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ABSTRACT

The radiative transport equation in a three-dimensional infinite medium is considered. The coefficients of the radiative transport equation are assumed to be constant. For a pencil beam, we extend the analytical discrete-ordinates method to three dimensions by rotating reference frames. Obtained results are compared to the Monte Carlo simulation.

1. Introduction

The discrete-ordinates method was first proposed by Wick [1] and Chandrasekhar [2]. In one-dimensional transport theory, analytical solutions are available in terms of singular eigenfunctions by Case's method [3–6]. The method of analytical discrete ordinates (ADO) [7–10] assumes the same separated solution as Case's method for the equation in which the cosine of the polar angle is discretized. Although the method was constructed for the one-dimensional transport equation, the searchlight problem in three dimensions was considered with ADO in the case of isotropic scattering [11]. ADO was developed for the one-dimensional transport equation with the scattering phase function which has the polar and azimuthal angles [12].

In this paper, we consider the three-dimensional radiative transport equation with general anisotropic scattering and construct ADO in three dimensions with the help of rotated reference frames [13]. We assume that the medium is homogeneous, and the scattering and absorption coefficients of the radiative transport equation are constants. Furthermore, we assume the pencil beam for the source term. The formulation is a direct extension of ADO developed in one dimension and the introduction of a pseudoproblem is not necessary. This is made possible by the knowledge of three-dimensional singular eigenfunctions obtained from the extension of Case's method to three dimensions [14]. For isotropic scattering in an infinite medium, solutions are known for different sources [15]. General anisotropic scattering can be treated in the numerical scheme proposed below.

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Kim and his collaborators developed discrete ordinates for the three-dimensional radiative transport equation [16–18]. The present method is similar to their formulation in the sense that the same structure of the plane-wave decomposition is derived and discrete ordinates are used. However, in the three-dimensional ADO which is developed in this paper, the explicit expression of eigenmodes are obtained and there is no need of computing eigenvalues for each Fourier vector.

The rotated reference frames were first introduced in the spherical-harmonics method [13, 19, 20]. In particular, Markel devised an efficient numerical algorithm called the method of rotated reference frames [13, 21, 22]. In the three-dimensional ADO, eigenmodes are obtained by the rotation of the eigenmodes for the original ADO in one-dimensional transport theory.

The remainder of the paper is organized as follows. In Section 2, the radiative transport equation is introduced. The specific intensity is then decomposed into the ballistic part and scattering part. In Section 3, eigenmodes are considered. Using these eigenmodes, the scattering part of the specific intensity is calculated in Section 4. The formula for the energy density is derived in Section 5. In Section 6, numerical tests are performed. Concluding remarks are given in Section 7. The fundamental solution is calculated in the Appendix.

2. Radiative transport equation

We consider the radiative transport equation in the three-dimensional space $\mathbb{R}^3$. Let $\mathbf{r} \in \mathbb{R}^3$ be the position vector with $\mathbf{r} = {}^t(\rho, z)$, $\rho = {}^t(x, y)$. The direction of propagation is specified by unit vector $\hat{\mathbf{s}} \in \mathbb{S}^2$. The specific intensity $I(\mathbf{r}, \hat{\mathbf{s}})$ obeys the following radiative transport equation:

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

where $\nabla = \partial/\partial \mathbf{r}$, and $\mu_t > 0$ and $\mu_s > 0$ are constants. Moreover, we assume that $\mu_a = \mu_t - \mu_s$ is positive. We have $I(\mathbf{r}, \hat{\mathbf{s}}) \to 0$ as $|\mathbf{r}| \to \infty$. Here, $p(\hat{\mathbf{s}}, \hat{\mathbf{s}}')$ is the scattering phase function which is assumed to be

$$p(\hat{\mathbf{s}}, \hat{\mathbf{s}}') = \frac{1}{4\pi} \sum_{l=0}^{l_{\max}} (2l + 1)g^l P_l(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}') = \sum_{l=0}^{l_{\max}} \sum_{m=-l}^{l} g^l Y_{lm}(\hat{\mathbf{s}}) Y_{lm}^*(\hat{\mathbf{s}}') \tag{2}$$

with $l_{\max} \geq 0$, Legendre polynomials P_l, and spherical harmonics Y_{lm}. Spherical harmonics are defined as

$$Y_{lm}(\hat{\mathbf{s}}) = Y_{lm}(\mu, \varphi) = \sqrt{\frac{2l + 1}{4\pi} \frac{(l - m)!}{(l + m)!}} P_l^m(\mu) \, e^{im\varphi}, \tag{3}$$

where $\mu \in [-1, 1]$ is the cosine of the polar angle of $\hat{\mathbf{s}}$, $\varphi \in [0, 2\pi)$ is the azimuthal angle of $\hat{\mathbf{s}}$, and $P_l^m(\mu)$ are associated Legendre polynomials. The constant $g \in [0, 1]$ is the anisotropic factor. We will consider the following source term:

$$f(\mathbf{r}, \hat{\mathbf{s}}) = \delta(\rho)\delta(z)\delta(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0), \tag{4}$$

where $\delta(\rho) = \delta(x)\delta(y)$ and $\hat{\mathbf{s}}_0 \in \mathbb{S}^2$. That is, $I(\mathbf{r}, \hat{\mathbf{s}})$ is the fundamental solution of the radiative transport equation. Here, $\hat{\mathbf{s}} \in \mathbb{S}^2$ is given by

$$\hat{\mathbf{s}} = \begin{pmatrix} \omega \\ \mu \end{pmatrix}, \quad \omega = \begin{pmatrix} \sqrt{1 - \mu^2} \cos\varphi \\ \sqrt{1 - \mu^2} \sin\varphi \end{pmatrix} \tag{5}$$

for $-1 \le \mu \le 1$, $0 \le \varphi < 2\pi$. We note that $\delta(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0) = \delta(\mu - \mu_0)\delta(\varphi - \varphi_0)$ with μ_0, φ_0 angles for $\hat{\mathbf{s}}_0$.

By dividing both sides of the above radiative transport Equation (1) by μ_t, we obtain

$$(\hat{\mathbf{s}} \cdot \nabla_* + 1)I_*(\mathbf{r}_*, \hat{\mathbf{s}}) = \varpi \int_{\mathbb{S}^2} p(\hat{\mathbf{s}}, \hat{\mathbf{s}}')I_*(\mathbf{r}_*, \hat{\mathbf{s}}') \, d\hat{\mathbf{s}}' + f_*(\mathbf{r}_*, \hat{\mathbf{s}}), \tag{6}$$

where $\mathbf{r}_* = \mu_t \mathbf{r}$, $\nabla_* = \partial/\partial \mathbf{r}_*$, $I_*(\mathbf{r}_*, \hat{\mathbf{s}}) = I(\mathbf{r}, \hat{\mathbf{s}})$, and

$$f_*(\mathbf{r}_*, \hat{\mathbf{s}}) = \frac{1}{\mu_t} f(\mathbf{r}, \hat{\mathbf{s}}) = \mu_t^2 \delta(\rho_*)\delta(z_*)\delta(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0). \tag{7}$$

Here, $\varpi = \mu_s/\mu_t \in (0, 1)$ is the albedo for single scattering. Hereafter, we will drop the subscript $*$.

We decompose the specific intensity into the ballistic and scattering terms as

$$I(\mathbf{r}, \hat{\mathbf{s}}) = I_b(\mathbf{r}, \hat{\mathbf{s}}) + I_s(\mathbf{r}, \hat{\mathbf{s}}). \tag{8}$$

The ballistic term I_b satisfies

$$(\hat{\mathbf{s}} \cdot \nabla + 1)I_b(\mathbf{r}, \hat{\mathbf{s}}) = f(\mathbf{r}, \hat{\mathbf{s}}) \quad \text{in } \mathbb{R}^3 \times \mathbb{S}^2. \tag{9}$$

The scattering term I_s satisfies

$$(\hat{\mathbf{s}} \cdot \nabla + 1)I_s(\mathbf{r}, \hat{\mathbf{s}}) = \varpi \int_{\mathbb{S}^2} p(\hat{\mathbf{s}}, \hat{\mathbf{s}}')I_s(\mathbf{r}, \hat{\mathbf{s}}') \, d\hat{\mathbf{s}}' + S(\mathbf{r}, \hat{\mathbf{s}}) \quad \text{in } \mathbb{R}^3 \times \mathbb{S}^2, \tag{10}$$

where

$$S(\mathbf{r}, \hat{\mathbf{s}}) = \varpi \int_{\mathbb{S}^2} p(\hat{\mathbf{s}}, \hat{\mathbf{s}}')I_b(\mathbf{r}, \hat{\mathbf{s}}') \, d\hat{\mathbf{s}}'. \tag{11}$$

Let us introduce the step function Θ as $\Theta(x) = 1$ for $x > 0$ and $\Theta(x) = 0$ for $x < 0$. We obtain

$$I_b(\mathbf{r}, \hat{\mathbf{s}}) = \Theta(\mu_0 z)\frac{\mu_t^2}{|\mu_0|}\delta(\rho - \omega_0 z/\mu_0) \, e^{-z/\mu_0}\delta(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0), \tag{12}$$

where ω_0, μ_0 are components of $\hat{\mathbf{s}}_0$. We note that

$$\delta(\rho - \omega z/\mu) = \frac{1}{|\rho|}\delta\left(|\rho| - z\frac{\sqrt{1 - \mu^2}}{\mu}\right)\delta(\varphi_\rho - \varphi)$$

$$= \left|\frac{z}{(\rho^2 + z^2)^{3/2}}\right|\left[\delta\left(\mu - \frac{z}{\sqrt{\rho^2 + z^2}}\right) + \delta\left(\mu + \frac{z}{\sqrt{\rho^2 + z^2}}\right)\right]\delta(\varphi_\rho - \varphi),$$

$$\tag{13}$$

where φ_ρ is the angle of ρ and $\rho = |\rho|$. Hence,

$$S(\mathbf{r}, \hat{\mathbf{s}}) = \varpi p(\hat{\mathbf{s}}, \hat{\mathbf{s}}_0) \Theta(\mu_0 z) \frac{\mu_t^2}{|\mu_0|} \delta(\rho - \omega_0 z/\mu_0) \, e^{-z/\mu_0}. \tag{14}$$

The Fourier transform $\tilde{I}_s(\mathbf{q}, z, \hat{\mathbf{s}})$ is given by

$$\tilde{I}_s(\mathbf{q}, z, \hat{\mathbf{s}}) = \int_{\mathbb{R}^2} e^{-i\mathbf{q}\cdot\rho} I_s(\mathbf{r}, \hat{\mathbf{s}}) \, d\rho, \tag{15}$$

where

$$\mathbf{q} = q \begin{pmatrix} \cos\varphi_\mathbf{q} \\ \sin\varphi_\mathbf{q} \end{pmatrix}, \quad q = |\mathbf{q}|, \ 0 \le \varphi_\mathbf{q} < 2\pi. \tag{16}$$

This $\tilde{I}_s(\mathbf{q}, z, \hat{\mathbf{s}})$ is obtained as the solution to the following equation:

$$\left(\mu\frac{\partial}{\partial z} + 1 + i\omega\cdot\mathbf{q}\right)\tilde{I}_s = \varpi \int_{\mathbb{S}^2} p(\hat{\mathbf{s}}, \hat{\mathbf{s}}')\tilde{I}_s(\mathbf{q}, z, \hat{\mathbf{s}}') \, d\hat{\mathbf{s}}' + \tilde{S}, \quad z \in \mathbb{R}, \quad \hat{\mathbf{s}} \in \mathbb{S}^2, \tag{17}$$

where

$$\tilde{S}(\mathbf{q}, z, \hat{\mathbf{s}}) = \varpi p(\hat{\mathbf{s}}, \hat{\mathbf{s}}_0) \Theta(\mu_0 z) \frac{\mu_t^2}{|\mu_0|} e^{-z/\mu_0} e^{-i\mathbf{q}\cdot\omega_0 z/\mu_0}. \tag{18}$$

The scattering term is given by

$$I_s(\mathbf{r}, \hat{\mathbf{s}}) = I_s(\rho, z, \hat{\mathbf{s}}) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} e^{i\mathbf{q}\cdot\rho}\tilde{I}_s(\mathbf{q}, z, \hat{\mathbf{s}}) \, d\mathbf{q}. \tag{19}$$

We note that

$$\omega\cdot\mathbf{q} = q\sqrt{1-\mu^2}\cos(\varphi - \varphi_\mathbf{q}). \tag{20}$$

We will obtain $\tilde{I}_s$ by using discrete ordinates:

$$\tilde{I}_s \approx \check{I}_s, \tag{21}$$

where $\check{I}_s$ is the solution to the following equation:

$$\left(\mu_i\frac{\partial}{\partial z} + 1 + i\omega_i\cdot\mathbf{q}\right)\check{I}_s = \varpi \sum_{i'=1}^{2N} w_{i'} \int_0^{2\pi} p(\hat{\mathbf{s}}_i, \hat{\mathbf{s}}_{i'})\check{I}_s(\mathbf{q}, z, \hat{\mathbf{s}}_{i'}) \, d\varphi' + \tilde{S} \tag{22}$$

for $z \in \mathbb{R}$, $\hat{\mathbf{s}}_i \in \mathbb{S}^2$. Here, we discretize the integral by discrete ordinates with the Gauss–Legendre quadrature of weights w_i ($i = 1, \ldots, N$). We use the Golub–Welsch algorithm [23]. We label μ_i ($i = 1, \ldots, N$) such that $0 < \mu_1 < \mu_2 < \cdots < \mu_N < 1$ and $-1 < \mu_{2N} < \cdots < \mu_{N+2} < \mu_{N+1} < 0$ ($\mu_{N+i} = -\mu_i$, $1 \le i \le N$). Furthermore, we introduced

$$\hat{\mathbf{s}}_i = \begin{pmatrix} \omega_i \\ \mu_i \end{pmatrix}, \quad \omega_i = \begin{pmatrix} \sqrt{1-\mu_i^2}\cos\varphi \\ \sqrt{1-\mu_i^2}\sin\varphi \end{pmatrix} \tag{23}$$

for $i = 1, 2, \ldots, 2N$, $0 \le \varphi < 2\pi$. We have

$$\omega_i\cdot\mathbf{q} = q\sqrt{1-\mu_i^2}\cos(\varphi - \varphi_\mathbf{q}). \tag{24}$$

Let us define

$$\omega_i^0(q, \varphi) = q\sqrt{1-\mu_i^2}\cos\varphi. \tag{25}$$

3. Eigenmodes

In order to obtain $\check{I}_s$ in (22), we find the solution $\check{I}$ to (28) below with separation of variables. We refer to $\check{I}$ as eigenmodes. The eigenmodes are labeled by a separation constant ν. This constant ν, which is referred to as an eigenvalue, is the reciprocal of the square roof of an eigenvalue of the eigenproblem (92) below or the negative of the reciprocal.

We begin by defining unit vector $\hat{\mathbf{k}}$ as [13]

$$\hat{\mathbf{k}} = \hat{\mathbf{k}}(\nu, \mathbf{q}) = \begin{pmatrix} -i\nu\mathbf{q} \\ \hat{k}_z(\nu q) \end{pmatrix}, \quad \hat{k}_z(\nu q) = \sqrt{1 + (\nu q)^2}, \tag{26}$$

where $\nu \in \mathbb{R}$. We will extend the rotation in $\mathbb{R}^3$ to $\mathbb{C}^3$ by analytic continuation (see (33) below) [21, 22]. To this end, we extend the usual dot product in $\mathbb{R}^3$ to $\mathbb{C}^3$ as $\alpha \cdot \beta = \alpha_1\beta_1 + \alpha_2\beta_2 + \alpha_3\beta_3$ for $\alpha, \beta \in \mathbb{C}^3$. We note that $\hat{\mathbf{k}} \cdot \hat{\mathbf{k}} = 1$. We have

$$\hat{\mathbf{s}}_i \cdot \hat{\mathbf{k}} = -i\nu q\sqrt{1 - \mu_i^2}\cos(\varphi - \varphi_{\mathbf{q}}) + \hat{k}_z(\nu q)\mu_i. \tag{27}$$

Let us consider the homogeneous equation below (i.e. the Equation (22) without the source term $\tilde{S}$).

$$\left(\mu_i\frac{\partial}{\partial z} + 1 + i\omega_i \cdot \mathbf{q}\right)\check{I}(\mathbf{q}, z, \hat{\mathbf{s}}_i) = \varpi \sum_{i'=1}^{2N} w_{i'} \int_0^{2\pi} p(\hat{\mathbf{s}}_i, \hat{\mathbf{s}}_{i'})\check{I}(\mathbf{q}, z, \hat{\mathbf{s}}_{i'})\,d\varphi' \tag{28}$$

for $\mathbf{q} \in \mathbb{R}^2, z \in \mathbb{R}, \hat{\mathbf{s}}_i \in \mathbb{S}^2$. Let $\mathcal{R}_{\hat{\mathbf{k}}}$ be the operator which rotates the reference frame in such a way that the z-axis is rotated to the direction of $\hat{\mathbf{k}}$ [24]. In ADO for the one-dimensional transport equation, the separated solution in which the spatial variable only exists in the exponential function was used [7–10]. In the same spirit, we assume the following separated solution:

$$\check{I}(\mathbf{q}, z, \hat{\mathbf{s}}_i) = \mathcal{R}_{\hat{\mathbf{k}}(\nu, \mathbf{q})}\Phi_\nu^m(\hat{\mathbf{s}}_i)\,e^{-\hat{k}_z(\nu q)z/\nu}, \tag{29}$$

where

$$\Phi_\nu^m(\hat{\mathbf{s}}_i) = \phi^m(\nu, \mu_i)(1 - \mu_i^2)^{|m|/2}\,e^{im\varphi}. \tag{30}$$

The function $\phi^m(\nu, \mu_i)$ is normalized as

$$\sum_{i=1}^{2N} w_i\phi^m(\nu, \mu_i)(1 - \mu_i^2)^{|m|} = 1. \tag{31}$$

The normalization condition (31) implies

$$\frac{1}{2\pi}\sum_{i=1}^{2N} w_i \int_0^{2\pi} \phi^m(\nu, \hat{\mathbf{s}}_i \cdot \hat{\mathbf{k}})[1 - (\hat{\mathbf{s}}_i \cdot \hat{\mathbf{k}})^2]^{|m|}\,d\varphi = 1. \tag{32}$$

We note that

$$\mathcal{R}_{\hat{\mathbf{k}}}Y_{lm}(\hat{\mathbf{s}}) = \sum_{m'=-l}^{l} e^{-im'\varphi_{\hat{\mathbf{k}}}}d_{m'm}^l(\theta_{\hat{\mathbf{k}}})Y_{lm'}(\hat{\mathbf{s}}), \tag{33}$$

where $d_{m'm}^l$ are Wigner's d-matrices [25]. If $\hat{\mathbf{k}} \in \mathbb{R}^3$, the operator $\mathcal{R}_{\hat{\mathbf{k}}}$ means the usual rotation of the reference frame in $\mathbb{R}^3$ such that the z-axis coincides with the direction of the

vector $\hat{\mathbf{k}}$ [13]. For $\hat{\mathbf{k}} \in \mathbb{C}^3$, the polar angle $\theta_{\hat{\mathbf{k}}}$ and azimuthal angle $\varphi_{\hat{\mathbf{k}}}$ of $\hat{\mathbf{k}}$ in the laboratory frame are analytically continued as follows [21, 22]. We write

$$\cos\theta_{\hat{\mathbf{k}}} = \hat{\mathbf{z}} \cdot \hat{\mathbf{k}} = \hat{k}_z, \quad \sin\theta_{\hat{\mathbf{k}}} = \sqrt{1 - \cos^2\theta_{\hat{\mathbf{k}}}} = \sqrt{\hat{k}_x^2 + \hat{k}_y^2} \tag{34}$$

and

$$\cos\varphi_{\hat{\mathbf{k}}} = \frac{\hat{k}_x}{\sqrt{\hat{k}_x^2 + \hat{k}_y^2}}, \quad \sin\varphi_{\hat{\mathbf{k}}} = \frac{\hat{k}_y}{\sqrt{\hat{k}_x^2 + \hat{k}_y^2}}. \tag{35}$$

We take square roots such that $0 \le \arg\sqrt{z} < \pi$ and $\Im\sqrt{z} \ge 0$ for all $z \in \mathbb{C}$ by drawing the branch cut on the positive real axis. The angles $\theta_{\hat{\mathbf{k}}}, \varphi_{\hat{\mathbf{k}}}$ of $\hat{\mathbf{k}}$ are given by

$$\cos\theta_{\hat{\mathbf{k}}(\nu,\mathbf{q})} = \hat{k}_z(\nu q), \quad \sin\theta_{\hat{\mathbf{k}}(\nu,\mathbf{q})} = i|\nu q| \tag{36}$$

and

$$\varphi_{\hat{\mathbf{k}}(\nu,\mathbf{q})} = \begin{cases} \varphi_{\mathbf{q}} + \pi & (\nu > 0), \\ \varphi_{\mathbf{q}} & (\nu < 0). \end{cases} \tag{37}$$

We can write

$$d^l_{mm'}(\theta_{\hat{\mathbf{k}}(\nu,\mathbf{q})}) = d^l_{mm'}[i\tau(\nu q)]. \tag{38}$$

Using $Y^*_{lm}(\hat{\mathbf{s}}) = (-1)^m Y_{l,-m}(\hat{\mathbf{s}})$, we have

$$\mathcal{R}_{\hat{\mathbf{k}}} Y^*_{lm}(\hat{\mathbf{s}}) = (-1)^m \sum_{m'=-l}^{l} e^{-im'\varphi_{\hat{\mathbf{k}}}} d^l_{m',-m}(\theta_{\hat{\mathbf{k}}}) Y_{lm'}(\hat{\mathbf{s}}) = \sum_{m'=-l}^{l} e^{im'\varphi_{\hat{\mathbf{k}}}} d^l_{m'm}(\theta_{\hat{\mathbf{k}}}) Y^*_{lm'}(\hat{\mathbf{s}}). \tag{39}$$

Moreover, we have

$$\mathcal{R}^{-1}_{\hat{\mathbf{k}}} Y_{lm}(\hat{\mathbf{s}}) = \sum_{m'=-l}^{l} e^{im'\varphi_{\hat{\mathbf{k}}}} d^l_{mm'}(\theta_{\hat{\mathbf{k}}}) Y_{lm'}(\hat{\mathbf{s}}), \tag{40}$$

$$\mathcal{R}^{-1}_{\hat{\mathbf{k}}} Y^*_{lm}(\hat{\mathbf{s}}) = \sum_{m'=-l}^{l} e^{-im'\varphi_{\hat{\mathbf{k}}}} d^l_{mm'}(\theta_{\hat{\mathbf{k}}}) Y^*_{lm'}(\hat{\mathbf{s}}). \tag{41}$$

The identity $\mathcal{R}^{-1}_{\hat{\mathbf{k}}} \mathcal{R}_{\hat{\mathbf{k}}} Y_{lm}(\hat{\mathbf{s}}) = Y_{lm}(\hat{\mathbf{s}})$ can be derived with the formula $\sum_{m'=-l}^{l} d^l_{m'm}(\theta_{\hat{\mathbf{k}}}) d^l_{m'm''}(\theta_{\hat{\mathbf{k}}}) = \delta_{mm''}$.

We note that $\mu_i = \hat{\mathbf{s}}_i \cdot \hat{\mathbf{z}}$, where $\hat{\mathbf{z}} = {}^t(0,0,1)$. We have

$$\mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}\mu_i = \hat{\mathbf{s}}_i \cdot \hat{\mathbf{k}}(\nu,\mathbf{q}) = -i\nu\omega_i \cdot \mathbf{q} + \hat{k}_z(\nu q)\mu_i. \tag{42}$$

This relation is also obtained as follows using $d_{00}^1(\theta) = \cos\theta$, $d_{10}^1(\theta) = -(1/\sqrt{2})\sin\theta$, and $d_{mm'}^l(\theta) = (-1)^{m+m'}d_{-m,-m'}^l(\theta)$:

$$\begin{aligned}
\mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}\mu_i &= \sqrt{\frac{4\pi}{3}}\,\mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}Y_{10}(\hat{\mathbf{s}}_i) \\
&= \sqrt{\frac{4\pi}{3}}\sum_{m'=-1}^{1} e^{-im'\varphi_{\hat{\mathbf{k}}}}d_{m'0}^1(\theta_{\hat{\mathbf{k}}})Y_{1m'}(\hat{\mathbf{s}}_i) \\
&= \sqrt{1-\mu_i^2}\sin\theta_{\hat{\mathbf{k}}}\cos(\varphi - \varphi_{\hat{\mathbf{k}}}) + \mu_i\cos\theta_{\hat{\mathbf{k}}} \\
&= \hat{k}_z(\nu q)\mu_i - i\nu q\sqrt{1-\mu_i^2}\cos(\varphi - \varphi_{\mathbf{q}}).
\end{aligned} \tag{43}$$

By substitution, we have

$$\left(1 - \frac{\hat{\mathbf{s}}_i \cdot \hat{\mathbf{k}}(\nu,\mathbf{q})}{\nu}\right)\mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}\Phi_\nu^m(\hat{\mathbf{s}}_i) = \varpi\sum_{i'=1}^{2N} w_{i'}\int_0^{2\pi} p(\hat{\mathbf{s}}_i,\hat{\mathbf{s}}_{i'})\mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}\Phi_\nu^m(\hat{\mathbf{s}}_{i'})\,d\varphi'. \tag{44}$$

Now, we view (44) in the reference frame whose z-axis is rotated to the direction of $\hat{\mathbf{k}}$. Note that $p(\hat{\mathbf{s}}_i,\hat{\mathbf{s}}_{i'})$ is invariant under rotation because it depends only on $\hat{\mathbf{s}}_i \cdot \hat{\mathbf{s}}_{i'}$. We note by (42)

$$\hat{\mathbf{s}}_i \cdot \hat{\mathbf{k}}(\nu,\mathbf{q}) = \mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}\hat{\mathbf{s}}_i \cdot \hat{\mathbf{z}}, \tag{45}$$

where $\hat{\mathbf{z}} = {}^t(0,0,1)$. If we operate $\mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}^{-1}$ on the left-hand side of (44), we obtain

$$\begin{aligned}
\mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}^{-1}\left(1 - \frac{\hat{\mathbf{s}}_i \cdot \hat{\mathbf{k}}(\nu,\mathbf{q})}{\nu}\right)\mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}\Phi_\nu^m(\hat{\mathbf{s}}_i) &= \mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}^{-1}\mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}\left(1 - \frac{\hat{\mathbf{s}}_i \cdot \hat{\mathbf{z}}}{\nu}\right)\Phi_\nu^m(\hat{\mathbf{s}}_i) \\
&= \left(1 - \frac{\hat{\mathbf{s}}_i \cdot \hat{\mathbf{z}}}{\nu}\right)\Phi_\nu^m(\hat{\mathbf{s}}_i).
\end{aligned} \tag{46}$$

Let us rewrite the right-hand side of (44) as

$$\begin{aligned}
&\varpi\sum_{i'=1}^{2N} w_{i'}\int_0^{2\pi} p(\hat{\mathbf{s}}_i,\hat{\mathbf{s}}_{i'})\mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}\Phi_\nu^m(\hat{\mathbf{s}}_{i'})\,d\varphi' \\
&= \varpi\sum_{i'=1}^{2N} w_{i'}\int_0^{2\pi} p(\mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}\hat{\mathbf{s}}_i, \mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}\hat{\mathbf{s}}_{i'})\mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}\Phi_\nu^m(\hat{\mathbf{s}}_{i'})\,d\varphi' \\
&\approx \varpi\sum_{i'=1}^{2N} w_{i'}\int_0^{2\pi} p(\mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}\hat{\mathbf{s}}_i, \hat{\mathbf{s}}_{i'})\Phi_\nu^m(\hat{\mathbf{s}}_{i'})\,d\varphi'.
\end{aligned} \tag{47}$$

In the last step of the above equation, we used the fact that the integral over all angles is invariant under the rotation of the reference frame. Similarly by operating $\mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}^{-1}$ on the

right-hand side of (44), we have

$$
\mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}^{-1} \, \varpi \sum_{i'=1}^{2N} w_{i'} \int_0^{2\pi} p(\hat{\mathbf{s}}_i, \hat{\mathbf{s}}_{i'}) \mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})} \Phi_\nu^m(\hat{\mathbf{s}}_{i'}) \, \mathrm{d}\varphi'
$$

$$
\approx \mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})}^{-1} \, \varpi \sum_{i'=1}^{2N} w_{i'} \int_0^{2\pi} p(\mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})} \hat{\mathbf{s}}_i, \hat{\mathbf{s}}_{i'}) \Phi_\nu^m(\hat{\mathbf{s}}_{i'}) \, \mathrm{d}\varphi'
$$

$$
= \varpi \sum_{i'=1}^{2N} w_{i'} \int_0^{2\pi} p(\hat{\mathbf{s}}_i, \hat{\mathbf{s}}_{i'}) \Phi_\nu^m(\hat{\mathbf{s}}_{i'}) \, \mathrm{d}\varphi'. \tag{48}
$$

Thus by inverse rotation, Equation (44) is reduced to

$$
\left(1 - \frac{\mu_i}{\nu}\right) \Phi_\nu^m(\hat{\mathbf{s}}_i) = \varpi \sum_{l'=0}^{l_{\max}} \sum_{m'=-l'}^{l'} g^{l'} Y_{l'm'}(\hat{\mathbf{s}}_i) \sum_{i'=1}^{2N} w_{i'} \int_0^{2\pi} Y_{l'm'}^*(\hat{\mathbf{s}}_{i'}) \Phi_\nu^m(\hat{\mathbf{s}}_{i'}) \, \mathrm{d}\varphi' \tag{49}
$$

for $i = 1, \ldots, 2N$. We have

$$
\sum_{i'=1}^{2N} w_{i'} \int_0^{2\pi} Y_{l'm'}^*(\hat{\mathbf{s}}_{i'}) \Phi_\nu^m(\hat{\mathbf{s}}_{i'}) \, \mathrm{d}\varphi' = \delta_{mm'} (-1)^m \sqrt{(2l'+1)\pi} \, g_{l'}^m(\nu), \tag{50}
$$

where

$$
g_l^m(\nu) = (-1)^m \sqrt{\frac{(l-m)!}{(l+m)!}} \sum_{i=1}^{2N} w_i \phi^m(\nu, \mu_i)(1-\mu_i^2)^{|m|/2} P_l^m(\mu_i). \tag{51}
$$

Noting that $P_l^{-m}(\mu_i) = (-1)^m [(l-m)!/(l+m)!] P_l^m(\mu_i)$ and $P_m^m(\mu_i) = (-1)^m (2m-1)!! (1-\mu_i^2)^{m/2}$ $(m \geq 0)$, we obtain

$$
g_m^m(\nu) = \frac{(2m-1)!!}{\sqrt{(2m)!}} = \frac{\sqrt{(2m)!}}{2^m m!}, \quad g_m^{-m}(\nu) = (-1)^m g_m^m(\nu) \tag{52}
$$

for $m \geq 0$. Equation (49) is written as

$$
\left(1 - \frac{\mu_i}{\nu}\right) \phi^m(\nu, \mu_i)(1-\mu_i^2)^{|m|/2} = \frac{\varpi}{2}(-1)^m \sum_{l'=|m|}^{l_{\max}} (2l'+1) g^{l'} \sqrt{\frac{(l'-m)!}{(l'+m)!}} P_{l'}^m(\mu_i) g_{l'}^m(\nu). \tag{53}
$$

Let us define

$$
p_l^m(\mu) = (-1)^m \sqrt{\frac{(l-m)!}{(l+m)!}} P_l^m(\mu)(1-\mu^2)^{-|m|/2}. \tag{54}
$$

We have

$$
p_m^m(\mu) = \frac{(2m-1)!!}{\sqrt{(2m)!}} = \frac{\sqrt{(2m)!}}{2^m m!}, \quad p_m^{-m}(\mu) = (-1)^m p_m^m(\mu) \tag{55}
$$

for $m \geq 0$. Moreover, from $(l-m+1)P_{l+1}^m(\mu) = (2l+1)\mu P_l^m(\mu) - (l+m)P_{l-1}^m(\mu)$,

$$
\sqrt{(l+1)^2 - m^2} \, p_{l+1}^m(\mu) = (2l+1)\mu p_l^m(\mu) - \sqrt{l^2 - m^2} \, p_{l-1}^m(\mu) \tag{56}
$$

for $l \geq |m| + 1$, and

$$p_{|m|+1}^m(\mu) = \sqrt{2|m| + 1}\mu p_{|m|}^m(\mu). \tag{57}$$

Thus,

$$(\nu - \mu_i)\phi^m(\nu, \mu_i) = \frac{\varpi \nu}{2} \sum_{l'=|m|}^{l_{max}} (2l' + 1)g^{l'} p_{l'}^m(\mu_i)g_{l'}^m(\nu). \tag{58}$$

We note that

$$g_l^m(\nu) = \sum_{i=1}^{2N} w_i\phi^m(\nu, \mu_i)p_l^m(\mu_i)(1 - \mu_i^2)^{|m|}. \tag{59}$$

The following recurrence relations are obtained.

$$\sqrt{(l+1)^2 - m^2}g_{l+1}^m(\nu) + \sqrt{l^2 - m^2}g_{l-1}^m(\nu)$$

$$= (2l+1)\nu g_l^m(\nu) - \frac{\varpi \nu}{2} \sum_{l'=|m|}^{l_{max}} (2l+1)(2l'+1)g^{l'} g_{l'}^m(\nu) \sum_{i=1}^{2N} w_i p_l^m(\mu_i)p_{l'}^m(\mu_i)(1 - \mu_i^2)^{|m|}. \tag{60}$$

Recall $\int_{-1}^{1} P_l^m(\mu)P_{l'}^m(\mu)\,d\mu = 2(l+m)!\delta_{ll'}/[(2l+1)(l-m)!]$. For sufficiently large N, the recurrence relations below are obtained.

$$\sqrt{(l+1)^2 - m^2}g_{l+1}^m(\nu) + \sqrt{l^2 - m^2}g_{l-1}^m(\nu) = \nu h_l g_l^m(\nu) \tag{61}$$

for $l \geq |m| + 1$, and

$$\sqrt{2|m| + 1}g_{|m|+1}^m(\nu) = \nu h_{|m|}g_{|m|}^m(\nu), \tag{62}$$

where

$$h_l = \begin{cases} (2l+1)(1 - \varpi g^l), & 0 \leq l \leq l_{max}, \\ 2l+1, & l > l_{max}. \end{cases} \tag{63}$$

The polynomials $g_l^m(\nu)$ are called the normalized Chandrasekhar polynomials [26, 27].

For numerical calculation, $g_l^m(\nu)$ can be computed using the recurrence relations. To compute $g_l^m(\nu)$ for $\nu > 1$, we define [27]

$$\bar{g}_l^m(\nu) = \frac{g_{l+1}^m(\nu)}{g_l^m(\nu)}. \tag{64}$$

Then we have

$$\bar{g}_{l-1}^m(\nu) = \frac{\sqrt{l^2 - m^2}}{\nu h_l - \sqrt{(l+1)^2 - m^2}\bar{g}_l^m(\nu)} \tag{65}$$

for $l = |m| + 1, |m| + 2, \ldots$. We can set $\bar{g}_l^m(\nu) = 0$ for sufficiently large l. Using $\bar{g}_l^m(\nu)$, we obtain

$$g_{l+1}^m(\nu) = \bar{g}_l^m(\nu)g_l^m(\nu), \quad l = |m|, |m| + 1, \ldots. \tag{66}$$

Suppose $\nu \neq \mu_i$. Then from (58),

$$\phi^m(\nu, \mu_i) = \frac{\varpi \nu}{2} \frac{g^m(\nu, \mu_i)}{\nu - \mu_i}, \tag{67}$$

where

$$g^m(\nu, \mu_i) = \sum_{l'=|m|}^{l_{max}} (2l' + 1) g^{l'} p_{l'}^m(\mu_i) g_{l'}^m(\nu). \tag{68}$$

We obtain

$$\Phi_\nu^m(\hat{\mathbf{s}}_i) = \frac{(-1)^m \varpi \nu}{\nu - \mu_i} \sum_{l=|m|}^{l_{max}} \sqrt{(2l+1)\pi} g^l g_l^m(\nu) Y_{lm}(\hat{\mathbf{s}}_i). \tag{69}$$

If $\nu \neq \hat{\mathbf{s}}_i \cdot \hat{\mathbf{k}}$, we have

$$\phi^m(\nu, \hat{\mathbf{s}}_i \cdot \hat{\mathbf{k}}(\nu, \mathbf{q})) = \frac{\varpi \nu}{2} \frac{g^m(\nu, \hat{\mathbf{s}}_i \cdot \hat{\mathbf{k}}(\nu, \mathbf{q}))}{\nu - \hat{\mathbf{s}}_i \cdot \hat{\mathbf{k}}(\nu, \mathbf{q})}. \tag{70}$$

Thus,

$$\mathcal{R}_{\hat{\mathbf{k}}(\nu, \mathbf{q})} \Phi_\nu^m(\hat{\mathbf{s}}_i) = \frac{(-1)^m \varpi \nu}{\nu - \hat{\mathbf{s}}_i \cdot \hat{\mathbf{k}}(\nu, \mathbf{q})} \sum_{l=|m|}^{l_{max}} \sqrt{(2l+1)\pi} g^l g_l^m(\nu) (\mathcal{R}_{\hat{\mathbf{k}}(\nu, \mathbf{q})} Y_{lm}(\hat{\mathbf{s}}_i)). \tag{71}$$

The above eigenmodes satisfy the orthogonality relation.

Lemma 3.1:

$$\sum_{i=1}^{2N} w_i \mu_i \int_0^{2\pi} (\mathcal{R}_{\hat{\mathbf{k}}(\nu, \mathbf{q})} \Phi_\nu^m(\hat{\mathbf{s}}_i)) (\mathcal{R}_{\hat{\mathbf{k}}(\nu', \mathbf{q})} \Phi_{\nu'}^{m'*}(\hat{\mathbf{s}}_i)) \, d\varphi = \mathcal{N}(\nu, q) \delta_{\nu\nu'} \delta_{mm'}, \tag{72}$$

where $\mathcal{N}(\nu, q)$ is a positive constant which depends on ν, q.

The factor $\mathcal{N}(\nu, q)$ in Lemma 3.1 satisfies $\mathcal{N}(-\nu, q) = -\mathcal{N}(\nu, q)$ because $g^m(-\nu, -\mu_i) = g^m(\nu, \mu_i)$. Note that

$$|\Phi_\nu^m(\hat{\mathbf{s}}_i)|^2 = \frac{\pi \varpi^2 \nu^2}{(\nu - \mu_i)^2} \left[\sum_{l=|m|}^{l_{max}} \sqrt{2l+1} g^l Y_{lm}(\mu_i, 0) g_l^m(\nu) \right]^2, \tag{73}$$

and for $\hat{\mathbf{k}} = \hat{\mathbf{k}}(\nu, \mathbf{q})$,

$$\mathcal{R}_{\hat{\mathbf{k}}}^{-1} \mu_i = \sqrt{\frac{4\pi}{3}} \mathcal{R}_{\hat{\mathbf{k}}}^{-1} Y_{10}(\hat{\mathbf{s}}_i) = \sqrt{\frac{4\pi}{3}} \sum_{m'=-1}^{1} d_{0m'}^1(\vartheta_{\hat{\mathbf{k}}}) Y_{1m'}(\hat{\mathbf{s}}_i)$$

$$= \hat{k}_z(\nu q) \mu_i - i|\nu q| \sqrt{1 - \mu_i^2} \cos\varphi. \tag{74}$$

Since integrals over all angles do not change their values if the reference frame is rotated, for sufficiently large N we have

$$\sum_{i=1}^{2N} w_i \mu_i \int_0^{2\pi} (\mathcal{R}_{\hat{\mathbf{k}}(v,\mathbf{q})} \Phi_v^m(\hat{\mathbf{s}}_i))(\mathcal{R}_{\hat{\mathbf{k}}(v,\mathbf{q})} \Phi_v^{m*}(\hat{\mathbf{s}}_i)) \, \mathrm{d}\varphi$$

$$= \sum_{i=1}^{2N} w_i \int_0^{2\pi} \mu_i \mathcal{R}_{\hat{\mathbf{k}}(v,\mathbf{q})} (\Phi_v^m(\hat{\mathbf{s}}_i) \Phi_v^{m*}(\hat{\mathbf{s}}_i)) \, \mathrm{d}\varphi$$

$$\approx \sum_{i=1}^{2N} w_i \int_0^{2\pi} \mathcal{R}_{\hat{\mathbf{k}}(v,\mathbf{q})}^{-1} [\mu_i \mathcal{R}_{\hat{\mathbf{k}}(v,\mathbf{q})} (\Phi_v^m(\hat{\mathbf{s}}_i) \Phi_v^{m*}(\hat{\mathbf{s}}_i))] \, \mathrm{d}\varphi$$

$$= \sum_{i=1}^{2N} w_i \int_0^{2\pi} (\mathcal{R}_{\hat{\mathbf{k}}(v,\mathbf{q})}^{-1} \mu_i) |\Phi_v^m(\hat{\mathbf{s}}_i)|^2 \, \mathrm{d}\varphi. \tag{75}$$

Hence we have

$$\mathcal{N}(v,q) \approx \sum_{i=1}^{2N} w_i \int_0^{2\pi} (\mathcal{R}_{\hat{\mathbf{k}}(v,\mathbf{q})}^{-1} \mu_i) |\Phi_v^m(\hat{\mathbf{s}}_i)|^2 \, \mathrm{d}\varphi$$

$$= 2\pi \hat{k}_z(vq) \sum_{i=1}^{2N} w_i \mu_i |\Phi_v^m(\hat{\mathbf{s}}_i)|^2. \tag{76}$$

Proof of Lemma 3.1.: We begin by expressing (44) as

$$\left(1 - \frac{\hat{\mathbf{s}}_i \cdot \hat{\mathbf{k}}(v,\mathbf{q})}{v}\right) \mathcal{R}_{\hat{\mathbf{k}}(v,\mathbf{q})} \Phi_v^m(\hat{\mathbf{s}}_i)$$

$$= \varpi \sum_{l=0}^{l_{max}} \sum_{m'=-l}^{l} g^l Y_{lm'}(\hat{\mathbf{s}}_i) \sum_{i'=1}^{2N} w_{i'} \int_0^{2\pi} Y_{lm'}^*(\hat{\mathbf{s}}_{i'}) \mathcal{R}_{\hat{\mathbf{k}}(v,\mathbf{q})} \Phi_v^m(\hat{\mathbf{s}}_{i'}) \, \mathrm{d}\varphi'. \tag{77}$$

Note that $v = v^m$ depends on m. Let us consider $\hat{\mathbf{k}}_1 = \hat{\mathbf{k}}(v_1^{m_1}, \mathbf{q})$ and $\hat{\mathbf{k}}_2 = \hat{\mathbf{k}}(v_2^{m_2}, \mathbf{q})$. We have

$$(\mathcal{R}_{\hat{\mathbf{k}}_2} \Phi_{v_2}^{m_2}(\hat{\mathbf{s}}_i)) \mathcal{R}_{\hat{\mathbf{k}}_1} \left(1 - \frac{\mu_i}{v_1}\right) \Phi_{v_1}^{m_1}(\hat{\mathbf{s}}_i)$$

$$= (\mathcal{R}_{\hat{\mathbf{k}}_2} \Phi_{v_2}^{m_2}(\hat{\mathbf{s}}_i)) \varpi \sum_{l=0}^{l_{max}} \sum_{m=-l}^{l} g^l Y_{lm}(\hat{\mathbf{s}}_i) \sum_{i'=1}^{2N} w_{i'} \int_0^{2\pi} Y_{lm}^*(\hat{\mathbf{s}}_{i'}) \mathcal{R}_{\hat{\mathbf{k}}_1} \Phi_{v_1}^{m_1}(\hat{\mathbf{s}}_{i'}) \, \mathrm{d}\varphi' \tag{78}$$

and

$$(\mathcal{R}_{\hat{\mathbf{k}}_1} \Phi_{v_1}^{m_1}(\hat{\mathbf{s}}_i)) \mathcal{R}_{\hat{\mathbf{k}}_2} \left(1 - \frac{\mu_i}{v_2}\right) \Phi_{v_2}^{m_2}(\hat{\mathbf{s}}_i)$$

$$= (\mathcal{R}_{\hat{\mathbf{k}}_1} \Phi_{v_1}^{m_1}(\hat{\mathbf{s}}_i)) \varpi \sum_{l=0}^{l_{max}} \sum_{m=-l}^{l} g^l Y_{lm}^*(\hat{\mathbf{s}}_i) \sum_{i'=1}^{2N} w_{i'} \int_0^{2\pi} Y_{lm}(\hat{\mathbf{s}}_{i'}) \mathcal{R}_{\hat{\mathbf{k}}_2} \Phi_{v_2}^{m_2}(\hat{\mathbf{s}}_{i'}) \, \mathrm{d}\varphi'. \tag{79}$$

By subtraction,

$$-\frac{1}{\nu_1}(\mathcal{R}_{\hat{\mathbf{k}}_2}\Phi_{\nu_2}^{m_2}(\hat{\mathbf{s}}_i))\mathcal{R}_{\hat{\mathbf{k}}_1}\mu_i\Phi_{\nu_1}^{m_1}(\hat{\mathbf{s}}_i)+\frac{1}{\nu_2}(\mathcal{R}_{\hat{\mathbf{k}}_1}\Phi_{\nu_1}^{m_1}(\hat{\mathbf{s}}_i))\mathcal{R}_{\hat{\mathbf{k}}_2}\mu_i\Phi_{\nu_2}^{m_2}(\hat{\mathbf{s}}_i)$$

$$=(\mathcal{R}_{\hat{\mathbf{k}}_2}\Phi_{\nu_2}^{m_2}(\hat{\mathbf{s}}_i))\varpi\sum_{l=0}^{l_{\max}}\sum_{m=-l}^{l}g^l Y_{lm}(\hat{\mathbf{s}}_i)\sum_{i'=1}^{2N}w_{i'}\int_0^{2\pi}Y_{lm}^*(\hat{\mathbf{s}}_{i'})\mathcal{R}_{\hat{\mathbf{k}}_1}\Phi_{\nu_1}^{m_1}(\hat{\mathbf{s}}_{i'})\,\mathrm{d}\varphi'$$

$$-(\mathcal{R}_{\hat{\mathbf{k}}_1}\Phi_{\nu_1}^{m_1}(\hat{\mathbf{s}}_i))\varpi\sum_{l=0}^{l_{\max}}\sum_{m=-l}^{l}g^l Y_{lm}^*(\hat{\mathbf{s}}_i)\sum_{i'=1}^{2N}w_{i'}\int_0^{2\pi}Y_{lm}(\hat{\mathbf{s}}_{i'})\mathcal{R}_{\hat{\mathbf{k}}_2}\Phi_{\nu_2}^{m_2}(\hat{\mathbf{s}}_{i'})\,\mathrm{d}\varphi'. \qquad (80)$$

Hence by summing both sides of the above two equations by $\sum_{i=1}^{2N}w_i\int_0^{2\pi}\,\mathrm{d}\varphi$,

$$\left(\frac{\hat{k}_z(\nu_2 q)}{\nu_2}-\frac{\hat{k}_z(\nu_1 q)}{\nu_1}\right)\sum_{i=1}^{2N}w_i\int_0^{2\pi}\mu_i(\mathcal{R}_{\hat{\mathbf{k}}_1}\Phi_{\nu_1}^{m_1}(\hat{\mathbf{s}}_i))(\mathcal{R}_{\hat{\mathbf{k}}_2}\Phi_{\nu_2}^{m_2}(\hat{\mathbf{s}}_i))\,\mathrm{d}\varphi=0. \qquad (81)$$

Suppose $\nu=\nu_1=\nu_2$ but $m_1\neq m_2$. In this case, $\hat{\mathbf{k}}=\hat{\mathbf{k}}_1=\hat{\mathbf{k}}_2$ and

$$\sum_{i=1}^{2N}w_i\int_0^{2\pi}\mu_i(\mathcal{R}_{\hat{\mathbf{k}}}\Phi_{\nu}^{m_1}(\hat{\mathbf{s}}_i))(\mathcal{R}_{\hat{\mathbf{k}}}\Phi_{\nu}^{m_2}(\hat{\mathbf{s}}_i))\,\mathrm{d}\varphi$$

$$=\sum_{i=1}^{2N}w_i\int_0^{2\pi}\mu_i(\mathcal{R}_{\hat{\mathbf{k}}}\Phi_{\nu}^{m_1}(\hat{\mathbf{s}}_i)\Phi_{\nu}^{m_2}(\hat{\mathbf{s}}_i))\,\mathrm{d}\varphi\propto\delta_{m_1,-m_2}. \qquad (82)$$

Noting that $\nu^{-m}=\nu^m$ and $\Phi_{\nu}^{-m}(\hat{\mathbf{s}}_i)=\Phi_{\nu}^{m*}(\hat{\mathbf{s}}_i)$, we have

$$\sum_{i=1}^{2N}w_i\int_0^{2\pi}\mu_i(\mathcal{R}_{\hat{\mathbf{k}}_1}\Phi_{\nu_1}^{m_1}(\hat{\mathbf{s}}_i))(\mathcal{R}_{\hat{\mathbf{k}}_2}\Phi_{\nu_2}^{m_2*}(\hat{\mathbf{s}}_i))\,\mathrm{d}\varphi\propto\delta_{\nu_1\nu_2}\delta_{m_1 m_2}. \qquad (83)$$

∎

Let us calculate eigenvalues. Equation (49) can be rewritten as ($i=1,\ldots,2N$, $-l_{\max}\leq m\leq l_{\max}$)

$$\left(1-\frac{\mu_i}{\nu}\right)\phi^m(\nu,\mu_i)=\frac{\varpi}{2}\sum_{l'=|m|}^{l_{\max}}g^{l'}(2l'+1)p_{l'}^m(\mu_i)\sum_{i'=1}^{2N}w_{i'}p_{l'}^m(\mu_{i'})(1-\mu_{i'}^2)^{|m|}\phi^m(\nu,\mu_{i'}). \qquad (84)$$

Hence, for $i=1,\ldots,N$,

$$\left(1-\frac{\mu_i}{\nu}\right)\phi^m(\nu,\mu_i)=\frac{\varpi}{2}\sum_{l'=|m|}l_{\max}g^{l'}(2l'+1)p_{l'}^m(\mu_i)$$

$$\times\sum_{i'=1}^{N}w_{i'}p_{l'}^m(\mu_{i'})(1-\mu_{i'}^2)^{|m|}[\phi^m(\nu,\mu_{i'})+(-1)^{l'+m}\phi^m(\nu,-\mu_{i'})], \qquad (85)$$

$$\left(1 + \frac{\mu_i}{\nu}\right)\phi^m(\nu, -\mu_i) = \frac{\varpi}{2} \sum_{l'=|m|}^{l_{max}} g^{l'}(2l'+1)p_{l'}^m(\mu_i)$$

$$\times \sum_{i'=1}^{N} w_{i'}p_{l'}^m(\mu_{i'})(1-\mu_{i'}^2)^{|m|}[(-1)^{l'+m}\phi^m(\nu, \mu_{i'}) + \phi^m(\nu, -\mu_{i'})].$$

(86)

We arrive at the following matrix-vector equation:

$$\left(I_N - \frac{1}{\nu}\Xi\right)\Phi_+^m(\nu) = \frac{\varpi}{2}[W_+^m\Phi_+^m(\nu) + W_-^m\Phi_-^m(\nu)],$$

$$\left(I_N + \frac{1}{\nu}\Xi\right)\Phi_-^m(\nu) = \frac{\varpi}{2}[W_-^m\Phi_+^m(\nu) + W_+^m\Phi_-^m(\nu)],$$

(87)

where I_N is the N-dimensional identity matrix. Matrix Ξ and vectors $\Phi_\pm^m$ are defined as

$$\Xi = \begin{pmatrix} \mu_1 & & \\ & \ddots & \\ & & \mu_N \end{pmatrix}, \quad \Phi_\pm^m(\nu) = \begin{pmatrix} \phi^m(\nu, \pm\mu_1) \\ \vdots \\ \phi^m(\nu, \pm\mu_N) \end{pmatrix}.$$

(88)

Elements of the matrices $W_\pm^m$ are given by

$$\{W_\pm^m\}_{ij} = w_j \sum_{l=|m|}^{l_{max}} (2l+1)g^l p_l^m(\pm\mu_i)p_l^m(\mu_j)(1-\mu_j^2)^{|m|}$$

$$= w_j \sum_{l=|m|}^{l_{max}} (2l+1)g^l \frac{(l-m)!}{(l+m)!}P_l^m(\pm\mu_i)P_l^m(\mu_j)(1-\mu_i^2)^{-|m|/2}(1-\mu_j^2)^{|m|/2}$$

$$= 4\pi w_j \sum_{l=|m|}^{l_{max}} g^l \frac{(1-\mu_j^2)^{|m|/2}}{(1-\mu_i^2)^{|m|/2}}Y_{lm}(\pm\mu_i, 0)Y_{lm}(\mu_j, 0),$$

(89)

where we wrote $Y_{lm}(\hat{s}_i) = Y_{lm}(\mu_i, \varphi)$. The fact $\Phi_\pm^m(-\nu) = \Phi_\mp^m(\nu)$ implies that $-\nu$ is an eigenvalue if ν is an eigenvalue.

According to [7, 28], we introduce

$$\mathbf{U}^m(\nu) = \Phi_+^m(\nu) + \Phi_-^m(\nu), \quad \mathbf{V}^m(\nu) = \Phi_+^m(\nu) - \Phi_-^m(\nu).$$

(90)

By adding and subtracting two equations, we obtain

$$\mathbf{U}^m(\nu) - \frac{1}{\nu}\Xi\mathbf{V}^m(\nu) = \frac{\varpi}{2}(W_+^m + W_-^m)\mathbf{U}^m(\nu),$$

$$\mathbf{V}^m(\nu) - \frac{1}{\nu}\Xi\mathbf{U}^m(\nu) = \frac{\varpi}{2}(W_+^m - W_-^m)\mathbf{V}^m(\nu).$$

(91)

Hence we arrive at [11, 29]

$$E_-^m E_+^m \Xi\mathbf{U}^m = \frac{1}{\nu^2}\Xi\mathbf{U}^m,$$

(92)

where

$$E_\pm^m = \left[I_N - \frac{\varpi}{2}(W_+^m \pm W_-^m) \right] \Xi^{-1}. \tag{93}$$

We note that (92) is not the only matrix-vector equation for $1/\nu^2$ (see [30]). From (92), the eigenvalues are obtained as

$$\nu = \nu_n^m > 0 \quad (n = 1, \ldots, N, \ m = 0, \ldots, l_{\max}) \tag{94}$$

with the relation $\nu_n^{-m} = \nu_n^m$. In addition, $-\nu_n^m$ are also eigenvalues.

4. Scattering term

Let φ_0 be the azimuthal angle of $\hat{\mathbf{s}}_{i_0}$ for some i_0. By setting $\tilde{S} = \delta(z - z')\delta_{ii_0}\delta(\varphi - \varphi_0)$ in (22) for $z' \in \mathbb{R}$, let us consider the fundamental solution $G_{\mathbf{q}}(z, \hat{\mathbf{s}}_i; z', \hat{\mathbf{s}}_{i_0})$:

$$\left(\mu_i \frac{\partial}{\partial z} + 1 + i\omega_i \cdot \mathbf{q} \right) G_{\mathbf{q}}(z, \hat{\mathbf{s}}_i; z', \hat{\mathbf{s}}_{i_0})$$

$$= \varpi \sum_{i'=1}^{2N} w_{i'} \int_0^{2\pi} p(\hat{\mathbf{s}}_i, \hat{\mathbf{s}}_{i'}) G_{\mathbf{q}}(z, \hat{\mathbf{s}}_{i'}; z', \hat{\mathbf{s}}_{i_0}) \, \mathrm{d}\varphi + \delta(z - z')\delta_{ii_0}\delta(\varphi - \varphi_0) \tag{95}$$

for $z \in \mathbb{R}$, $1 \le i \le 2N$, $\varphi \in [0, 2\pi)$. We obtain (see Appendix)

$$G_{\mathbf{q}}(z, \hat{\mathbf{s}}_i; z', \hat{\mathbf{s}}_{i_0}) = \sum_{m=-l_{\max}}^{l_{\max}} \sum_{n=1}^{N} \frac{w_{i_0}}{\mathcal{N}(\nu_n^m, q)} \mathrm{e}^{\mp \hat{k}_z(\nu_n^m q)(z-z')/\nu_n^m}$$

$$\times (\mathcal{R}_{\hat{\mathbf{k}}_\pm} \Phi_{\pm\nu_n^m}^m(\hat{\mathbf{s}}_i))(\mathcal{R}_{\hat{\mathbf{k}}_\pm} \Phi_{\pm\nu_n^m}^{m*}(\hat{\mathbf{s}}_{i_0})), \tag{96}$$

where upper (lower) signs are taken for $z > z'$ ($z < z'$) and

$$\hat{\mathbf{k}}_\pm = \hat{\mathbf{k}}(\pm\nu_n^m, \mathbf{q}). \tag{97}$$

Let us define

$$C(\tau; \zeta, \eta) = \frac{\mathrm{e}^{-\tau/\zeta} - \mathrm{e}^{-\tau/\eta}}{\zeta - \eta}. \tag{98}$$

We note that $C(-\tau; -\zeta, -\eta) = -C(\tau; \zeta, \eta)$ and

$$C(\tau; \eta, \eta) = \frac{\tau}{\eta^2}. \tag{99}$$

The solution $\check{I}_s$ to (22) is obtained as

$$\check{I}_s(\mathbf{q}, z, \hat{\mathbf{s}}_i) = \sum_{i'=1}^{2N} \int_0^{2\pi} \int_{-\infty}^{\infty} G_{\mathbf{q}}(z, \hat{\mathbf{s}}_i; z', \hat{\mathbf{s}}_{i'})\tilde{S}(\mathbf{q}, z', \hat{\mathbf{s}}_{i'}) \, \mathrm{d}z'\mathrm{d}\varphi'$$

$$= \frac{\varpi \mu_t^2}{|\mu_0|} \int_{-\infty}^{\infty} \Theta(\mu_0 z') \left[\sum_{i'=1}^{2N} \int_0^{2\pi} G_{\mathbf{q}}(z, \hat{\mathbf{s}}_i; z', \hat{\mathbf{s}}_{i'}) p(\hat{\mathbf{s}}_{i'}, \hat{\mathbf{s}}_{i_0}) \, \mathrm{d}\varphi' \right] \mathrm{e}^{-(1+i\mathbf{q}\cdot\omega_0)z'/\mu_0} \, \mathrm{d}z'. \tag{100}$$

Since $p(\hat{\mathbf{s}}_{i'}, \hat{\mathbf{s}}_{i_0}) = p(\mathcal{R}_{\hat{\mathbf{k}}}\hat{\mathbf{s}}_{i'}, \mathcal{R}_{\hat{\mathbf{k}}}\hat{\mathbf{s}}_{i_0})$ for a unit vector $\hat{\mathbf{k}} \in \mathbb{C}$, we have

$$\sum_{l=0}^{l_{\max}} \sum_{m=-l}^{l} g^l Y_{lm}(\hat{\mathbf{s}}_{i'}) Y_{lm}^*(\hat{\mathbf{s}}_{i_0}) = \sum_{l=0}^{l_{\max}} \sum_{m=-l}^{l} g^l (\mathcal{R}_{\hat{\mathbf{k}}} Y_{lm}(\hat{\mathbf{s}}_{i'}))(\mathcal{R}_{\hat{\mathbf{k}}} Y_{lm}^*(\hat{\mathbf{s}}_{i_0})). \tag{101}$$

We obtain

$$\sum_{i'=1}^{2N} \int_0^{2\pi} G_{\mathbf{q}}(z, \hat{\mathbf{s}}_i; z', \hat{\mathbf{s}}_{i'}) p(\hat{\mathbf{s}}_{i'}, \hat{\mathbf{s}}_{i_0}) \, d\varphi'$$

$$= \sum_{m=-l_{\max}}^{l_{\max}} \sum_{n=1}^{N} \frac{1}{\mathcal{N}(\nu_n^m, q)} e^{\mp \hat{k}_z (\nu_n^m q)(z-z')/\nu_n^m} (\mathcal{R}_{\hat{\mathbf{k}}_{\pm}} \Phi_{\pm \nu_n^m}^m(\hat{\mathbf{s}}_i))$$

$$\times \sum_{l=0}^{l_{\max}} \sum_{m'=-l}^{l} g^l (\mathcal{R}_{\hat{\mathbf{k}}_{\pm}} Y_{lm'}^*(\hat{\mathbf{s}}_{i_0})) \sum_{i'=1}^{2N} w_{i'} \int_0^{2\pi} (\mathcal{R}_{\hat{\mathbf{k}}_{\pm}} \Phi_{\pm \nu_n^m}^{m*}(\hat{\mathbf{s}}_{i'}))(\mathcal{R}_{\hat{\mathbf{k}}_{\pm}} Y_{lm'}(\hat{\mathbf{s}}_{i'})) \, d\varphi'$$

$$\approx \sum_{m=-l_{\max}}^{l_{\max}} \sum_{n=1}^{N} \frac{1}{\mathcal{N}(\nu_n^m, q)} e^{\mp \hat{k}_z (\nu_n^m q)(z-z')/\nu_n^m} (\mathcal{R}_{\hat{\mathbf{k}}_{\pm}} \Phi_{\pm \nu_n^m}^m(\hat{\mathbf{s}}_i))$$

$$\times \sum_{l=0}^{l_{\max}} \sum_{m'=-l}^{l} g^l (\mathcal{R}_{\hat{\mathbf{k}}_{\pm}} Y_{lm'}^*(\hat{\mathbf{s}}_{i_0})) \sum_{i'=1}^{2N} w_{i'} \int_0^{2\pi} \Phi_{\pm \nu_n^m}^{m*}(\hat{\mathbf{s}}_{i'}) Y_{lm'}(\hat{\mathbf{s}}_{i'}) \, d\varphi'. \tag{102}$$

To reach the rightmost side of the above equation, we used the fact that the discretized integral over all angles is numerically unchanged about the rotation of the reference frame for sufficiently large N. Hence,

$$\sum_{i'=1}^{2N} \int_0^{2\pi} G_{\mathbf{q}}(z, \hat{\mathbf{s}}_i; z', \hat{\mathbf{s}}_{i'}) p(\hat{\mathbf{s}}_{i'}, \hat{\mathbf{s}}_{i_0}) \, d\varphi'$$

$$\approx \sum_{m=-l_{\max}}^{l_{\max}} \sum_{n=1}^{N} \frac{1}{\mathcal{N}(\nu_n^m, q)} e^{\mp \hat{k}_z (\nu_n^m q)(z-z')/\nu_n^m} (\mathcal{R}_{\hat{\mathbf{k}}_{\pm}} \Phi_{\pm \nu_n^m}^m(\hat{\mathbf{s}}_i))$$

$$\times \sum_{l=0}^{l_{\max}} \sum_{m'=-l}^{l} g^l \mathcal{R}_{\hat{\mathbf{k}}_{\pm}} Y_{lm'}^*(\hat{\mathbf{s}}_{i_0}) \sum_{i'=1}^{2N} w_{i'} \int_0^{2\pi} \Phi_{\pm \nu_n^m}^{m*}(\hat{\mathbf{s}}_{i'}) Y_{lm'}(\hat{\mathbf{s}}_{i'}) \, d\varphi'$$

$$= \sum_{m=-l_{\max}}^{l_{\max}} \sum_{n=1}^{N} \frac{(-1)^m}{\mathcal{N}(\nu_n^m, q)} e^{\mp \hat{k}_z (\nu_n^m q)(z-z')/\nu_n^m} (\mathcal{R}_{\hat{\mathbf{k}}_{\pm}} \Phi_{\pm \nu_n^m}^m(\hat{\mathbf{s}}_i))$$

$$\times \sum_{l=|m|}^{l_{\max}} \sqrt{(2l+1)\pi} g^l g_l^m(\pm \nu_n^m)(\mathcal{R}_{\hat{\mathbf{k}}_{\pm}} Y_{lm}^*(\hat{\mathbf{s}}_{i_0})), \tag{103}$$

where we used (50).

Hereafter, we assume

$$\hat{\mathbf{s}}_0 = \hat{\mathbf{z}} = {}^t(0, 0, 1).$$ (104)

Since

$$\mathcal{R}_{\hat{\mathbf{k}}_\pm} Y_{lm}(\hat{\mathbf{z}}) = \sqrt{\frac{2l+1}{4\pi}} d^l_{0m}[i\tau(\nu_n q)],$$ (105)

we have

$$\mathcal{R}_{\hat{\mathbf{k}}_\pm} Y^*_{lm}(\hat{\mathbf{s}}_{i_0}) = \mathcal{R}_{\hat{\mathbf{k}}(\pm\nu_n^m, \mathbf{q})} Y^*_{lm}(\hat{\mathbf{z}}) = \sqrt{\frac{2l+1}{4\pi}} d^l_{0m}[i\tau(\nu_n^m q)].$$ (106)

If (103) is substituted into (100), $\check{I}_s(\mathbf{q}, z, \hat{\mathbf{s}}_i)$ is calculated as

$$
\begin{aligned}
\check{I}_s(\mathbf{q}, z, \hat{\mathbf{s}}_i) = {} & \frac{\varpi \mu_t^2}{2} \int_{-\infty}^z \Theta(z') \left[\sum_{m=-l_{\max}}^{l_{\max}} \sum_{n=1}^N \frac{(-1)^m}{\mathcal{N}(\nu_n^m, q)} e^{-\hat{k}_z(\nu_n^m q)(z-z')/\nu_n^m} (\mathcal{R}_{\hat{\mathbf{k}}_+} \Phi^m_{\nu_n^m}(\hat{\mathbf{s}}_i)) \right. \\
& \left. \times \sum_{l=|m|}^{l_{\max}} (2l+1) g^l g_l^m(\nu_n^m) d^l_{0m}[i\tau(\nu_n^m q)] \right] e^{-z'/\mu_0} \, dz' \\
& + \frac{\varpi \mu_t^2}{2} \int_z^\infty \Theta(z') \left[\sum_{m=-l_{\max}}^{l_{\max}} \sum_{n=1}^N \frac{(-1)^m}{\mathcal{N}(\nu_n^m, q)} e^{\hat{k}_z(\nu_n^m q)(z-z')/\nu_n^m} (\mathcal{R}_{\hat{\mathbf{k}}_-} \Phi^m_{-\nu_n^m}(\hat{\mathbf{s}}_i)) \right. \\
& \left. \times \sum_{l=|m|}^{l_{\max}} (2l+1) g^l g_l^m(-\nu_n^m) d^l_{0m}[i\tau(\nu_n^m q)] \right] e^{-z'/\mu_0} \, dz'.
\end{aligned}
$$ (107)

In the above equation, we assumed that N is large enough that the approximation in (103) is numerically exact. Thus we have

$$\check{I}_s(\mathbf{q}, z, \hat{\mathbf{s}}_i) = \frac{\varpi \mu_t^2}{2} \sum_{m=-l_{\max}}^{l_{\max}} \sum_{n=1}^N \frac{(-1)^m \nu_n^m}{\mathcal{N}(\nu_n^m, q)\hat{k}_z(\nu_n^m q)} [\Theta(z)(\psi_1 + \psi_2) + (1 - \Theta(z))\psi_3],$$ (108)

where

$$\psi_1 = C\left(z; 1, \frac{\nu_n^m}{\hat{k}_z(\nu_n^m q)}\right) (\mathcal{R}_{\hat{\mathbf{k}}_+} \Phi^m_{\nu_n^m}(\hat{\mathbf{s}}_i)) \sum_{l=|m|}^{l_{\max}} (2l+1) g^l g_l^m(\nu_n^m) d^l_{0m}[i\tau(\nu_n q)],$$ (109)

$$\psi_2 = \frac{e^{-z\hat{k}_z(\nu_n^m q)}}{\nu_n^m + \hat{k}_z(\nu_n^m q)} (\mathcal{R}_{\hat{\mathbf{k}}_-} \Phi^m_{-\nu_n^m}(\hat{\mathbf{s}}_i)) \sum_{l=|m|}^{l_{\max}} (2l+1) g^l g_l^m(-\nu_n^m) d^l_{0m}[i\tau(\nu_n q)],$$ (110)

$$\psi_3 = \frac{e^{\hat{k}_z(\nu_n^m q)z/\nu_n^m} \hat{k}_z(\nu_n^m q)}{\nu_n^m + \hat{k}_z(\nu_n^m q)} (\mathcal{R}_{\hat{\mathbf{k}}_-} \Phi^m_{-\nu_n^m}(\hat{\mathbf{s}}_i)) \sum_{l=|m|}^{l_{\max}} (2l+1) g^l g_l^m(-\nu_n^m) d^l_{0m}[i\tau(\nu_n q)].$$ (111)

5. Energy density

In this section, we return to the original unit of length and put the subscript $*$ for the scaled space variables. We suppose $\rho \neq \mathbf{0}$. The energy density $U(\mathbf{r})$ is given by

$$U(\mathbf{r}) = \int_{\mathbb{S}^2} I(\mathbf{r}, \hat{\mathbf{s}}) \, \mathrm{d}\hat{\mathbf{s}}. \tag{112}$$

Noting $\tilde{I}_s \approx \check{I}_s$ by the discretization of the cosine μ of the polar angle, we have

$$U(\mathbf{r}) = \int_{\mathbb{S}^2} I_b(\mathbf{r}, \hat{\mathbf{s}}) \, \mathrm{d}\hat{\mathbf{s}} + \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} e^{i\mathbf{q}\cdot\rho\mu_t} \int_{\mathbb{S}^2} \tilde{I}_s(\mathbf{q}, z_*, \hat{\mathbf{s}}) \, \mathrm{d}\hat{\mathbf{s}} \, \mathrm{d}\mathbf{q}$$

$$\approx \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} e^{i\mathbf{q}\cdot\rho\mu_t} \sum_{i=1}^{2N} w_i \int_0^{2\pi} \check{I}_s(\mathbf{q}, z_*, \hat{\mathbf{s}}_i) \, \mathrm{d}\varphi \, \mathrm{d}\mathbf{q}$$

$$= \frac{1}{2\pi} \int_0^\infty q J_0(q\rho_*) \sum_{i=1}^{2N} w_i \int_0^{2\pi} \check{I}_s(\mathbf{q}, z_*, \hat{\mathbf{s}}_i) \, \mathrm{d}\varphi \, \mathrm{d}q$$

$$= U(\rho, z), \tag{113}$$

where $\rho_* = \mu_t\rho$, $z_* = \mu_t z$, and we used the Hansen–Bessel formula

$$J_0(x) = \frac{1}{2\pi} \int_0^{2\pi} e^{ix\cos\varphi} \, \mathrm{d}\varphi \tag{114}$$

with $J_0(x)$ $(x \geq 0)$ the Bessel function of order 0. Note that

$$\sum_{i=1}^{2N} w_i \int_0^{2\pi} \mathcal{R}_{\hat{\mathbf{k}}(\nu,\mathbf{q})} \Phi_\nu^m(\hat{\mathbf{s}}_i) \, \mathrm{d}\varphi \approx 2\pi\delta_{m0} \tag{115}$$

for sufficiently large N because $\int_{\mathbb{S}^2} \mathcal{R}_{\hat{\mathbf{k}}} \Phi_\nu^m(\hat{\mathbf{s}}) \, \mathrm{d}\hat{\mathbf{s}} = \int_{\mathbb{S}^2} \Phi_\nu^m(\hat{\mathbf{s}}) \, \mathrm{d}\hat{\mathbf{s}}$. Within this approximation we have

$$U(\rho, z) = \frac{\varpi\mu_t^2}{2} \int_0^\infty q J_0(q\rho_*) F(q, z_*) \, \mathrm{d}q, \tag{116}$$

where

$$F(q, z_*) = \sum_{n=1}^N \frac{\nu_n^0}{\mathcal{N}(\nu_n^0, q)} \left[\Theta(z_*) \frac{e^{-z_*} - e^{-\hat{k}_z(\nu_n^0 q)z_*/\nu_n^0}}{\hat{k}_z(\nu_n^0 q) - \nu_n^0} \sum_{l=0}^{l_{max}} (2l+1) g^l g_l^0(\nu_n^0) d_{00}^l[i\tau(\nu_n q)] \right.$$

$$+ \Theta(z_*) \frac{e^{-z_*}}{\hat{k}_z(\nu_n^0 q) + \nu_n^0} \sum_{l=0}^{l_{max}} (-1)^l(2l+1) g^l g_l^0(\nu_n^0) d_{00}^l[i\tau(\nu_n q)]$$

$$\left. + (1 - \Theta(z_*)) \frac{e^{\hat{k}_z(\nu_n^0 q)z_*/\nu_n^0}}{\hat{k}_z(\nu_n^0 q) + \nu_n^0} \sum_{l=0}^{l_{max}} (-1)^l(2l+1) g^l g_l^0(\nu_n^0) d_{00}^l[i\tau(\nu_n q)] \right]. \tag{117}$$

For the purpose of numerical calculation, we use the asymptotic expression of the Bessel function:

$$J_0(x) = \sqrt{\frac{2}{\pi x}} \left[\left(1 - \frac{9}{128x^2} + O(x^{-4}) \right) \cos \left(x - \frac{\pi}{4} \right) \right.$$
$$\left. + \left(\frac{1}{8x} - \frac{75}{1024x^3} + O(x^{-5}) \right) \sin \left(x - \frac{\pi}{4} \right) \right]. \tag{118}$$

We define

$$d(q, \rho_*)$$

$$= qJ_0(q\rho_*) - \sqrt{\frac{2q}{\pi\rho_*}}$$

$$\times \left[\left(1 - \frac{9}{128(q\rho_*)^2} \right) \cos \left(q\rho_* - \frac{\pi}{4} \right) + \left(\frac{1}{8q\rho_*} - \frac{75}{1024(q\rho_*)^3} \right) \sin \left(q\rho_* - \frac{\pi}{4} \right) \right]. \tag{119}$$

Let us set

$$a = \frac{\pi}{4\rho_*}. \tag{120}$$

We have

$$U(\rho, z) = \frac{\varpi \mu_t^2}{2} \int_0^a qJ_0(q\rho_*)F(q, z_*) \, dq + \frac{\varpi \mu_t^2}{2} \int_a^\infty d(q, \rho_*)F(q, z_*) \, dq$$

$$+ \frac{\varpi \mu_t^2}{\sqrt{2\pi\rho_*}} \int_0^\infty [F_1(s, \mathbf{r}_*) + F_2(s, \mathbf{r}_*)] \, ds, \tag{121}$$

where $s = q - a$,

$$F_1(s, \mathbf{r}_*) = \sqrt{s + \frac{\pi}{4\rho_*}} \left(1 - \frac{9}{128(s\rho_* + \frac{\pi}{4})^2} \right) F \left(s + \frac{\pi}{4\rho_*}, z_* \right) \cos(s\rho_*),$$

$$F_2(s, \mathbf{r}_*) = \sqrt{s + \frac{\pi}{4\rho_*}} \left(\frac{1}{8(s\rho_* + \frac{\pi}{4})} - \frac{75}{1024(s\rho_* + \frac{\pi}{4})^3} \right) F \left(s + \frac{\pi}{4\rho_*}, z_* \right) \sin(s\rho_*). \tag{122}$$

The integrals $\int_0^\infty F_1(q) \, dq$ and $\int_0^\infty F_2(q) \, dq$ can be evaluated by the double-exponential formula [31–33]. Define

$$\phi(t) = \frac{t}{1 - e^{-6\sinh t}} \tag{123}$$

with

$$\phi'(t) = \frac{1 - (1 + 6t\cosh t) \, e^{-6\sinh t}}{(1 - e^{-6\sinh t})^2}. \tag{124}$$

With the approximation of the double-exponential formula, we can write

$$\int_0^\infty F_1(s, \mathbf{r}_*) \, ds \approx \frac{\pi}{\rho_*} \sum_{k=-N_k}^{N_k} F_1 \left(\frac{\pi}{h\rho_*} \phi \left(kh + \frac{h}{2} \right), \mathbf{r}_* \right) \phi' \left(kh + \frac{h}{2} \right),$$

$$\int_0^\infty F_2(s, \mathbf{r}_*) \, ds \approx \frac{\pi}{\rho_*} \sum_{k=-N_k}^{N_k} F_2\left(\frac{\pi}{h\rho_*}\phi(kh), \mathbf{r}_*\right) \phi'(kh), \tag{125}$$

where $N_k > 0$ is an integer and h is a mesh size.

6. Numerical tests

Let us compute $U(\mathbf{r}) = U(\rho, z) = \int_{\mathbb{S}^2} I(\mathbf{r}, \hat{\mathbf{s}}) \, d\hat{\mathbf{s}}$ in (112), where $I(\mathbf{r}, \hat{\mathbf{s}})$ is the solution of the radiative transport Equation (1) for the source term $f(\mathbf{r}, \hat{\mathbf{s}}) = \delta(\rho)\delta(z)\delta(\hat{\mathbf{s}} - \hat{\mathbf{s}}_0)$ given in (4). As was assumed in (104), $\hat{\mathbf{s}}_0 = \hat{\mathbf{z}}$.

Numerical calculation was conducted for

$$\mu_a = 0.01 \, \text{mm}^{-1}, \quad \mu_s = 10 \, \text{mm}^{-1}, \quad g = 0 \text{ or } 0.9. \tag{126}$$

When the integral (116) over q is computed for $U(\rho, z)$ making use of the double-exponential formula, we set $h = 0.01$, and $N_k = 400$. The trapezoidal rule was used for the first two integrals in (121) with 10^4 trapezoids. The upper limit of the second integral was set to 1. We took 101 points on the z-axis between -50 and $50 \, \text{mm}(g = 0.9)$ or -5 and $5 \, \text{mm}(g = 0)$. Results are shown in Figures 1– 4.

We set $g = 0.9$ in Figures 1 and 2. We first set $\rho = 5$ mm. In Figure 1(a), $U(\rho, z)$ in (121) is plotted for $l_{\max} = 9$. A smooth curve is obtained when $N = 9$ and $N = 11$. Figure 1(b) shows that the calculation with $l_{\max} = 3$ and $N = 3$ is almost identical to the result for $l_{\max} = 9$ and $N = 11$. Using FORTRAN (gfortran), the computation time was 5.6 s for $l_{\max} = 9, N = 11$ and 0.5 s for $l_{\max} = 3, N = 3$ on a laptop computer (Apple, MacBook Pro, 2.3 GHz Intel Core i5). Next we set $\rho = 2$ mm. Figure 2(a) shows that only the case of $N \geq 11$ is successful when $l_{\max} = 9$. In Figure 2(b), the result for $l_{\max} = 3, N = 3$ is close to the curve for $l_{\max} = 9$, $N = 11$, which gives the converged curve.

In Figures 3 and 4, $U(\rho, z)$ in (121) is compared to Monte Carlo simulation. The Monte-Carlo RTE solver MC [34] was used with the number of photons 10^8. The Monte Carlo simulation uses the Henyey–Greenstein model ($l_{\max} = \infty$). Parameters were chosen as $l_{\max} = 3, N = 3$. In Figure 3, we set $g = 0.9$. In Figure 4, g is set to 0. In both figures, $U(\rho, z)$
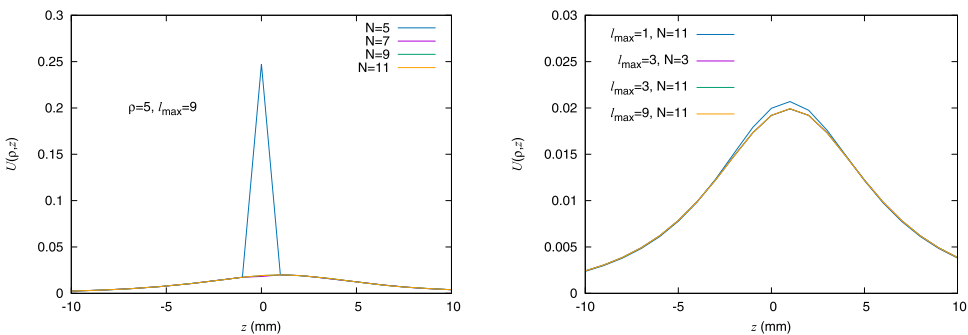
(a) Dependence on N for $l_{\max} = 9$. (b) Convergence behavior.

Figure 1. The energy density $U(\rho, z)$ in (121) is plotted for $\rho = 5$ mm. The parameters are set to $\mu_a = 0.01, \mu_s = 10$, and $g = 0.9$. (a) Dependence on N for $l_{\max} = 9$. (b) Convergence behavior.
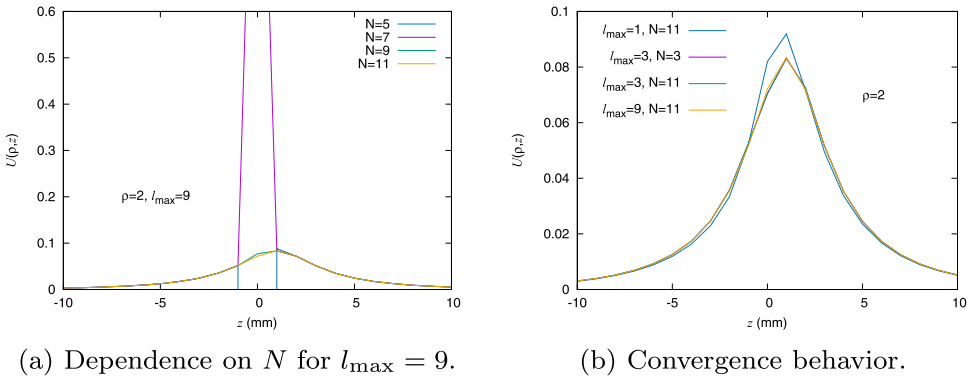
(a) Dependence on N for $l_{\max} = 9$.

(b) Convergence behavior.

Figure 2. Same as Figure 1 but $\rho = 2$ mm. (a) Dependence on N for $l_{\max} = 9$. (b) Convergence behavior.
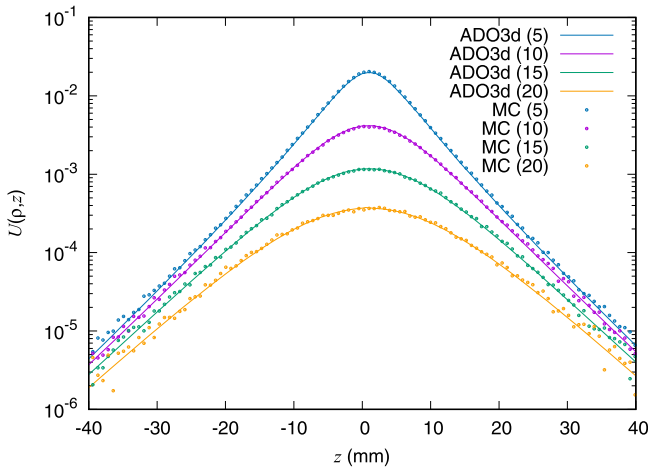

Figure 3. The energy density $U(\rho, z)$ is plotted. Results from (121) are compared to Monte Carlo simulation. From the top, $\rho = 5, 10, 15,$ and 20 mm. The parameters are set to $\mu_a = 0.01$, $\mu_s = 10$, and $g = 0.9$.

are plotted as functions of z for different ρ. Good agreement is seen in each line of Figures 3 and 4.

7. Concluding remarks

In one dimension, the equivalence between the discrete-ordinates method and spherical-harmonics method is known [4, 35]. In three dimensions, eigenmodes of the method of rotated reference frames [13] are obtained by expanding singular eigenfunctions with spherical harmonics [36] and then rotating the resulting expressions. However, the series expansion in the method of rotated reference frames diverges because components of $\hat{\mathbf{k}}$ become very large even if $\hat{\mathbf{k}} \cdot \hat{\mathbf{k}} = 1$ always holds.

Kim and Keller [17] and Kim [16] established discrete-ordinates with plane-wave decomposition for the three-dimensional radiative transport equation. Their method can be
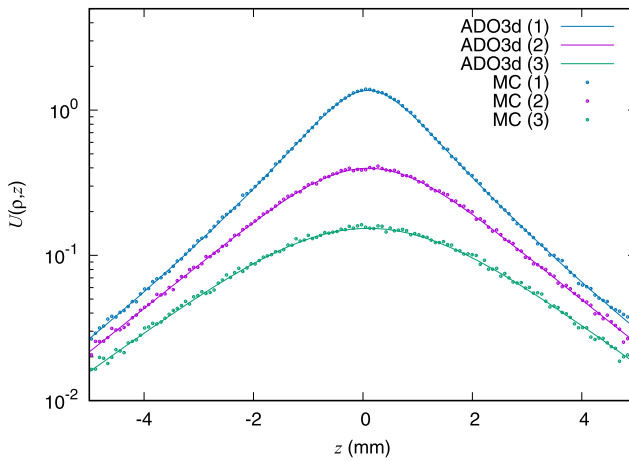
Figure 4. Same as Figure 3, but $g = 0$. From the top, $\rho = 1, 2$, and 3 mm.

viewed as separation of variables assuming the form

$$\check{I}(\mathbf{q}, z, \hat{\mathbf{s}}_i) = V_\lambda(\hat{\mathbf{s}}_i, \mathbf{q})\, e^{\lambda(\mathbf{q})z}. \tag{127}$$

The eigenvalues λ and eigenvectors V_λ are numerically computed for each $\mathbf{q} \in \mathbb{R}^2$. In the present paper, on the other hand, the form (29) was assumed. The explicit form of the eigenvectors is obtained and we can compute eigenvalues ν by diagonalizing a matrix once.

In Section 6, we computed the energy density. For the computation of the specific intensity itself, the post-processing procedure [28, 37], which was proposed in the original ADO is expected to help obtaining stable numerical solutions.

In this paper, the pencil beam (4) was assumed. For a general source function $f(\mathbf{r}, \hat{\mathbf{s}})$, the solution $I(\mathbf{r}, \hat{\mathbf{s}})$ to (1) is given by

$$I(\mathbf{r}, \hat{\mathbf{s}}) = \int_{\mathbb{S}^2} \int_{\mathbb{R}^3} G(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}', \hat{\mathbf{s}}') f(\mathbf{r}', \hat{\mathbf{s}}')\, d\mathbf{r}'\, d\hat{\mathbf{s}}', \tag{128}$$

where $G(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}', \hat{\mathbf{s}}')$ ($\mathbf{r}' = {}^t(\rho', z')$) is the solution of (1) for the source term $\delta(\rho - \rho')\delta(z - z')\delta(\hat{\mathbf{s}} - \hat{\mathbf{s}}')$. For any $\hat{\mathbf{s}}_0$, we can obtain $G(\mathbf{r}, \hat{\mathbf{s}}; \mathbf{r}', \hat{\mathbf{s}}_0)$ simply by shifting ρ, z by ρ', z' in the solution $I(\mathbf{r}, \hat{\mathbf{s}})$ to (1) for the source term (4). Moreover, the solution to (1) can be computed without the decomposition (8) if the source term is smooth. In this alternative approach for smooth f, the solution to (1) is obtained as $I_s(\mathbf{r}, \hat{\mathbf{s}})$ in (10) in which $S(\mathbf{r}, \hat{\mathbf{s}})$ is replaced by $f(\mathbf{r}, \hat{\mathbf{s}})$. Accordingly, $\tilde{S}$ in (100) is replaced by the Fourier transform of f. Then the calculation in Sec. 4 is modified in a straightforward way.

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M. MACHIDA AND K. DAS

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Appendix. Fundamental solution

Let us obtain $G_{\mathbf{q}}(z, \hat{\mathbf{s}}_i; z', \hat{\mathbf{s}}_{i_0})$ which satisfies (95). Since $G_{\mathbf{q}} \to 0$ as $z \to \pm\infty$, we can write

$$
\begin{aligned}
&G_{\mathbf{q}}(z, \hat{\mathbf{s}}_i; z', \hat{\mathbf{s}}_{i_0}) \\
&= \begin{cases}
\displaystyle\sum_{m=-l_{\max}}^{l_{\max}} \sum_{n=1}^{N} A_n^m \mathcal{R}_{\hat{\mathbf{k}}(\nu_n^m, \mathbf{q})} \Phi_{\nu_n^m}^m(\hat{\mathbf{s}}_i)\, e^{-\hat{k}_z(\nu_n^m q)(z-z')/\nu_n^m}, \\
\quad z > z', \\
\displaystyle\sum_{m=-l_{\max}}^{l_{\max}} \sum_{n=1}^{N} B_n^m \mathcal{R}_{\hat{\mathbf{k}}(-\nu_n^m, \mathbf{q})} \Phi_{-\nu_n^m}^m(\hat{\mathbf{s}}_i)\, e^{\hat{k}_z(\nu_n^m q_0)(z-z')/\nu_n^m}, \\
\quad z < z',
\end{cases}
\end{aligned}
\tag{A1}
$$

where coefficients $A_n^m = A_n^m(\mathbf{q}, \hat{\mathbf{s}}_{i_0})$, $B_n^m = B_n^m(\mathbf{q}, \hat{\mathbf{s}}_{i_0})$ will be determined from the source term. With the source term, the jump condition is written as

$$
\begin{aligned}
&\mu_i [G_{\mathbf{q}}(z' + 0, \hat{\mathbf{s}}_i; z', \hat{\mathbf{s}}_{i_0}) - G_{\mathbf{q}}(z' - 0, \hat{\mathbf{s}}_i; z', \hat{\mathbf{s}}_{i_0})] \\
&= \delta_{ii_0} \delta(\varphi - \varphi_0).
\end{aligned}
\tag{A2}
$$

Hence,

$$
\begin{aligned}
&\mu_i \sum_{m=-l_{\max}}^{l_{\max}} \sum_{n=1}^{N} \left[A_n^m \mathcal{R}_{\hat{\mathbf{k}}(\nu_n^m, \mathbf{q})} \Phi_{\nu_n^m}^m(\hat{\mathbf{s}}_i) - B_n^m \mathcal{R}_{\hat{\mathbf{k}}(-\nu_n^m, \mathbf{q})} \Phi_{-\nu_n^m}^m(\hat{\mathbf{s}}_i) \right] \\
&= \delta_{ii_0} \delta(\varphi - \varphi_0).
\end{aligned}
\tag{A3}
$$

Using the orthogonality relation in Lemma (3.1), we obtain

$$
\begin{aligned}
A_n^m &= \frac{w_{i_0}}{\mathcal{N}(\nu_n^m, q)} \mathcal{R}_{\hat{\mathbf{k}}(\nu_n^m, \mathbf{q})} \Phi_{\nu_n^m}^{m*}(\hat{\mathbf{s}}_{i_0}), \\
B_n^m &= \frac{-w_{i_0}}{\mathcal{N}(-\nu_n^m, q)} \mathcal{R}_{\hat{\mathbf{k}}(-\nu_n^m, \mathbf{q})} \Phi_{-\nu_n^m}^{m*}(\hat{\mathbf{s}}_{i_0}).
\end{aligned}
\tag{A4}
$$

Thus we arrive at (96).