# Singular eigenfunctions for the three-dimensional radiative transport equation

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Case's method obtains solutions to the radiative transport equation as superpositions of elementary solutions when the specific intensity depends on one spatial variable. In this paper, we find elementary solutions when the specific intensity depends on three spatial variables in three-dimensional space. By using the reference frame whose z axis lies in the direction of the wave vector, the angular part of each elementary solution becomes the singular eigenfunction for the one-dimensional radiative transport equation. Thus, Case's method is generalized. © 2013 Optical Society of America

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### 1. INTRODUCTION

We consider light propagating in random media, such as fog, cloud, and biological tissue. Then the specific intensity of light obeys the radiative transport equation. Although different numerical methods have been developed [1-3], the analytical approach is preferable particularly for the sake of medical imaging and optical tomography [4,5].

Case's method is a method of obtaining solutions to the equation as superpositions of elementary solutions [6]. Although the method gives insight into the theoretical structure of the specific intensity, it works only when the specific intensity carries one spatial variable and is independent of two spatial variables in three-dimensional space. While the extension of Case's method to anisotropic scattering was soon done [7,8], there has been no real success in extending the method to three dimensions despite considerable efforts [9-15]. In particular, Kaper proposed elementary solutions of the form of a plane wave and developed a singular eigenfunction theory by reducing the problem to a one-dimensional equation by changing angular variables to a new complex variable [10]. However, this singular eigenfunction is complicated (for example, the dispersion function  $\Lambda$  is given by a threedimensional integral) [13]. Even for an infinite medium with isotropic scattering, calculation is quite complicated. Duderstadt and Martin wrote, "Although there have been many attempts to extend these methods (the integral transform and singular eigenfunction methods) to two- and threedimensional problems, these extensions have usually encountered extreme mathematical complexity and have met with only marginal success" ([2], p. 122).

In this paper, we extend Case's method to a general case where the specific intensity depends on three spatial variables in addition to two angular variables. We evaluate the singular eigenfunction in each elementary solution with the reference frame whose z axis is taken in the direction of the wave vector. That is, the reference frame is rotated depending on the transverse buckling constants. This point is the key difference from Kaper's singular eigenfunctions. Indeed, the idea of rotated reference frames was first used by Markel [<u>16</u>]; the angular part of elementary solutions was expanded by rotated spherical harmonics.

The remainder of the paper is organized as follows. In Section 2, we introduce the radiative transport equation. In Section 3, we develop singular eigenfunctions and obtain elementary solutions. In Section 4, we consider eigenvalues. We see the relation to the method of rotated reference frames in Section 5. In Section 6, we obtain the three-dimensional Green's function in an infinite medium. Then the energy density is calculated as a numerical example in Section 7. Finally, we give summary in Section 8. Polar and azimuthal angles in rotated reference frames are presented in Appendix A. The expansion coefficients in the method of rotated reference frames are calculated in Appendix B.

### 2. RADIATIVE TRANSPORT EQUATION

Let  $I(\mathbf{r}, \hat{\mathbf{s}})$  be the specific intensity at position  $\mathbf{r} \in \mathbb{R}^3$  in direction  $\hat{\mathbf{s}} \in \mathbb{S}^2$ . We consider the time-independent radiative transport equation, which is given by

$$\hat{\mathbf{s}} \cdot \nabla I(\mathbf{r}, \hat{\mathbf{s}}) + (\mu_a + \mu_s)I(\mathbf{r}, \hat{\mathbf{s}}) = \mu_s \int_{\mathbb{S}^2} f(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}')I(\mathbf{r}, \hat{\mathbf{s}}') d\hat{\mathbf{s}}' + S(\mathbf{r}, \hat{\mathbf{s}}),$$
(1)

where  $\mu_a$  and  $\mu_s$  are the absorption and scattering coefficients, respectively, and  $S(\mathbf{r}, \hat{\mathbf{s}})$  is the source term. We suppose  $\mu_a$  and  $\mu_s$  are positive constants, and the scattering phase function  $f(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}')$  can be modeled by a polynomial of spherical harmonics of degree *N*:

$$f(\hat{\mathbf{s}}\cdot\hat{\mathbf{s}}') = \sum_{l=0}^{N} \sum_{m=-l}^{l} f_l Y_{lm}(\hat{\mathbf{s}}) Y_{lm}^*(\hat{\mathbf{s}}').$$
(2)

We choose  $f_l$  so that f is normalized as

$$\int_{\mathbb{S}^2} f(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}') \mathrm{d}\hat{\mathbf{s}}' = 1.$$
(3)

We have  $N = 0, f_0 = 1$  in the case of isotropic scattering, and have  $N = 1, f_0 = 1, f_1 = \int_{\mathbb{S}^2} (\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}') f(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}') d\hat{\mathbf{s}}'$  in the case of linear scattering. For the Henyey–Greenstein model [17], we have  $N = \infty, f_l = f_1^l$ . By dividing both sides of Eq. (1) by  $\mu_t = \mu_a + \mu_s$ , we obtain

$$\hat{\mathbf{s}} \cdot \nabla_{\tilde{\mathbf{r}}} I(\tilde{\mathbf{r}}/\mu_t, \hat{\mathbf{s}}) + I(\tilde{\mathbf{r}}/\mu_t, \hat{\mathbf{s}}) = c \int_{\mathbb{S}^2} f(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}') I(\tilde{\mathbf{r}}/\mu_t, \hat{\mathbf{s}}') d\hat{\mathbf{s}}' + \frac{1}{\mu_t} S(\tilde{\mathbf{r}}/\mu_t, \hat{\mathbf{s}}), \qquad (4)$$

where  $c = \mu_s / \mu_t$  is a constant, 0 < c < 1, and  $\tilde{\mathbf{r}} = \mu_t \mathbf{r}$ . By writing

$$\tilde{I}(\tilde{\mathbf{r}}, \hat{\mathbf{s}}) = I(\tilde{\mathbf{r}}/\mu_t, \hat{\mathbf{s}}), \tag{5}$$

we obtain

$$\hat{\mathbf{s}} \cdot \nabla_{\tilde{\mathbf{r}}} \tilde{I}(\tilde{\mathbf{r}}, \hat{\mathbf{s}}) + \tilde{I}(\tilde{\mathbf{r}}, \hat{\mathbf{s}}) = c \int_{\mathbb{S}^2} f(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}') \tilde{I}(\tilde{\mathbf{r}}, \hat{\mathbf{s}}') \mathrm{d}\hat{\mathbf{s}}' + \frac{1}{\mu_t} S(\tilde{\mathbf{r}}/\mu_t, \hat{\mathbf{s}}).$$
(6)

Hereafter, we will take the unit of length to be  $1/\mu_t$  and drop tildes.

The specific intensity I in Eq. (6) is given as a superposition of elementary solutions, which are solutions to the following homogeneous equation:

$$\hat{\mathbf{s}} \cdot \nabla I(\mathbf{r}, \hat{\mathbf{s}}) + I(\mathbf{r}, \hat{\mathbf{s}}) = c \int_{\mathbb{S}^2} f(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}') I(\mathbf{r}, \hat{\mathbf{s}}') d\hat{\mathbf{s}}'.$$
 (7)

Let  $\mu = \cos \theta$  be the cosine of the polar angle of  $\hat{\mathbf{s}}$  and  $\varphi$  be the azimuthal angle of  $\hat{\mathbf{s}}$ . Following [7], we express  $f(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}')$  in Eq. (2) as

$$f(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}') = \sum_{l=0}^{N} \sum_{m=-l}^{l} f_{l} \frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!} (1-\mu^{2})^{|m|/2} \times (1-\mu'^{2})^{|m|/2} p_{l}^{m}(\mu) p_{l}^{m}(\mu') e^{im(\varphi-\varphi')}.$$
(8)

Here the polynomials  $p_l^m(\mu)$  are related to associated Legendre polynomials  $P_l^m(\mu)$  as [7]

$$P_l^m(\mu) = (-1)^m (1 - \mu^2)^{|m|/2} p_l^m(\mu).$$
(9)

They satisfy the following recurrence relations and orthogonality relations:

$$(l-m+1)p_{l+1}^m(\mu) = (2l+1)\mu p_l^m(\mu) - (l+m)p_{l-1}^m(\mu), \quad (10)$$

$$\int_{-1}^{1} p_{l}^{m}(\mu) p_{l'}^{m}(\mu) \mathrm{d}m(\mu) = \frac{2(l+m)!}{(2l+1)(l-m)!} \delta_{ll'}, \qquad (11)$$

where we introduced

$$dm(\mu) = (1 - \mu^2)^{|m|} d\mu.$$
(12)

Furthermore, we have

$$p_{|m|}^{m}(\mu) = \begin{cases} \frac{2^{m}m!}{2^{m}m!} & \text{for } m \ge 0, \\ \frac{(-1)^{m}}{2^{|m|}(|m|!)} & \text{for } m < 0. \end{cases}$$
(13)

### **3. ELEMENTARY SOLUTIONS**

We seek solutions of the form of plane-wave decomposition  $[\underline{10,18,19}]$ . We introduce  $\nu \in \mathbb{R}$  and  $\mathbf{q} \in \mathbb{R}^2$ , and define vector  $\mathbf{k} \in \mathbb{C}^3$  as

$$\mathbf{k} = \frac{1}{\nu} \hat{\mathbf{k}}, \qquad \hat{\mathbf{k}} = \begin{pmatrix} -i\nu \mathbf{q} \\ Q(\nu q) \end{pmatrix}, \qquad Q(\nu q) = \sqrt{1 + (\nu q)^2}, \quad (14)$$

where  $q = |\mathbf{q}|$ . We emphasize that  $\mathbf{k}$  and  $\hat{\mathbf{k}}$  are functions of  $\nu$  and  $\mathbf{q}$ . We assume the specific intensity of the form

$$I_{\nu}^{m}(\mathbf{r},\hat{\mathbf{s}};\mathbf{q}) = \Phi_{\nu}^{m}(\hat{\mathbf{s}};\hat{\mathbf{k}})e^{-\mathbf{k}\cdot\mathbf{r}},$$
(15)

where

$$\Phi^m_{\nu}(\hat{\mathbf{s}}; \hat{\mathbf{k}}) = \phi^m(\nu, \mu(\hat{\mathbf{k}}))(1 - \mu(\hat{\mathbf{k}})^2)^{|m|/2} e^{im\varphi(\hat{\mathbf{k}})}.$$
 (16)

Here,  $\mu(\hat{\mathbf{k}})$  and  $\varphi(\hat{\mathbf{k}})$  are the cosine of the polar angle of  $\hat{\mathbf{s}}$  and the azimuthal angle of  $\hat{\mathbf{s}}$ , respectively, in the rotated reference frame whose z axis coincides with the direction of  $\hat{\mathbf{k}}$  (see Appendix <u>A</u>). Note that in the laboratory frame ( $\hat{\mathbf{k}} = \hat{\mathbf{z}}$ ), Eq. (<u>15</u>) reduces to the form used in [7]. We will determine elementary solutions  $I_{\nu}^{m}(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{q})$  in Eq. (<u>15</u>) so that they satisfy Eq. (7). We normalize  $\phi^{m}$  as

$$\frac{1}{2\pi} \int_{\mathbb{S}^2} \phi^m(\nu, \mu(\hat{\mathbf{k}})) (1 - \mu(\hat{\mathbf{k}})^2)^{|m|} d\hat{\mathbf{s}} = \int_{-1}^1 \phi^m(\nu, \mu) dm(\mu) = 1.$$
(17)

We will calculate singular eigenfunctions  $\phi^m$  below.

By plugging Eq.  $(\underline{15})$  into the radiative transport equation (7), we obtain

$$\begin{split} & \left(1 - \frac{\mu(\hat{\mathbf{k}})}{\nu}\right) \phi^m(\nu, \mu(\hat{\mathbf{k}})) (1 - \mu(\hat{\mathbf{k}})^2)^{|m|/2} e^{im\varphi(\hat{\mathbf{k}})} \\ &= c \int_{\mathbb{S}^2} f(\hat{\mathbf{s}}(\hat{\mathbf{k}}) \cdot \hat{\mathbf{s}}'(\hat{\mathbf{k}})) \phi^m(\nu, \mu'(\hat{\mathbf{k}})) (1 - \mu'(\hat{\mathbf{k}})^2)^{|m|/2} e^{im\varphi'(\hat{\mathbf{k}})} \mathrm{d}\hat{\mathbf{s}}', \end{split}$$
(18)

where we used  $\hat{\mathbf{s}} \cdot \hat{\mathbf{k}} = \mu(\hat{\mathbf{k}})$  and expressed  $f(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}')$  in the rotated reference frame. The right-hand side is calculated as

RHS = 
$$2\pi c \Theta (N - |m|) (1 - \mu(\hat{\mathbf{k}})^2)^{|m|/2} e^{im\varphi(\hat{\mathbf{k}})}$$
  
  $\times \sum_{l'=|m|}^{N} f_l \frac{2l' + 1}{4\pi} \frac{(l' - m)!}{(l' + m)!}$   
  $\times p_{l'}^m(\mu(\hat{\mathbf{k}})) \int_{-1}^{1} p_{l'}^m(\mu') \phi^m(\nu, \mu') dm(\mu'),$  (19)

where the step function  $\Theta(\cdot)$  is defined as  $\Theta(x) = 1$  for  $x \ge 0$ and = 0 for x < 0. Hence, ~

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$$(\nu - \mu(\mathbf{k}))\phi^{m}(\nu, \mu(\mathbf{k})) = 2\pi c\nu\Theta(N - |m|) \\ \times \sum_{l'=|m|}^{N} f_{l'} \frac{2l' + 1}{4\pi} \frac{(l' - m)!}{(l' + m)!} p_{l'}^{m}(\mu(\hat{\mathbf{k}}))h_{l'}^{m}(\nu),$$
(20)

where we defined

$$h_l^m(\nu) = \int_{-1}^1 \phi^m(\nu, \mu) p_l^m(\mu) \mathrm{d}m(\mu).$$
(21)

The polynomials  $h_l^m$  were introduced by Mika [8] for m = 0and then generalized by McCormick and Kuščer [7] for general m. Since the right-hand side of Eq. (20) is zero for |m| > N and then  $\phi^m = 0$ , hereafter we suppose

$$0 \le |m| \le N. \tag{22}$$

Let us define

$$\sigma_l = 1 - cf_l \Theta(N - l). \tag{23}$$

From Eq. (20), we obtain

$$\sigma_l \nu h_l^m(\nu) = \int_{-1}^1 \mu \phi^m(\nu, \mu) p_l^m(\mu) \mathrm{d}m(\mu).$$
(24)

Equation (24) implies the three-term recurrence relation for  $h_l^m(\nu)$  [20]:

$$\nu(2l+1)\sigma_l h_l^m(\nu) - (l-m+1)h_{l+1}^m(\nu) - (l+m)h_{l-1}^m(\nu) = 0$$
(25)

with

$$h_{|m|}^{m}(\nu) = p_{|m|}^{m} \tag{26}$$

and

$$h_{|m|+1}^{|m|}(\nu) = (2|m|+1)\nu\sigma_{|m|}h_{|m|}^{|m|}(\nu).$$
(27)

We also have

$$h_l^{-|m|}(\nu) = (-1)^{|m|} \frac{(l-|m|)!}{(l+|m|)!} h_l^{|m|}(\nu).$$
(28)

The functions  $h_l^m(\nu)$  are computed using Eq. (25).

Let us define

$$g^{m}(\nu,\mu(\hat{\mathbf{k}})) = \sum_{l'=|m|}^{N} (2l'+1) f_{l'} \frac{(l'-m)!}{(l'+m)!} p_{l'}^{m}(\mu(\hat{\mathbf{k}})) h_{l'}^{m}(\nu).$$
(29)

We note that  $g^{-m}(\nu,\mu(\hat{\mathbf{k}})) = g^m(\nu,\mu(\hat{\mathbf{k}}))$ . The function  $\phi^m$  is obtained as

$$\phi^{m}(\nu,\mu(\hat{\mathbf{k}})) = \frac{c\nu}{2} \mathcal{P}\frac{g^{m}(\nu,\mu(\hat{\mathbf{k}}))}{\nu-\mu(\hat{\mathbf{k}})} + \lambda^{m}(\nu)(1-\nu^{2})^{-|m|}\delta(\nu-\mu(\hat{\mathbf{k}})),$$
(30)

where  $\lambda^m(\nu)$  is given below.

### 4. DISCRETE EIGENVALUES AND CONTINUOUS SPECTRUM

By multiplying  $(1 - \mu(\hat{\mathbf{k}})^2)^{|m|}$  and integrating over  $\hat{\mathbf{s}}$ , Eq. (30) becomes

$$1 = \frac{c\nu}{2} \mathcal{P} \int_{-1}^{1} \frac{g^m(\nu,\mu)}{\nu-\mu} \mathrm{d}m(\mu) + \int_{-1}^{1} \lambda^m(\nu) \delta(\nu-\mu) \mathrm{d}\mu.$$
(31)

For  $\nu \in (-1, 1)$ , we obtain

$$\lambda^{m}(\nu) = 1 - \frac{c\nu}{2} \mathcal{P} \int_{-1}^{1} \frac{g^{m}(\nu, \mu)}{\nu - \mu} \mathrm{d}m(\mu).$$
(32)

Note that  $\lambda^{-m}(\nu) = \lambda^{m}(\nu)$  and hence  $\phi^{-m}(\nu,\mu(\hat{\mathbf{k}})) = \phi^{m}(\nu,\mu(\hat{\mathbf{k}}))$ . Let us define

$$\Lambda^{m}(z) = 1 - \frac{cz}{2} \int_{-1}^{1} \frac{g^{m}(z,\mu)}{z-\mu} \mathrm{d}m(\mu), \qquad (33)$$

where  $z \in \mathbb{C}$ . Eigenvalues  $\nu \notin [-1, 1]$  are solutions to

$$\Lambda^m(\nu) = 0. \tag{34}$$

We write these discrete eigenvalues as  $\pm \nu_j^m$  ( $\nu_0^m > \nu_1^m > \cdots > \nu_{M-1}^m > 1$ ). Note that  $\nu_j^{-m} = \nu_j^m$ . The number of discrete eigenvalues M depends on |m| and we have [7,8]  $M \le N - |m| + 1$ . For  $\nu \in (-1, 1)$ , we have the continuous spectrum.

## 5. METHOD OF ROTATED REFERENCE FRAMES

Let us expand singular eigenfunctions with spherical harmonics. By introducing  $c_i^m(\nu)$ , we write

$$\Phi^m_{\nu}(\hat{\mathbf{s}}; \hat{\mathbf{k}}) = \sum_{l=|m|}^{\infty} c^m_l(\nu) Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{k}}).$$
(35)

The calculation of the specific intensity by this expansion is called the method of rotated reference frames [ $\underline{16},\underline{21}-\underline{23}$ ]. From Eq. (18), we obtain

$$c_l^m(\nu) - \frac{1}{\nu} \sum_{l'=|m|}^{\infty} \left( \int_{\mathbb{S}^2} \mu Y_{l'm}(\hat{\mathbf{s}}) Y_{lm}^*(\hat{\mathbf{s}}) \mathrm{d}\hat{\mathbf{s}} \right) c_l^m(\nu)$$
  
=  $cf_l \Theta(N-l) c_l^m(\nu).$  (36)

Hence, we arrive at an eigenproblem:

$$B^{m}|\psi^{m}(\nu)\rangle = \nu|\psi^{m}(\nu)\rangle, \qquad (37)$$

where

$$B_{ll'}^{m} = \frac{1}{\sqrt{\sigma_{l}\sigma_{l'}}} \int_{\mathbb{S}^{2}} \mu Y_{l'm}(\hat{\mathbf{s}}) Y_{lm}^{*}(\hat{\mathbf{s}}) d\hat{\mathbf{s}}$$
  
=  $\sqrt{\frac{l^{2} - m^{2}}{(4l^{2} - 1)\sigma_{l}\sigma_{l-1}}} \delta_{l',l-1} + \sqrt{\frac{(l+1)^{2} - m^{2}}{(4(l+1)^{2} - 1)\sigma_{l+1}\sigma_{l}}} \delta_{l',l+1}, (38)$ 

$$\langle l|\psi^m(\nu)\rangle = \frac{1}{\sqrt{Z^m(\nu)}}\sqrt{\sigma_l}c_l^m(\nu),\tag{39}$$

where the normalization factor  $Z^m(\nu)$  will be determined below so that  $\langle \psi^m(\nu) | \psi^m(\nu) \rangle = 1$  is satisfied. Note that  $\Phi^m_{\nu}$  and  $| \psi^m(\nu) \rangle$  are related as

$$\Phi_{\nu}^{m}(\hat{\mathbf{s}};\hat{\mathbf{k}}) = \sqrt{Z^{m}(\nu)} \sum_{l=|m|}^{\infty} \frac{\langle l | \psi^{m}(\nu) \rangle}{\sqrt{\sigma_{l}}} Y_{lm}(\hat{\mathbf{s}};\hat{\mathbf{k}}).$$
(40)

In Appendix B, expansion coefficients  $c_l^m(\nu)$  in Eq. (35) are calculated using Eqs. (39) and (40).

### 6. GREEN'S FUNCTION

Let us consider the Green's function of the radiative transport equation in an infinite medium. The Green's function obeys

$$\hat{\mathbf{s}} \cdot \nabla G(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}_0, \hat{\mathbf{s}}_0) + G(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}_0, \hat{\mathbf{s}}_0)$$
  
=  $c \int_{\mathbb{S}^2} f(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}') G(\mathbf{r}, \hat{\mathbf{s}}'; \mathbf{r}_0, \hat{\mathbf{s}}_0) d\hat{\mathbf{s}}' + \delta(\mathbf{r} - \mathbf{r}_0) \delta(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0).$  (41)

To proceed, we introduce  $\tilde{\Phi}^m_{\nu}(\hat{\mathbf{s}}; \hat{\mathbf{k}})$  such that

$$\int_{\mathbb{S}^2} \mu \Phi^m_{\nu}(\hat{\mathbf{s}}; \hat{\mathbf{k}}) [\tilde{\Phi}^m_{\nu'}(\hat{\mathbf{s}}; \hat{\mathbf{k}}')]^* \mathrm{d}\hat{\mathbf{s}} = \delta_{\nu\nu'}, \qquad (42)$$

where the Kronecker delta  $\delta_{\nu\nu'}$  is understood as the Dirac delta  $\delta(\nu - \nu')$  for the continuous spectrum. The function  $\tilde{\Phi}_{\nu}^{m}(\hat{\mathbf{s}}; \hat{\mathbf{k}})$  will be determined as we compute the Green's function.

We replace the source term in Eq.  $(\underline{41})$  by a jump condition and solve

 $\begin{cases} \hat{\mathbf{s}} \cdot \nabla G(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}_{0}, \hat{\mathbf{s}}_{0}) + G(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}_{0}, \hat{\mathbf{s}}_{0}) = c \int_{\mathbb{S}^{2}} f(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}') G(\mathbf{r}, \hat{\mathbf{s}}'; \mathbf{r}_{0}, \hat{\mathbf{s}}_{0}) d\hat{\mathbf{s}}', \\ G(\rho, z_{0} + 0, \hat{\mathbf{s}}; \mathbf{r}_{0}, \hat{\mathbf{s}}_{0}) - G(\rho, z_{0} - 0, \hat{\mathbf{s}}; \mathbf{r}_{0}, \hat{\mathbf{s}}_{0}) = \frac{1}{\hat{\mathbf{s}}\hat{\mathbf{z}}} \delta(\rho - \rho_{0}) \delta(\hat{\mathbf{s}} - \hat{\mathbf{s}}_{0}), \end{cases}$ (43)

with the condition  $\lim_{|\mathbf{r}|\to\infty} G(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}_0, \hat{\mathbf{s}}_0) = 0$  and  $\mathbf{r} = (\rho, z)$  $(\rho \in \mathbb{R}^2, z \in \mathbb{R})$ , where  $\rho = (x, y)$ . Let us expand the Green's function using elementary solutions or normal modes Eq. (15). To find  $\tilde{\Phi}^m_{\nu}$ , we note that the Green's function obtained with the method of rotated reference frames [21] is expressed as

$$G(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}_{0}, \hat{\mathbf{s}}_{0}) = \frac{1}{(2\pi)^{2}} \int_{\mathbb{R}^{2}} e^{i\mathbf{q}\cdot(\rho-\rho_{0})} \sum_{\nu>0} \sum_{m=-N}^{N} \frac{1}{\nu Q(\nu q) Z^{m}(\nu)} \times \Phi_{\pm\nu}^{m}(\hat{\mathbf{s}}, \hat{\mathbf{k}}) [\Phi_{\pm\nu}^{m}(\hat{\mathbf{s}}_{0}; \hat{\mathbf{k}})]^{*} e^{-Q(\nu q)|z-z_{0}|/\nu} \mathrm{d}\mathbf{q}, \qquad (47)$$

where we used the relation  $(\underline{40})$ . By comparing Eqs.  $(\underline{46})$  and  $(\underline{47})$ , we obtain

$$\tilde{\Phi}^m_{\pm\nu}(\hat{\mathbf{s}};\hat{\mathbf{k}}) = \Phi^m_{+\nu}(\hat{\mathbf{s}};\hat{\mathbf{k}})[\pm\nu Q(\nu q)Z^m(\nu)]^{-1}.$$
(48)

To determine  $Z^m(\nu)$ , we consider the one-dimensional case. By integrating the Green's function over  $\rho_0$ , we obtain

$$G(z, \hat{\mathbf{s}}; z_0, \hat{\mathbf{s}}_0) = \pm \sum_{m=-N}^{N} \left\{ \sum_{j=0}^{M-1} \Phi_{j\pm}^m(\hat{\mathbf{s}}; \hat{\mathbf{z}}) [\tilde{\Phi}_{j\pm}^m(\hat{\mathbf{s}}_0; \hat{\mathbf{z}})]^* e^{-|z-z_0|/\nu_j^m} + \int_0^1 \Phi_{\pm\nu}^m(\hat{\mathbf{s}}; \hat{\mathbf{z}}) [\tilde{\Phi}_{\pm\nu}^m(\hat{\mathbf{s}}_0; \hat{\mathbf{z}})]^* e^{-|z-z_0|/\nu} d\nu \right\}.$$
 (49)

On the other hand, the one-dimensional Green's function is given by  $[\underline{7,8}]$ 

$$\begin{cases} G(\boldsymbol{\rho}, z, \hat{\mathbf{s}}; \boldsymbol{\rho}_{0}, z_{0}, \hat{\mathbf{s}}_{0}) &= \sum_{m=-N}^{N} \int_{\mathbb{R}^{2}} \left[ \sum_{j=0}^{M-1} a_{j+}^{m}(\mathbf{q}) I_{j+}^{m}(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{q}) + \int_{0}^{1} A_{\nu}^{m}(\mathbf{q}) I_{\nu}^{m}(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{q}) d\nu \right] \frac{d\mathbf{q}}{(2\pi)^{2}}, \quad z > z_{0}, \\ G(\boldsymbol{\rho}, z, \hat{\mathbf{s}}; \boldsymbol{\rho}_{0}, z_{0}, \hat{\mathbf{s}}_{0}) &= -\sum_{m=-N}^{N} \int_{\mathbb{R}^{2}} \left[ \sum_{j=0}^{M-1} a_{j-}^{m}(\mathbf{q}) I_{j-}^{m}(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{q}) + \int_{0}^{1} A_{\nu}^{m}(\mathbf{q}) I_{\nu}^{m}(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{q}) d\nu \right] \frac{d\mathbf{q}}{(2\pi)^{2}}, \quad z < z_{0}, \end{cases}$$
(44)

From the jump condition, coefficients  $a_{j\pm}^m$  and  $A_{\nu}^m$  are determined as

$$a_{j\pm}^{m}(\mathbf{q}) = e^{-i\mathbf{q}\cdot\rho_{0}}e^{\pm Q(\nu_{j}^{m}q)z_{0}/\nu_{j}^{m}}[\tilde{\Phi}_{j\pm}^{m}(\hat{\mathbf{s}}_{0};\hat{\mathbf{k}})]^{*},$$
  

$$A_{\nu}^{m}(\mathbf{q}) = e^{-i\mathbf{q}\cdot\rho_{0}}e^{Q(\iota q)z_{0}/\nu}[\tilde{\Phi}_{\nu}^{m}(\hat{\mathbf{s}}_{0};\hat{\mathbf{k}})]^{*}.$$
(45)

Hence, the Green's function is written as

$$G(\boldsymbol{\rho}, \boldsymbol{z}, \hat{\mathbf{s}}; \boldsymbol{\rho}_{0}, \boldsymbol{z}_{0}, \hat{\mathbf{s}}_{0}) = \frac{\pm 1}{(2\pi)^{2}} \int_{\mathbb{R}^{2}} e^{i\mathbf{q}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}_{0})} \sum_{m=-N}^{N} \left\{ \sum_{j=0}^{M-1} \times \Phi_{j\pm}^{m}(\hat{\mathbf{s}}; \hat{\mathbf{k}}) [\tilde{\Phi}_{j\pm}^{m}(\hat{\mathbf{s}}_{0}; \hat{\mathbf{k}})]^{*} e^{-Q(\nu_{j}^{m}q)|\boldsymbol{z}-\boldsymbol{z}_{0}|/\nu_{j}^{m}} + \int_{0}^{1} \Phi_{\pm\nu}^{m}(\hat{\mathbf{s}}; \hat{\mathbf{k}}) [\tilde{\Phi}_{\pm\nu}^{m}(\hat{\mathbf{s}}_{0}; \hat{\mathbf{k}})]^{*} \times e^{-Q(\nu q)|\boldsymbol{z}-\boldsymbol{z}_{0}|/\nu} d\nu \right\} d\mathbf{q}, \qquad (46)$$

$$G(z, \hat{\mathbf{s}}; z_0, \hat{\mathbf{s}}_0) = \frac{1}{2\pi} \sum_{m=-N}^{N} \left\{ \sum_{j=0}^{M-1} \frac{1}{\mathcal{N}_j^m} \phi^m(\pm \nu_j^m, \mu) \phi^m(\pm \nu_j^m, \mu_0) \right. \\ \left. \times (1 - \mu^2)^{|m|} e^{im(\varphi - \varphi_0)} e^{-|z - z_0|/\nu_j^m} \right. \\ \left. + \int_0^1 \frac{1}{\mathcal{N}^m(\nu)} \phi^m(\pm \nu, \mu) \phi^m(\pm \nu, \mu_0) \right. \\ \left. \times (1 - \mu^2)^{|m|} e^{im(\varphi - \varphi_0)} e^{-|z - z_0|/\nu} \, \mathrm{d}\nu \right\},$$
(50)

where

$$\mathcal{N}_{j}^{m} = \mathcal{N}^{m}(\nu_{j}^{m}) = \frac{c}{2}(\nu_{j}^{m})^{2}g(\nu_{j}^{m},\nu_{j}^{m})\frac{\mathrm{d}\Lambda^{m}(z)}{\mathrm{d}z}\Big|_{z=\nu_{j}^{m}},$$
(51)

and for  $\nu \in (-1, 1)$ ,

$$\mathcal{N}^{m}(\nu) = \nu \Lambda^{m+}(\nu) \Lambda^{m-}(\nu) (1 - \nu^{2})^{-|m|}.$$
 (52)

Here,  $\Lambda^{m\pm}(\nu) = \lim_{\epsilon \to 0+} \Lambda^m(\nu \pm i\epsilon)$ . By comparing Eqs. (49) and (50), we obtain

$$\nu_j^m Z^m(\nu_j^m) = 2\pi \mathcal{N}_j^m, \qquad \nu Z^m(\nu) = 2\pi \mathcal{N}^m(\nu), \qquad (53)$$

where  $\nu$  belongs to the continuous spectrum. Finally, we obtain

$$\tilde{\Phi}^m_{\nu}(\hat{\mathbf{s}}; \hat{\mathbf{k}}) = \Phi^m_{\nu}(\hat{\mathbf{s}}; \hat{\mathbf{k}}) [2\pi Q(\nu q) \mathcal{N}^m(\nu)]^{-1}, \qquad (54)$$

where  $\nu = \pm \nu_i^m$  or  $\nu \in (-1, 1)$ . The Green's function is obtained as

$$\begin{aligned} G(\boldsymbol{\rho}, z, \hat{\mathbf{s}}; \boldsymbol{\rho}_{0}, z_{0}, \hat{\mathbf{s}}_{0}) &= \frac{1}{(2\pi)^{3}} \int_{\mathbb{R}^{2}} e^{i\mathbf{q}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}_{0})} \sum_{m=-N}^{N} \left\{ \sum_{j=0}^{M-1} \frac{1}{Q(\nu_{j}^{m}q)\mathcal{N}_{j}^{m}} \right. \\ &\times \Phi_{j\pm}^{m}(\hat{\mathbf{s}}; \hat{\mathbf{k}}) [\Phi_{j\pm}^{m}(\hat{\mathbf{s}}_{0}; \hat{\mathbf{k}})]^{*} e^{-Q(\nu_{j}^{m}q)|z-z_{0}|/\nu_{j}^{m}} \\ &+ \int_{0}^{1} \frac{1}{Q(\nu q)\mathcal{N}^{m}(\nu)} \Phi_{\pm\nu}^{m}(\hat{\mathbf{s}}; \hat{\mathbf{k}}) \\ &\times [\Phi_{\pm\nu}^{m}(\hat{\mathbf{s}}_{0}; \hat{\mathbf{k}})]^{*} e^{-Q(\nu q)|z-z_{0}|/\nu} \mathrm{d}\nu \} \mathrm{d}\mathbf{q}. \end{aligned}$$

$$(55)$$

As the simplest case, let us consider the isotropic scattering N = 0. We then have

$$\Phi^0_{\nu}(\hat{\mathbf{s}};\hat{\mathbf{k}}) = \frac{c\nu}{2} \mathcal{P} \frac{1}{\nu - \mu(\hat{\mathbf{k}})} + \lambda^0(\nu)\delta(\nu - \mu(\hat{\mathbf{k}})) = \phi^0(\nu, \mu(\hat{\mathbf{k}})), \quad (56)$$

where

$$\lambda^{0}(\nu) = 1 - \frac{c\nu}{2} \mathcal{P} \int_{-1}^{1} \frac{1}{\nu - \mu} d\mu = 1 - c\nu \tanh^{-1}\nu.$$
 (57)

In this case M = 1 and the discrete eigenvalues  $\pm \nu_0^0 = \pm \nu_0$ are solutions to

$$\Lambda^{0}(z) = 1 - \frac{cz}{2} \int_{-1}^{1} \frac{1}{z - \mu} d\mu = 1 - cz \tanh^{-1} \frac{1}{z} = 0.$$
 (58)

The Green's function is obtained as

The energy density U is given by

$$U(z) = \frac{1}{v} \int_{\mathbb{S}^2} I(\boldsymbol{\rho} = \mathbf{0}, z, \hat{\mathbf{s}}) \mathrm{d}\hat{\mathbf{s}}, \tag{60}$$

where v is the speed of light in the medium and I is the specific intensity obeying Eq. (1).

First we place an isotropic source at the origin,  $S = S_a \delta(\mathbf{r})$ with constant  $S_a$  in Eq. (1) [see Fig. <u>1(a)</u>]. We have

$$I(\mathbf{0}, z, \hat{\mathbf{s}}) = \mu_t^2 S_a \int_{\mathbb{R}^3 \times \mathbb{S}^2} G(\mathbf{0}, z, \hat{\mathbf{s}}; \boldsymbol{\rho}_0, z_0, \hat{\mathbf{s}}_0) \\ \times \delta(\boldsymbol{\rho}_0) \delta(z_0) d\boldsymbol{\rho}_0 dz_0 d\hat{\mathbf{s}}_0,$$
(61)

where  $z, \rho, z_0$  are measured in the unit of  $1/\mu_t$ . In this case, U is spherically symmetric. Using Eq. (55) we obtain

$$\frac{U(z)}{\mu_t^2 S_a} = \int_{\mathbb{S}^2 \times \mathbb{S}^2} G(\mathbf{0}, z, \hat{\mathbf{s}}; \mathbf{0}, 0, \hat{\mathbf{s}}_0) d\hat{\mathbf{s}} d\hat{\mathbf{s}}_0 
= \frac{1}{vz} \left[ \frac{e^{-z/\nu_0}}{\nu_0 \mathcal{N}_0} + \int_0^1 \frac{e^{-z/\nu}}{v \mathcal{N}(\nu)} d\nu \right], \qquad z > 0.$$
(62)

Here,  $\nu_0$  is the positive solution to  $\Lambda^0(\nu_0) = 0$ , where

$$\Lambda^{0}(\nu_{0}) = 1 - \frac{c\nu_{0}}{2} \int_{-1}^{1} \frac{g^{0}(\nu_{0},\mu)}{\nu_{0}-\mu} d\mu.$$
(63)

We consider the following three cases: (i)  $\mu_a = 0.03 \text{ cm}^{-1}$ ,  $\mu_s = 100 \text{ cm}^{-1}$ ,  $f_1 = 0$  (c = 0.9997); (ii)  $\mu_a = 0.03 \text{ cm}^{-1}$ ,  $\mu_s = 100 \text{ cm}^{-1}$ ,  $f_1 = 0.3$  (c = 0.9997) [24]; and (iii)  $\mu_a = 0.3 \text{ cm}^{-1}$ ,  $\mu_s = 100 \text{ cm}^{-1}$ ,  $f_1 = 0.3$  (c = 0.9977). In the case (i) with  $f_1 = 0$ , the density can also be obtained with the Fourier transform. The Green's function is obtained as

$$G(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}_{0}, \hat{\mathbf{s}}_{0}) = G_{0}(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}_{0}, \hat{\mathbf{s}}_{0}) + \frac{c}{4\pi(2\pi)^{3}} \int_{\mathbb{R}^{3}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_{0})} \\ \times \frac{1}{(1+i\mathbf{k}\cdot\hat{\mathbf{s}})(1+i\mathbf{k}\cdot\hat{\mathbf{s}}_{0})} \left[1 - \frac{c}{|\mathbf{k}|} \tan^{-1}(|\mathbf{k}|)\right]^{-1} d\mathbf{k},$$
(64)

$$G(\boldsymbol{\rho}, \boldsymbol{z}, \hat{\mathbf{s}}; \boldsymbol{\rho}_{0}, \boldsymbol{z}_{0}, \hat{\mathbf{s}}_{0}) = \frac{1}{(2\pi)^{3}} \int_{\mathbb{R}^{2}} e^{i\mathbf{q}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}_{0})} \left\{ \frac{1}{Q(\nu_{0}q)\mathcal{N}_{0}} \phi^{0}(\pm\nu_{0}, \mu(\hat{\mathbf{k}})) \phi^{0*}(\pm\nu_{0}, \mu_{0}(\hat{\mathbf{k}})) e^{-Q(\nu_{0}q)|\boldsymbol{z}-\boldsymbol{z}_{0}|/\nu_{0}} + \int_{0}^{1} \frac{1}{Q(\nu q)\mathcal{N}(\nu)} \phi^{0}(\pm\nu, \mu(\hat{\mathbf{k}})) \phi^{0*}(\pm\nu, \mu_{0}(\hat{\mathbf{k}})) e^{-Q(\nu q)|\boldsymbol{z}-\boldsymbol{z}_{0}|/\nu} d\nu \right\} d\mathbf{q}.$$
(59)

If we integrate Eq. (59) with respect to  $\rho_0$ , G in Eq. (59) becomes the one-dimensional Green's function written in the book by Case and Zweifel [1].

### 7. ENERGY DENSITY

Let us calculate the energy density U. For simplicity, we assume linear scattering, N = 1. We measure U along the z axis. where

$$G_0(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}_0, \hat{\mathbf{s}}_0) = \frac{e^{-|\mathbf{r}-\mathbf{r}_0|}}{|\mathbf{r}-\mathbf{r}_0|^2} \delta\left(\hat{\mathbf{s}} - \frac{\mathbf{r}-\mathbf{r}_0}{|\mathbf{r}-\mathbf{r}_0|}\right) \delta(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0).$$
(65)

Using Eqs. (64) and (65), we obtain



Fig. 1. Energy density U(z) for (a) the point source and (b) the source of length  $\ell$  on the x axis.

$$\frac{U(z)}{\mu_t^2 S_a} = \frac{e^{-|z|}}{vz^2} + \frac{2c}{\pi v} \int_0^\infty \frac{\sin(kz)}{z} \frac{(\tan^{-1}k)^2}{k - c \tan^{-1}k} dk.$$
(66)

In Fig. 2, we plot  $U(z)v/\mu_t^2 S_a$  as a function of z. In addition to Eq. (62), densities by Eq. (66) and by Monte Carlo simulation are shown. We see perfect agreement.

Next we consider the source of length  $\ell$  on the x axis [see Fig. <u>1(b)</u>], i.e., we put  $S = S_b \Theta(\ell - x)\Theta(x)\delta(y)\delta(z)$  with constant  $S_b$  in Eq. (1). We have

$$I(\mathbf{0}, z, \hat{\mathbf{s}}) = \mu_t S_b \int_{\mathbb{R}^3 \times \mathbb{S}^2} G(\mathbf{0}, z, \hat{\mathbf{s}}; x_0, y_0, z_0, \hat{\mathbf{s}}_0) \\ \times \Theta(\mu_t \ell' - x_0) \Theta(x_0) \delta(y_0) \delta(z_0) \mathrm{d}x_0 \mathrm{d}y_0 \mathrm{d}z_0 \mathrm{d}\hat{\mathbf{s}}_0, \quad (67)$$

where z,  $x_0$ ,  $y_0$ ,  $z_0$  are measured in the unit of  $1/\mu_t$ . We compute I using Eq. (55) and obtain

$$\frac{U(z)}{\mu_t S_b} = \int_{\mathbb{R}^2} \int_{\mathbb{S}^2 \times \mathbb{S}^2} G(\mathbf{0}, z, \hat{\mathbf{s}}; \boldsymbol{\rho}_0, 0, \hat{\mathbf{s}}_0) \\
\times \Theta(\mu_t \ell' - x_0) \Theta(x_0) \delta(y_0) d\hat{\mathbf{s}} d\hat{\mathbf{s}}_0 d\boldsymbol{\rho}_0 \\
= \frac{1}{v} \int_0^\infty \left( \int_0^{\mu_t \ell q} J_0(t) dt \right) \left[ \frac{e^{-Q(\nu_0 q) z/\nu_0}}{Q(\nu_0 q) \mathcal{N}_0} \\
+ \int_0^1 \frac{e^{-Q(\nu q) z/\nu}}{Q(\nu q) \mathcal{N}(\nu)} d\nu \right] dq, \quad z > 0, \quad (68)$$

where  $\nu_0$  is the positive root of Eq. (63) and  $J_0(u)$  is the zerothorder Bessel function of the first kind. In addition, with the Fourier transform, we obtain



Fig. 2. Energy density Eq. (62) is plotted together with Eq. (66) and results from Monte Carlo simulation. The optical parameters ( $\mu_a, \mu_s, f_1$ ) are, from the top, (0.03 cm<sup>-1</sup>, 100 cm<sup>-1</sup>, 0), (0.03 cm<sup>-1</sup>, 100 cm<sup>-1</sup>, 0.3), and (0.3 cm<sup>-1</sup>, 100 cm<sup>-1</sup>, 0.3).



Fig. 3. Energy density Eq. (68) is plotted. The optical parameters  $(\mu_a, \mu_s, f_1)$  are, from the top,  $(0.03 \text{ cm}^{-1}, 100 \text{ cm}^{-1}, 0)$ ,  $(0.03 \text{ cm}^{-1}, 100 \text{ cm}^{-1}, 0.3)$ , and  $(0.3 \text{ cm}^{-1}, 100 \text{ cm}^{-1}, 0.3)$ . The blue line from Fig. 2 shows Eq. (62) for  $(\mu_a, \mu_s, f_1) = (0.03 \text{ cm}^{-1}, 100 \text{ cm}^{-1}, 0.3)$ .

$$\frac{U(z)}{\mu_t S_b} = \frac{1}{v} \int_0^{\mu_t \ell} \left[ \frac{e^{-\sqrt{x_0^2 + z^2}}}{x_0^2 + z^2} + \frac{2c}{\pi} \int_0^\infty \frac{\sin\left(k\sqrt{x_0^2 + z^2}\right)}{\sqrt{x_0^2 + z^2}} \frac{(\tan^{-1}k)^2}{k - c\tan^{-1}k} dk \right] dx_0. \quad (69)$$

Let us put  $\mu_{\ell}\ell = 1$ . In Fig. 3, we plot Eq. (68) together with Eq. (69). Moreover, Eq. (62) for  $(\mu_a, \mu_s, f_1) = (0.03 \text{ cm}^{-1}, 100 \text{ cm}^{-1}, 0.3)$  is plotted for comparison. We see that U is similar to the density in Fig. 2 except for small z.

### 8. SUMMARY

We have constructed elementary solutions of the radiative transport equation in three dimensions. Each elementary solution carries the wave vector  $\mathbf{k}$ , and is labeled by Case's discrete eigenvalues and continuous spectrum. By virtue of rotated reference frames, the angular part of each elementary solution is given by the singular eigenfunction for the one-dimensional radiative transport equation.

Using the elementary solutions, the Green's function in an infinite medium is obtained. Moreover, the energy density is computed for different sources and optical parameters.

### APPENDIX A: POLAR AND AZIMUTHAL ANGLES IN ROTATED REFERENCE FRAMES

Let  $\theta$  and  $\varphi$  be the polar and azimuthal angles of  $\hat{\mathbf{s}}$  in the laboratory frame. Let  $\varphi_{\hat{\mathbf{k}}}$  and  $\theta_{\hat{\mathbf{k}}}$  be the polar and azimuthal angles of  $\hat{\mathbf{k}}$  in the laboratory frame. For  $\hat{\mathbf{k}} = (-i\nu\mathbf{q}, Q(\nu q))$ , we obtain

$$\cos \theta_{\hat{\mathbf{k}}} = \hat{\mathbf{k}} \cdot \hat{\mathbf{z}} = Q(\nu q), \qquad \sin \theta_{\hat{\mathbf{k}}} = \sqrt{1 - \cos^2 \theta_{\hat{\mathbf{k}}}} = i|\nu \mathbf{q}|$$
(A1)

and

$$\varphi_{\hat{\mathbf{k}}} = \begin{cases} \varphi_{\mathbf{q}} + \pi & \text{for } \nu > 0, \\ \varphi_{\mathbf{q}} & \text{for } \nu < 0, \end{cases}$$
(A2)

where  $\varphi_{\mathbf{q}}$  is the angle of  $\mathbf{q}$ . Therefore, we have

$$\mu(\hat{\mathbf{k}}) = \hat{\mathbf{s}} \cdot \hat{\mathbf{k}} = -i\nu q \sin \theta \cos(\varphi - \varphi_{\mathbf{q}}) + Q(\nu q) \cos \theta.$$
(A3)

In general, we can rotate functions as follows. Let us introduce rotated spherical harmonics  $Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{k}})$  [16]:

$$Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{k}}) = \mathcal{D}(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{s}}) = \sum_{m'=-l}^{l} D_{m'm}^{l}(\varphi_{\hat{\mathbf{k}}}, \theta_{\hat{\mathbf{k}}}, 0) Y_{lm'}(\hat{\mathbf{s}}), \quad (A4)$$

where  $D_{m'm}^{l}(\varphi_{\hat{\mathbf{k}}}, \theta_{\hat{\mathbf{k}}}, 0) = e^{-im'\varphi_{\hat{\mathbf{k}}}} d_{m'm}^{l}(\theta_{\hat{\mathbf{k}}})$ . Here,  $d_{m'm}^{l}$  are the Wigner *d*-matrices [25]. That is,  $Y_{lm}(\hat{\mathbf{s}}, \hat{\mathbf{k}})$  are spherical harmonics defined in a rotated reference frame whose *z* axis co-incides with the direction of the unit vector  $\hat{\mathbf{k}}$ . We have  $Y_{lm}(\hat{\mathbf{s}}) = Y_{lm}(\hat{\mathbf{s}}; \hat{\mathbf{z}})$ . We write analytically continued Wigner's *d* matrices as

$$d_{m'm}^l(\theta_{\hat{\mathbf{k}}}) = d_{m'm}^l[i\tau(\nu q)]. \tag{A5}$$

First, a few matrices are obtained as

$$d_{00}^0 = 1,$$
 (A6)

$$d_{00}^1 = \sqrt{1+x^2}, \qquad d_{01}^1 = \frac{i}{\sqrt{2}}|x|, \qquad d_{1\pm 1}^1 = \frac{1\pm\sqrt{1+x^2}}{2}.$$
 (A7)

We note that  $d_{mm'}^l = (-1)^{m+m'} d_{-m-m'}^l = (-1)^{m+m'} d_{m'm}^l$ . All  $d_{m'm}^l[i\tau(\nu q)]$  are computed using the recurrence relations [23]. We obtain

$$e^{im\varphi(\hat{\mathbf{k}})} = (1 - \mu(\hat{\mathbf{k}})^2)^{-|m|/2} \frac{(-1)^m \sqrt{4\pi(2m+1)!}}{(2m+1)!!} \times \sum_{m'=-m}^m e^{-im'\varphi_{\hat{\mathbf{k}}}} d_{m'm}^m(\theta_{\hat{\mathbf{k}}}) Y_{mm'}(\hat{\mathbf{s}}),$$
(A8)

where  $\theta$  satisfies  $\cos \theta = \mu$  with  $\mu$  in Eq. (15).

### **APPENDIX B: EXPANSION COEFFICIENTS**

Here, we calculate  $c_l^m(\nu)$ . We have

$$c_{l}^{m}(\nu) = \int_{\mathbb{S}^{2}} \left[ \frac{c\nu}{2} \mathcal{P} \frac{g^{m}(\nu,\mu)}{\nu-\mu} + \lambda^{m}(\nu)(1-\nu^{2})^{-|m|} \delta(\nu-\mu) \right] \\ \times (1-\mu^{2})^{|m|/2} e^{im\varphi} Y_{lm}^{*}(\hat{\mathbf{s}}) d\hat{\mathbf{s}}.$$
(B1)

Hence,

$$c_{l}^{m}(\nu) = 2\pi \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} \bigg[ \frac{c\nu}{2} \sum_{l'=|m|}^{N} f_{l''}(2l''+1) \\ \times \frac{(l''-m)!}{(l''+m)!} h_{l''}^{m}(\nu)(-1)^{m} \mathcal{P} \int_{-1}^{1} \frac{P_{l'}^{m}(\mu)P_{l}^{m}(\mu)}{\nu-\mu} d\mu \\ + \lambda^{m}(\nu)(1-\nu^{2})^{-|m|/2} P_{l}^{m}(\nu) \int_{-1}^{1} \delta(\nu-\mu) d\mu \bigg].$$
(B2)

Note that  $c_l^m(-\nu) = (-1)^{l+m} c_l^m(\nu)$  because  $P_l^m(-\nu) = (-1)^{l+m} P_l^m(\nu)$ . Therefore, we obtain for  $\nu \notin [-1, 1]$ 

$$c_{l}^{m}(\nu) = 2\pi \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} \frac{c\nu}{2} \sum_{l'=|m|}^{N} f_{l'}(2l''+1)$$
$$\times \frac{(l''-m)!}{(l''+m)!} h_{l''}^{m}(\nu)(-1)^{m} 2Q_{\max(l,l'')}^{m}(\nu) P_{\min(l,l'')}^{m}(\nu),$$
(B3)

where  $Q_{\max(l,l'')}^m(\nu)$  and  $P_{\min(l,l'')}^m(\nu)$  have a branch cut from  $-\infty$  to 1 [26], and for  $\nu \in (-1, 1)$ 

$$\begin{aligned} c_{l}^{m}(\nu) &= 2\pi \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} \bigg[ \frac{c\nu(-1)^{m}}{2} \sum_{l''=|m|}^{N} f_{l''}(2l''+1) \\ &\times \frac{(l''-m)!}{(l''+m)!} h_{l'}^{m}(\nu) \\ &\times \left( -i\pi P_{l'}^{m}(\nu) P_{l}^{m}(\nu) - \int_{0}^{\pi} \frac{P_{l'}^{m}(e^{i\theta}) P_{l}^{m}(e^{i\theta})}{\nu - e^{i\theta}} i e^{i\theta} d\theta \right) \\ &+ \lambda^{m}(\nu) (1-\nu^{2})^{-|m|/2} P_{l}^{m}(\nu) \bigg]. \end{aligned}$$
(B4)

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