new problem:

$$\begin{pmatrix} -\mu'\mathbf{E}_4 & \mathbf{0} \\ \mathbf{0} & \mu'\mathbf{E}_4 \end{pmatrix}\begin{pmatrix} \boldsymbol{\psi}_k(-\mu') \\ \boldsymbol{\psi}_k(\mu') \end{pmatrix}\boldsymbol{\lambda}_k = \int_0^1 \mathrm{d}\mu\mathbf{H}^+(\mu',\mu)\begin{pmatrix} \boldsymbol{\psi}_k(-\mu) \\ \boldsymbol{\psi}_k(\mu) \end{pmatrix}. \tag{A.70}$$

Multiply both sides with $[\boldsymbol{\varphi}_j^{\mathrm{T}}(-\mu')\ \ \boldsymbol{\varphi}_j^{\mathrm{T}}(\mu')]$, integrate over μ' from 0 to 1, transpose on both sides, and note that $\mathbf{H}^+ = \mathbf{H}^{\mathrm{T}}$, we obtain

$$\boldsymbol{\lambda}_k\mathbf{N}_{kj} = \int_0^1 \mathrm{d}\mu\begin{pmatrix} \boldsymbol{\psi}_k(-\mu) \\ \boldsymbol{\psi}_k(\mu) \end{pmatrix}^{\mathrm{T}}\int_0^1 \mathrm{d}\mu'\mathbf{H}(\mu,\mu')\begin{pmatrix} \boldsymbol{\varphi}_j(-\mu') \\ \boldsymbol{\varphi}_j(\mu') \end{pmatrix}. \tag{A.71}$$

Eq. (A.63) and Eq. (A.71) have the same RHS, therefore

$$\mathbf{N}_{kj}\boldsymbol{\lambda}_j = \boldsymbol{\lambda}_k\mathbf{N}_{kj}. \tag{A.72}$$

This equation means that, when $j \neq k$, all elements of $\mathbf{N}_{kj}$ must be 0, and when $j = k$, $\mathbf{N}_{kj}$ must be diagonal, i.e.,

$$\int_0^1 \mathrm{d}\mu\begin{pmatrix} \boldsymbol{\psi}_k(-\mu) \\ \boldsymbol{\psi}_k(\mu) \end{pmatrix}^{\mathrm{T}}\begin{pmatrix} -\mu\mathbf{E}_4 & \mathbf{0} \\ \mathbf{0} & \mu\mathbf{E}_4 \end{pmatrix}\begin{pmatrix} \boldsymbol{\varphi}_j(-\mu) \\ \boldsymbol{\varphi}_j(\mu) \end{pmatrix} = \mathbf{N}_j\delta_{jk}, \tag{A.73}$$

where $\mathbf{N}_j$ are 4×4 diagonal matrices. By expanding Eq. (A.73) we can rewrite it as

$$\int_{-1}^1 \boldsymbol{\psi}_k^{\mathrm{T}}(\mu)\mu\boldsymbol{\varphi}_j(\mu)\,\mathrm{d}\mu = \mathbf{N}_j\delta_{jk}. \tag{A.74}$$

The orthogonal property is obtained.

References

[1] Green G. An essay on the application of mathematical analysis to the theories of electricity and magnetism, printed by T. Wheelhouse, Nottingham; 1828.

[2] Stakgold I. Green's functions and boundary value problems, New York: Wiley; 1979. 638pp.

[3] Case KM, Zweifel PF. Linear transport theory. Reading, MA: Addison-Wesley; 1967. 342pp.

[4] Bell GI, Glasstone S. Nuclear reactor theory. New York: Van Nostrand Reinholt; 1970. 619pp.

[5] Siewert CE. A concise and accurate solution to Chandrasekhar's basic problem in radiative transfer. JQSRT 2000;64:109–30.

[6] Siewert CE. A discrete-ordinate solution for radiative transfer models that include polarization effects. JQSRT 2000;64:227–54.

[7] Barichello LB, Garcia RDM, Siewert CE. Particular solution for the discrete-ordinates method. JQSRT 2000; 64:219–26.

[8] Qin Y, Box MA, Jupp DLB. Particular solution of discrete-ordinate method. Appl Opt 2004;43:3717–25.

[9] Spurr RJD. Simultaneous derivation of intensities and weighting functions in a general pseudo-spherical discrete ordinate radiative transfer treatment. JQSRT 2002;75:129–75.

[10] Chandrasekhar S. Radiative transfer. New York: Dover; 1960. 393pp.

[11] Stamnes K, Tsay S, Wiscombe W, Jayaweera K. Numerically stable algorithm for discrete-ordinate-method radiative transfer in multiple scattering and emitting layered media. Appl Opt 1988;27:2502–10.

[12] Lyapustin A, Knyazikhin Y. Green's function method for the radiative transfer problem. I. Homogeneous non-Lambertian surface. Appl Opt 2001;40:3495–501.

[13] Lyapustin A, Knyazikhin Y. Green's function method in the radiative transfer problem. II. Spatially heterogeneous anisotropic surface. Appl Opt 2002;41:5600–6.
[14] Liou KN. An Introduction to Atmospheric Radiation. New York: Academic Press; 1980.
[15] Landgraf J, Hasekamp OP, Trautmann T. Linearization of radiative transfer with respect to surface properties. JQSRT 2002;72:327–39.
[16] Box MA, Keevers M, McKellar BHJ. On the perturbation series for radiative effects. JQSRT 1988;39:219–23.
[17] Trautmann T, Elliott P, Box MA. Shortwave radiative effects of standard aerosol models: a perturbation approach. Beitr Phys Atmos 1992;65:59–78.
[18] Box MA, Polonsky IN, Davis AB. Higher order perturbation theory applied to radiative transfer in non-plane-parallel media. JQSRT 2003;78:105–18.
[19] Polonsky IN, Box MA. General perturbation technique for the calculation of radiative effects in scattering and absorbing media. J Opt Soc Am 2002;19:2281–92.
[20] Qin Y, Jupp DLB, Box MA. Extension of the Discrete-Ordinate algorithm and high efficient radiative transfer calculation. JQSRT 2002;74:767–81.
[21] Qin Y, Box MA, Trautmann T. Accelerated higher order radiative perturbation computation: an application of GDOM. JQSRT 2004;92:73–83.
[22] Benedetti A, Gabriel P, Stephens GL. Properties of reflected sunlight derived from a Green's function method. JQSRT 2002;72:201–25.
[23] Davis AB, Marshak A. Space-time characteristics of light transmitted through dense clouds: a Green's function analysis. J Atmos Sci 2002;59:2713–27.
[24] Davis AB, Cahalan RF, Spinehirne D, McGill MJ, Love SP. Off-beam Lidar: an emerging technique in cloud remote-sensing based on radiative Green-function theory in the diffusion domain. Phys Chem Earth (B) 1999; 24:177–85.
[25] Knyazikhin Y, Marshak A. Mathematical aspects of BRDF modelling: adjoint problem and Green's function. Rem Sens Rev 2000;18:263–80.
[26] Tezcan C, Kaskas A, Gulecyuz MC. The H-N method for solving linear transport equation: theory and applications. JQSRT 2003;78:243–54.
[27] Hong SG, Cho NZ. The infinite medium Green's function method for multigroup discrete ordinate transport problems in multi-layered slab geometry. Ann Nuclear Energy 2001;28:1101–14.
[28] Hovenier JW. Symmetry relationships for scattering of polarized light in a slab of randomly oriented particles. J Atmos Sci 1969;26:488–9.
[29] Anderson E, Bai Z, Bischof C, Blackford S, Demmel J, Dongarra J, Du Croz J, Greenbaum A, Hammarling S, McKenney A, Sorensen D. LAPACK Users' Guide, 3rd ed. Philadelphia, PA: Society for Industrial and Applied Mathematics; 1999 (electronic version is available at: www.netlib.org/lapack).
[30] Asano S. On the discrete ordinates method for radiative transfer. J Meteo Soc Jpn 1975;53:92–5.
[31] Gelfand IM, Sapiro ZY. Representation of the group rotations of 3-dimensional space and their applications. Amer Math Soc Trans 1956;2:207–316.
[32] Siewert CE. On the equation of transfer relevant to the scattering of polarized light. The Astrophysical J 1981;245:1080–6.
[33] Siewert CE. On the phase matrix to the scattering of polarized light. Astron Astrophys 1982;109:195–200.