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How to Construct Three-Dimensional Transport Theory Using Rotated Reference Frames

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ABSTRACT

In linear transport theory, 3D equations reduce to 1D equations by means of rotated reference frames. In this paper, we illustrate how the technique works and 3D transport theories are obtained.

KEYWORDS

Linear transport theory; rotated reference frames; singular eigenfunctions

1. Introduction

In linear transport theory, 3D equations reduce to 1D equations with rotated reference frames when the angular flux has the structure of separation of variables. Although the technique can be used for anisotropic scattering in the presence of boundaries, calculation becomes complicated in such general cases and sometimes the essence is buried in straightforward but lengthy and tedious calculations. In this paper, aiming at elucidating how rotated reference frames help construct linear transport theory in three dimensions, we will consider the case of isotropic scattering in an infinite medium.

To the best of the author’s knowledge, rotated reference frames were first introduced in transport theory by Dede (1964) in the context of the $P_N$ method, and then Kobayashi (1977) expanded Dede’s calculation. Forty years after Dede’s finding, Markel (2004) devised an efficient numerical algorithm of computing solutions to the 3D transport equation by reinventing rotated reference frames. The method is called the method of rotated reference frames. A lot of numerical calculations (Panasyuk et al., 2006; Xu and Patterson, 2006a,b; Machida et al., 2010; Liemert and Kienle, 2011a,b,c, 2012a,b,c,d,e, 2013a,b,c, 2015) done during the last decade have proved the usefulness and efficiency of this method. It was then found that the technique of rotated reference frames is not merely for the particular numerical method but is a tool to build bridges between 3D transport theory and 1D transport theory. Case’s method (Case, 1960; Mika, 1961; McCormick and Kuščer, 1966; Case and Zweifel, 1967) was extended to three dimensions (Machida, 2014), and the $F_N$ method (Siewert, 1978; Siewert and Benoist, 1979) was also extended to three
dimensions (Machida, 2015). Recently, the angular flux of the 3D transport equation with anisotropic scattering was computed using the Fourier transform by making use of rotated reference frames (Machida, 2016). The technique of rotated reference frames is also applied to optical tomography (Schotland and Markel, 2007; Machida et al., 2016; Machida, in press).

There have been many attempts to construct multi-dimensional transport theory especially since Case’s method (1960) of singular eigenfunctions appeared. In addition to trials of direct extension of the singular-eigenfunction approach (Williams, 1967; Kaper, 1969; Case and Hazeltine, 1970; Gibbs, 1969; Cannon, 1973; Pomraning, 1996), there were approaches based on the integral transform (Bareiss and Abu-Shumays, 1967; Williams, 1968; Schreiner et al., 1969; Garrettson and Leonard, 1970; Leonard, 1971; Lam and Leonard, 1971, 1973; Williams, 1982). However, the efforts of extending the singular-eigenfunction approach ended up with formal complicated calculations and could not arrive at useful formulas.

Let us consider the following transport equation in a 3D infinite medium:

$$\left(\hatOmega \cdot \nabla + 1\right) \psi(r, \hatOmega) = \frac{\sigma_T}{4\pi} \int_{S^2} \psi(r, \hatOmega) \, d\hatOmega + S(r, \hatOmega),$$

where $r \in \mathbb{R}^3$, $\hatOmega \in S^2$, and $\sigma_T \in (0, 1)$ is the albedo for single scattering. Here, $\psi(r, \hatOmega)$ is the angular flux and $S(r, \hatOmega)$ is the source term. The unit vector $\hatOmega$ has the polar angle $\theta$ and azimuthal angle $\varphi$. We let $\mu$ denote the cosine of $\theta$, i.e., $\mu = \cos \theta$.

Let $\hat{k} \in \mathbb{C}^3$ be a unit vector. For a function $f(\hatOmega)$, we introduce an operator $R_{\hat{k}}$ such that $R_{\hat{k}} f(\hatOmega)$ is the value of $f$ in which $\hatOmega$ is measured in the reference frame whose $z$-axis lies in the direction of $\hat{k}$. For example, when $f(\hatOmega) = \mu$, we have

$$R_{\hat{k}} \mu = \hat{k} \cdot \hatOmega.$$ 

Such reference frames which are rotated in directions of given unit vectors $\hat{k}$ are called rotated reference frames. We define spherical harmonics by

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

where $P_l^m(\mu)$ are associated Legendre polynomials. We have the following calculation for spherical harmonics:

$$R_{\hat{k}} Y_{lm}(\hatOmega) = \sum_{m' = -l}^{l} D_{lm'}^{m} (\varphi, \theta, 0) \, Y_{lm'}(\hatOmega),$$

where $\theta$ and $\varphi$ are the polar and azimuthal angles of $\hat{k}$ in the laboratory frame, and $D_{lm'}^{m}$ are Wigner’s D-matrices (Varshalovich et al., 1988). The function $D_{lm'}^{m}(\alpha, \beta, \gamma)$, where $\alpha, \beta, \gamma$ are called the Euler angles, expresses rotation of the reference frame. If we set $\alpha = \varphi$, $\beta = \theta$, and $\gamma = 0$, we can rotate the laboratory frame to the reference frame whose $z$-axis lies in the direction of $\hat{k}$. That is, by $D_{lm'}^{m}(\varphi, \theta, 0)$, the reference frame is rotated about the original $z$-axis by $\varphi$ and then about the new $x$-axis by $\theta$. As a result, the new $z$-axis coincides with $\hat{k}$.
\( \gamma \) is non-zero, we further rotate the reference frame about the resulting \( z \)-axis by the angle \( \gamma \). We note that if we rotate the obtained rotated reference frame about the \( x \)-axis by \(-\theta_k^*\) and then rotate it on the \( x-y \) plane by \(-\varphi_k^*\), the reference frame returns to the laboratory frame. The rotated reference frame also comes back to the laboratory frame by the following successive rotations: the rotation about the new \( z \)-axis or the vector \( \mathbf{k} \) by \( \pi \), the rotation about the flipped \( x \)-axis by \( \theta_k^* \) and the rotation on the \( x-y \) plane by \( \pi - \varphi_k^* \). From the above consideration, we have

\[
Y_{lm}(\mathbf{\hat{\Omega}}) = \sum_{m'=-l}^{l} D_{m'm}^{l}(0, -\theta_k^*, -\varphi_k^*) \mathcal{R}_k Y_{lm}(\mathbf{\hat{\Omega}})
= \sum_{m'=-l}^{l} D_{m'm}^{l}(\pi, \theta_k^*, \pi - \varphi_k^*) \mathcal{R}_k Y_{lm}(\mathbf{\hat{\Omega}}).
\]

It is possible to write \( D_{m'm}^{l}(\alpha, \beta, \gamma) = e^{-im\alpha} d_{m'm}^{l}(\beta) e^{-im\gamma} \), where \( d_{m'm}^{l}(\beta) \) are called Wigner’s \( d \)-matrices. We have

\[
d_{m'm}^{l}(\beta) = \xi_{m'm} \sqrt{s!(s+m_1+m_2)!} \left( \frac{1 - \cos \beta}{2} \right)^{m_1/2} \left( \frac{1 + \cos \beta}{2} \right)^{m_2/2} P_s^{(m_1, m_2)}(\cos \beta),
\]

where \( \xi_{m'm} = 1 \) for \( m \geq m' \), \((-1)^{m-m'} \) for \( m < m' \), \( m_1 = |m'-m|, m_2 = |m'+m| \), \( s = l - (m_1 + m_2)/2 \), and the Jacobi polynomials \( P_s^{(m_1, m_2)}(\mu) \) are given by

\[
P_s^{(m_1, m_2)}(\mu) = \frac{1}{2^s} \sum_{j=0}^{s} \frac{(s+m_1)!}{(s-j)!(m_1+j)!} \frac{(s+m_2)!}{j!(s+m_2-j)!} (\mu - 1)^j (\mu + 1)^{s-j}.
\]

We note that \( d_{m'm}^{l}(\beta) = (-1)^{m'-m} d_{-m',-m}^{l}(\beta) = (-1)^{m'-m} d_{m'm}^{l}(\beta) \) and

\[
d_{00}^{l}(\beta) = 1, \quad d_{00}^{l}(\beta) = \cos \beta, \quad d_{10}^{l}(\beta) = -\frac{1}{\sqrt{2}} \sin \beta, \quad d_{1\pm1}^{l}(\beta) = \frac{1 \pm \cos \beta}{2}.
\]

2. Case’s method in three dimensions

For a unit vector \( \mathbf{k} \), we assume the following separated solutions with separation parameter \( \nu \):

\[
\psi_{\nu}(r, \mathbf{\hat{\Omega}}; \mathbf{\hat{k}}) = \Phi_{\nu}(\mathbf{\hat{\Omega}}; \mathbf{\hat{k}}) e^{-\mathbf{k} \cdot r / \nu},
\]

where the unknown function \( \Phi_{\nu}(\mathbf{\hat{\Omega}}; \mathbf{\hat{k}}) \) is normalized as

\[
\frac{1}{2\pi} \int_{S^2} \Phi_{\nu}(\mathbf{\hat{\Omega}}; \mathbf{\hat{k}}) \, d\mathbf{\hat{\Omega}} = 1.
\]

We plug the above \( \psi_{\nu}(r, \mathbf{\hat{\Omega}}; \mathbf{\hat{k}}) \) into the homogeneous equation

\[
\left( \mathbf{\hat{\Omega}} \cdot \nabla + 1 \right) \psi(r, \mathbf{\hat{\Omega}}) = \frac{\nu^2}{4\pi} \int_{S^2} \psi(r, \mathbf{\hat{\Omega}}) \, d\mathbf{\hat{\Omega}}.
\]
and obtain

\[
\left(1 - \frac{\hat{k} \cdot \hat{\Omega}}{v}\right) \Phi_v(\hat{\Omega}; \hat{k}) = \frac{\sigma}{2}.
\]  

Let us express \( \Phi_v(\hat{\Omega}; \hat{k}) \) as

\[
\Phi_v(\hat{\Omega}; \hat{k}) = R_k \phi(v, \mu),
\]

where

\[
\int_{-1}^{1} \phi(v, \mu) d\mu = 1.
\]

We will see below that \( \phi(v, \mu) \) is independent of \( \varphi \). Then, Equation (3) is written as

\[
\left(1 - \frac{R_k \mu}{v}\right) R_k \phi(v, \mu) = \frac{\sigma}{2}.
\]  

(4)

Since the right-hand side of Equation (4) is a scalar, by operating \( R_k^{-1} \), Equation (4) reduces to

\[
\left(1 - \frac{\mu}{v}\right) \phi(v, \mu) = \frac{\sigma}{2}.
\]  

(5)

The above Equation (5) is the equation appearing in 1D transport theory (Case, 1960; Case and Zweifel, 1967). This is different from the pseudo-problem approach (Williams, 1967, 1968, 1982) and the coefficients in the corresponding 1D transport equation remains constant. That is, in one dimension, Equation (5) is derived from the following equation:

\[
\left(\mu \frac{\partial}{\partial z} + 1\right) \psi(z, \mu) = \frac{\sigma}{2} \int_{-1}^{1} \psi(z, \mu) d\mu,
\]

where

\[
\psi(z, \mu) = \phi(v, \mu) e^{-z/v}.
\]

Therefore, it turns out that \( \phi(v, \mu) \) are singular eigenfunctions (Case, 1960), which are obtained as

\[
\phi(v, \mu) = \frac{\sigma v}{2} \mathcal{P} \frac{1}{v - \mu} + \lambda(v) \delta(v - \mu),
\]

where

\[
\lambda(v) = 1 - \frac{\sigma v}{2} \mathcal{P} \int_{-1}^{1} \frac{1}{v - \mu} d\mu = 1 - \sigma v \tanh^{-1}(v).
\]

The separation constant \( v \) takes values in \((-1, 1)\) in addition to \( \pm v_0 \), where \( v_0 > 1 \) is the positive root of \( \Lambda(v) \) such that \( \Lambda(v_0) = 0 \). Here, the function \( \Lambda(w) \) is defined for \( w \in \mathbb{C} \setminus [-1, 1] \) as

\[
\Lambda(w) = 1 - \frac{\sigma w}{2} \int_{-1}^{1} \frac{1}{w - \mu} d\mu.
\]  

(6)
Thus, $\nu_0$ is given as the positive solution to the transcendental equation

$$1 - \omega \nu_0 \tanh^{-1} \left( \frac{1}{\nu_0} \right) = 0.$$  

When $\omega$ is near 1, which is typical for light propagating in biological tissue, $\nu_0$ is approximately calculated as Case and Zweifel (1967)

$$\nu_0 \approx \frac{1}{\sqrt{3(1 - \omega)}}.$$  

Now, we return to eigenmodes (2) in three dimensions. We obtain

$$\psi_{\nu}(\mathbf{r}, \hat{\Omega} \hat{k}) = \mathcal{R}_k \phi(\nu, \mu) e^{-\hat{k} \cdot \mathbf{r} / \nu} = \phi(\nu, \hat{k} \cdot \hat{\Omega}) e^{-\hat{k} \cdot \mathbf{r} / \nu}.$$ (7)

The angular flux in Equation (1) is given by a superposition of eigenmodes $\psi_{\nu}(\mathbf{r}, \hat{\Omega} \hat{k})$.

So far, $\hat{k} \in \mathbb{C}^3$ has been arbitrary as long as $\hat{k} \cdot \hat{k} = 1$ is satisfied. Let us write $\hat{k} = (\hat{k}_x, \hat{k}_y, \hat{k}_z)^T$. We see that $\hat{k} \cdot \hat{k} = 1$ cannot be achieved if $\Re \hat{k}_x = \Re \hat{k}_y = \Re \hat{k}_z = 0$. Therefore, at least one component of $\hat{k}$ must have a non-zero real part. Hereafter, we consider $\hat{k}$ of the following form, so that the Green's function (10) is given as plane-wave decomposition:

$$\hat{k}(\nu, \mathbf{q}) = \begin{pmatrix} -i \nu \mathbf{q} \\ \hat{k}_z(\nu \mathbf{q}) \end{pmatrix},$$

where $\mathbf{q} \in \mathbb{R}^2$, $\mathbf{q} = \mathbf{q} \cdot |\mathbf{q}|$, and $\hat{k}_z(\nu \mathbf{q}) = \sqrt{1 + (\nu \mathbf{q})^2}$. Below, the Green's function (10) is given as a superposition of all possible $\hat{k}$ and $\nu$. It turns out that the above form of $\hat{k}(\nu, \mathbf{q})$ is enough to construct a complete set (Panasyuk et al., 2006; Kim, 2004). The present formulation is similar to the pseudo-problem approach (Williams, 1967, 1968, 1982) in the sense that Fourier transform is taken for the 2D position vector $\mathbf{r}$. However, as is seen below, the structure of the Green's function (10) becomes much simpler thanks to the use of rotated reference frames. The angles $\theta_k$ and $\varphi_k$ are introduced as

$$\hat{k}(\nu, \mathbf{q}) = \begin{pmatrix} \sin \theta_k \cos \varphi_k \\ \sin \theta_k \sin \varphi_k \\ \cos \theta_k \end{pmatrix}.$$  

We see that $\cos \theta_k = \hat{k}_z(\nu \mathbf{q})$. Moreover, we have $\sin \theta_k = \sqrt{1 - \cos^2 \theta_k} = i|\nu \mathbf{q}|$ by choosing the branch cut on the positive real axis, i.e., we have $0 \leq \Im \sqrt{z}$ for any $z \in \mathbb{C}$. We can write the vector $\mathbf{q}$ as

$$\mathbf{q} = \begin{pmatrix} \cos \varphi_q \\ \sin \varphi_q \end{pmatrix}.$$
We have \( \varphi_\kappa = \varphi_q + \pi \) (\( v > 0 \)) and \( \varphi_\kappa = \varphi_q \) (\( v < 0 \)). We can rotate the reference frame using \( \hat{\mathbf{k}} \). For this \( \hat{\mathbf{k}} \), we have

\[
\mathcal{R}_{k(v, q, u)} \mu = \sqrt{\frac{4\pi}{3}} \mathcal{R}_{k(v, q, u, \kappa)} Y_{10}(\hat{\Omega})
\]

\[
= \sqrt{\frac{4\pi}{3}} \sum_{m'=-1}^1 D_{m'0}(\varphi^*_\kappa, \theta^*_\kappa, 0) Y_{1m'}(\hat{\Omega})
\]

\[
= \sum_{m'=-1}^1 d_{m'0}^1(\theta^*_\kappa) \sqrt{(1 - m')! (1 + m')!} P_{m'}(\mu)e^{im\varphi - \varphi^*_\kappa} \cos \theta^*_\kappa \cos \theta - \sqrt{1 - \cos^2 \theta^*_\kappa} \sin \theta \cos (\varphi - \varphi^*_\kappa)
\]

\[
= \hat{k}_z(vq) \mu - ivq \sqrt{1 - \mu^2} \cos (\varphi - \varphi^*_\kappa),
\]

where we used \( P_{m}^{-1}(\mu) = \frac{1}{2} \sin \theta, \ P_{1}(\mu) = \cos \theta, \ P_{1}^{1}(\mu) = -\sin \theta, \ d_{00}^1(\theta^*_\kappa) = \cos \theta^*_\kappa \), and \( d_{\pm 10}^1(\theta^*_\kappa) = \pm \frac{1}{\sqrt{2}} \sin \theta^*_\kappa \). Similarly, we obtain

\[
\mathcal{R}_{k(v, q, u)}^{-1} \mu = \sqrt{\frac{4\pi}{3}} \mathcal{R}_{k(v, q, u)}^{-1} Y_{10}(\hat{\Omega})
\]

\[
= \sqrt{\frac{4\pi}{3}} \sum_{m'=-1}^1 D_{m'0}(0, -\theta^*_\kappa, -\varphi^*_\kappa) Y_{1m'}(\hat{\Omega})
\]

\[
= \sqrt{\frac{4\pi}{3}} \sum_{m'=-1}^1 D_{m'0}(\pi, \theta^*_\kappa, \pi - \varphi^*_\kappa) Y_{1m'}(\hat{\Omega})
\]

\[
= \sum_{m'=-1}^1 (-1)^{m'} d_{m'0}^1(\theta^*_\kappa) \sqrt{(1 - m')! (1 + m')!} P_{m'}(\mu)e^{im\varphi} \cos \theta^*_\kappa \cos \theta + \sqrt{1 - \cos^2 \theta^*_\kappa} \sin \theta \cos \varphi
\]

\[
= \hat{k}_z(vq) \mu - ivq \sqrt{1 - \mu^2} \cos \varphi.
\]

**Theorem 2.1** (Orthogonality relations (Machida, 2014, 2015)). For 3D singular eigenfunctions, we have

\[
\int_{\mathbb{S}^2} \mu \left[ \mathcal{R}_{k(v, q, u)} \phi(v, \mu) \right] \left[ \mathcal{R}_{k(v', q, u)}^{-1} \phi(v', \mu) \right] d\hat{\Omega} = 2\pi \hat{k}_z(vq) \mathcal{N}(v) \delta_{vv'}.
\]

Here, the Kronecker delta \( \delta_{vv'} \) is read as the Dirac delta function \( \delta(v - v') \) when \( v, v' \) are in the continuous spectrum \((-1, 1)\). The normalization factor \( \mathcal{N}(v) \) is from 1D transport theory and given by

\[
\mathcal{N}(v) = \begin{cases} 
\frac{\sigma}{2} v^3 \left( \frac{\sigma}{\nu + 1} - \frac{1}{\nu^2} \right), & \nu = \pm \nu_0, \\
\nu \left[ (1 - \sigma \nu \tanh^{-1}(\nu)) + \left( \frac{\nu}{2} \right)^2 \right], & \nu \in (-1, 1).
\end{cases}
\]
Proof. For fixed $\mathbf{q}$, we consider two eigenvalues $v_1$ and $v_2$. Correspondingly, we write $\mathbf{\hat{k}}_1 = \mathbf{\hat{k}}(v_1, \mathbf{q})$ and $\mathbf{\hat{k}}_2 = \mathbf{\hat{k}}(v_2, \mathbf{q})$. We multiply Equation (3) for $v_1$ by $\mathcal{R}_{\mathbf{\hat{k}}_2} \phi(v_2, \mu)$ and multiply Equation (3) for $v_2$ by $\mathcal{R}_{\mathbf{\hat{k}}_1} \phi(v_1, \mu)$. We have

$$
\left[ \mathcal{R}_{\mathbf{\hat{k}}_1} \phi(v_1, \mu) \right] \left( 1 - \frac{\mathbf{\hat{k}}_1 \cdot \mathbf{\hat{\Omega}}}{v_1} \right) \mathcal{R}_{\mathbf{\hat{k}}_1} \phi(v_1, \mu) = \frac{\sigma}{2} \mathcal{R}_{\mathbf{\hat{k}}_1} \phi(v_2, \mu),
$$

$$
\left[ \mathcal{R}_{\mathbf{\hat{k}}_1} \phi(v_1, \mu) \right] \left( 1 - \frac{\mathbf{\hat{k}}_1 \cdot \mathbf{\hat{\Omega}}}{v_2} \right) \mathcal{R}_{\mathbf{\hat{k}}_1} \phi(v_2, \mu) = \frac{\sigma}{2} \mathcal{R}_{\mathbf{\hat{k}}_1} \phi(v_1, \mu).
$$

By integrating both sides and subtracting the latter from former, we obtain

$$
\int_{S^2} \left( \frac{\mathcal{R}_{\mathbf{\hat{k}}_2} \mu}{v_2} - \frac{\mathcal{R}_{\mathbf{\hat{k}}_1} \mu}{v_1} \right) \left[ \mathcal{R}_{\mathbf{\hat{k}}_1} \phi(v_1, \mu) \right] \left[ \mathcal{R}_{\mathbf{\hat{k}}_2} \phi(v_2, \mu) \right] d\mathbf{\hat{\Omega}} = 0.
$$

Therefore,

$$
\int_{S^2} \mu \left[ \mathcal{R}_{\mathbf{\hat{k}}_1} \phi(v_1, \mu) \right] \left[ \mathcal{R}_{\mathbf{\hat{k}}_2} \phi(v_2, \mu) \right] d\mathbf{\hat{\Omega}} = 0, \quad v_1 \neq v_2.
$$

When $v_1 = v_2 = v$, we have

$$
\int_{S^2} \mu \left[ \mathcal{R}_{\mathbf{\hat{k}}} \phi(v, \mu) \right]^2 d\mathbf{\hat{\Omega}} = \int_{S^2} \left[ \mathcal{R}_{\mathbf{\hat{k}}}^{-1} \mu \right] \phi(v, \mu)^2 d\mathbf{\hat{\Omega}}
$$

$$
= 2\pi \mathbf{\hat{k}}_z(v) \int_{-1}^{1} \mu \phi(v, \mu)^2 d\mu.
$$

The proof is completed by noticing $\mathcal{N}(v) = \int_{-1}^{1} \mu \phi(v, \mu)^2 d\mu$ (Case and Zweifel, 1967).

By using 3D singular eigenfunctions, let us compute the Green's function. When the source term in Equation (1) is given by

$$
S(r, \mathbf{\hat{\Omega}}) = \delta(r)\delta(\mathbf{\hat{\Omega}} - \mathbf{\hat{\Omega}}_0),
$$

the angular flux becomes the Green's function:

$$
G(r, \mathbf{\hat{\Omega}}; \mathbf{\hat{\Omega}}_0) = \psi(r, \mathbf{\hat{\Omega}}).
$$

With some coefficients $a_{\pm}(\mathbf{q})$, $A_v(\mathbf{q})$, we can write $G(r, \mathbf{\hat{\Omega}}; \mathbf{\hat{\Omega}}_0)$ in terms of the eigenmodes $\psi_v$ in Equation (7) as

$$
G(r, \mathbf{\hat{\Omega}}; \mathbf{\hat{\Omega}}_0) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \left[ a_+(\mathbf{q}) \psi_{v_0} \left( r, \mathbf{\hat{\Omega}}; \mathbf{\hat{k}}(v_0, \mathbf{q}) \right) + a_-(\mathbf{q}) \psi_{-v_0} \left( r, \mathbf{\hat{\Omega}}; \mathbf{\hat{k}}(-v_0, \mathbf{q}) \right) + \int_{-1}^{1} A_v(\mathbf{q}) \psi_v \left( r, \mathbf{\hat{\Omega}}; \mathbf{\hat{k}}(v, \mathbf{q}) \right) dv \right] d\mathbf{q}.
$$
Since the Green’s function vanishes at infinity, particularly \( G(\mathbf{r}, \hat{\mathbf{Ω}}; \hat{\mathbf{Ω}}_0) \to 0 \) as \(|z| \to \infty\), we can write \( G(\mathbf{r}, \hat{\mathbf{Ω}}; \hat{\mathbf{Ω}}_0) \) as

\[
G(\mathbf{r}, \hat{\mathbf{Ω}}; \hat{\mathbf{Ω}}_0) = \begin{cases} 
\frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \left[ a_+ (\mathbf{q}) \psi_{v_0} (\mathbf{r}, \hat{\mathbf{Ω}}; \hat{\mathbf{k}}) + \int_0^1 A_v (\mathbf{q}) \psi_v (\mathbf{r}, \hat{\mathbf{Ω}}; \hat{\mathbf{k}}) \, dv \right] \, d\mathbf{q}, & z > 0, \\
-\frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \left[ a_- (\mathbf{q}) \psi_{-v_0} (\mathbf{r}, \hat{\mathbf{Ω}}; \hat{\mathbf{k}}) + \int_{-1}^0 A_v (\mathbf{q}) \psi_v (\mathbf{r}, \hat{\mathbf{Ω}}; \hat{\mathbf{k}}) \, dv \right] \, d\mathbf{q}, & z < 0,
\end{cases}
\]

where coefficients \( a_\pm (\mathbf{q}), A_v (\mathbf{q}) \) are determined below. We let \( \rho \in \mathbb{R}^2 \) be the position vector in the plane perpendicular to the \( z \)-axis, i.e., \( \mathbf{r} = (\rho, z) \) and \( \rho = (x, y) \). The jump condition is written as

\[
G(\rho, 0^+, \hat{\mathbf{Ω}}; \hat{\mathbf{Ω}}_0) - G(\rho, 0^-, \hat{\mathbf{Ω}}; \hat{\mathbf{Ω}}_0) = \frac{1}{\mu} \delta(\rho) \delta(\hat{\mathbf{Ω}} - \hat{\mathbf{Ω}}_0).
\]

Let us multiply \( e^{-iQ\cdot\rho} \) on both sides of the above-mentioned jump condition and integrate both sides over \( \rho \). As a result, we obtain

\[
a_\pm (\mathbf{q}) \mathcal{R}_{\hat{k}(v_0, \mathbf{q})} \phi (v_0, \mu) + a_- (\mathbf{q}) \mathcal{R}_{\hat{k}(-v_0, q)} \phi (-v_0, \mu) \\
+ \int_{-1}^1 A_v (\mathbf{q}) \mathcal{R}_{\hat{k}(v, \mathbf{q})} \phi (v, \mu) \, dv = \frac{1}{\mu} \delta(\hat{\mathbf{Ω}} - \hat{\mathbf{Ω}}_0).
\]

By using the orthogonality relations in Theorem 2.1, we can determine the coefficients as

\[
a_\pm (\mathbf{q}) = \frac{1}{2\pi \hat{k}_z (v_0 q) \mathcal{N}(v_0)} \mathcal{R}_{\hat{k}(\pm v_0, \mathbf{q})} \phi (\pm v_0, \mu_0),
\]

\[
A_v (\mathbf{q}) = \frac{1}{2\pi \hat{k}_z (v q) \mathcal{N}(v)} \mathcal{R}_{\hat{k}(v, \mathbf{q})} \phi (v, \mu_0).
\]

We note that

\[
\mathcal{R}_{\hat{k}(v, \mathbf{q})} \phi (v, \mu) = \phi \left( v, \hat{k}(v, \mathbf{q}) \cdot \hat{\mathbf{Ω}} \right).
\]

Finally, the Green’s function is obtained as Machida (2014)

\[
G(\mathbf{r}, \hat{\mathbf{Ω}}; \hat{\mathbf{Ω}}_0) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} e^{i\mathbf{q} \cdot \rho} \\
\times \left[ \frac{1}{\hat{k}_z (v_0 q) \mathcal{N}(v_0)} \phi (\pm v_0, \hat{k}(\pm v_0, \mathbf{q}) \cdot \hat{\mathbf{Ω}}) \phi (\pm v_0, \hat{k}(\pm v_0, \mathbf{q}) \cdot \hat{\mathbf{Ω}}_0) e^{i\hat{k}_z (v_0 q) z/v_0} \\
+ \int_{-1}^1 \frac{1}{\hat{k}_z (v q) \mathcal{N}(v)} \phi (\pm v, \hat{k}(\pm v, \mathbf{q}) \cdot \hat{\mathbf{Ω}}) \phi (\pm v, \hat{k}(\pm v, \mathbf{q}) \cdot \hat{\mathbf{Ω}}_0) e^{i\hat{k}_z (v q) z/v} \, dv \right] \, d\mathbf{q},
\]

where upper signs are used for \( z > 0 \) and lower signs are chosen for \( z < 0 \). We can readily extend Equation (10) to the case of anisotropic scattering (Machida, 2014).

The right-hand side of Equation (10) has the form of plane-wave decomposition. The fact implies that \( \mathcal{R}_{\hat{k}} \phi \) are complete if \( \phi \) form a complete set in the 1D transport.
theory (Panasyuk et al., 2006; Kim, 2004). The structure of the right-hand side of Equation (10) is similar to Williams (1967) and Garrettson and Leonard (1970) in the sense that Fourier transforms are used in the \((x, y)\) directions and the dependence of the integrand on \(z\) is exponentially decaying.

Let us consider the energy density \(U(\rho, z)\) for an isotropic point source \(1/4\pi \delta(r)\), i.e.,

\[
U(\rho, z) = \frac{1}{4\pi} \int \int_{S^2} G(r, \hat{\Omega}; \hat{\Omega}_0) \, d\hat{\Omega} d\hat{\Omega}_0.
\]

It is worth mentioning that the singular eigenfunctions do not appear in \(U(\rho, z)\). We have

\[
U(\rho, z) = \frac{1}{8\pi^2} \int_{\mathbb{R}^2} e^{i\mathbf{q} \cdot \rho} e^{-\hat{k}_z(vq)z/v} \left[ \frac{1}{\hat{k}_z(vq)} \mathcal{N}(v) + \int_0^1 \frac{1}{\hat{k}_z(vq)} \mathcal{N}(v) \, dv \right] \, dq.
\]

Let us suppose \(z > 0\). We note that for \(v > 0\)

\[
\int_{\mathbb{R}^2} e^{i\mathbf{q} \cdot \rho} e^{-\hat{k}_z(vq)z/v} \, dq = \frac{2\pi}{v} \int_0^\infty J_0(q\rho) \frac{e^{-z\sqrt{(1/v^2) + q^2}}}{\sqrt{(1/v^2) + q^2}} \, dq = \frac{2\pi}{v^2} \int_0^\infty J_0\left(\frac{\rho}{v}u\right) e^{-(z/v)\sqrt{u^2 + 1}} \frac{u}{\sqrt{u^2 + 1}} \, du = \frac{2\pi}{v^2} \frac{1}{\rho(v)^2 + (z/v)^2} e^{-\sqrt{(\rho/v)^2 + (z/v)^2}},
\]

where \(J_0\) is the Bessel function of the zeroth order and we used \(u = vq\). Thus, we obtain

\[
U(\rho, z) = \frac{1}{4\pi r} \left[ \frac{e^{-r/v_0}}{v_0 \mathcal{N}(v_0)} + \int_0^1 \frac{e^{-r/v}}{v \mathcal{N}(v)} \, dv \right],
\]

where \(r = \sqrt{\rho^2 + z^2}\). In some special cases such as the above \(U(\rho, z)\), it is possible to arrive at the same expression without introducing the 3D singular eigenfunctions. Indeed, in Ganapol and Kornreich (1995), Ganapol and Kornreich obtained exactly the same formula (11) using the Fourier transform and pseudo-problem. In Ganapol and Kornreich (1995), \(\int_{S^2} G(r, \hat{\Omega}; \hat{\Omega}_0) \, d\hat{\Omega}\) and the case of an isotropic line source are also calculated.

### 3. Ganapol’s Fourier-transform approach

Alternative expressions of the Green’s function (10) can be obtained with the Fourier transform. We obtain (Ishimaru, 1978)

\[
G(r, \hat{\Omega}; \hat{\Omega}_0) = \frac{1}{r^2} e^{-r} \delta\left(\hat{\Omega} - \frac{\hat{\Omega}_0}{r}\right) \delta(\hat{\Omega} - \hat{\Omega}_0)
\]

\[
+ \frac{\sigma}{2(2\pi)^2} \int_{\mathbb{R}^3} e^{ik \cdot r} \left[ 1 - \frac{\sigma}{r} \tan^{-1}(k) \right]^{-1} \, dk,
\]

(12)
where \( r = |r| \) and \( k = |k| \). The extension of Equation (12) to anisotropic scattering is also possible by using rotated reference frames (Machida, 2016). Cassell and Williams proposed an alternative expression of the Green’s function (12) by separating the once-collided term in addition to the uncollided term. This expression is more useful for benchmarking purposes (Cassell and Williams, 2000). In one dimension, Ganapol has developed an alternative Fourier-transform approach (Ganapol, 2000, 2015), which is different from the conventional derivation that yields the 1D version of Equation (12). The new formula is potentially more suitable for numerical calculation. Here, we compute the 3D Green’s function using Ganapol’s approach.

In this section, we use the source term (8). The angular flux or the Green’s function is then symmetric about the azimuthal angle. Using the Fourier transform of the Green’s function

\[
\tilde{G}(k, \hat{\Omega} ; \hat{\Omega}_0) = \int_{\mathbb{R}^3} e^{-i k \cdot r} G(r, \hat{\Omega} ; \hat{\Omega}_0) \, dr,
\]

in the Fourier space, the transport equation is written as

\[
\left( 1 + i k \cdot \hat{\Omega} \right) \tilde{G}(k, \hat{\Omega} ; \hat{\Omega}_0) = \frac{\sigma}{4\pi} \int_{\mathbb{S}^2} \tilde{G}(k, \hat{\Omega} ; \hat{\Omega}_0) \, d\hat{\Omega} + \delta(\hat{\Omega} - \hat{\Omega}_0).
\]  

Note that

\[
G(r, \hat{\Omega} ; \hat{\Omega}_0) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \tilde{G}(k, \hat{\Omega} ; \hat{\Omega}_0) e^{i k \cdot r} \, dk,
\]

has the structure of separation of variables in the sense that \( \tilde{G} \) depends on \( \hat{\Omega} \) and \( r \) exists only in \( e^{i k \cdot r} \). Keeping in mind the notation (9), let us define

\[
\tilde{\psi}_l(k) = \int_{\mathbb{S}^2} \left[ R_k P_l(\mu) \right] \tilde{G}(k, \hat{\Omega} ; \hat{\Omega}_0) \, d\hat{\Omega}.
\]  

We will use a new variable

\[
z = \frac{i}{k}.
\]

Noting the recurrence relation

\[
(2l + 1) \mu P_l(\mu) = (l + 1) P_{l+1}(\mu) + l P_{l-1}(\mu),
\]

we obtain

\[
zh_l \tilde{\psi}_l(k) - (l + 1) \tilde{\psi}_{l+1}(k) - l \tilde{\psi}_{l-1}(k) = zS_l(\hat{k}),
\]  

where

\[
h_l = 2l + 1 - \sigma \delta_{l0},
\]

and

\[
S_l(\hat{k}) = (2l + 1) R_k P_l(\mu_0) = (2l + 1) P_l(\hat{k} \cdot \hat{\Omega}_0).
\]
Chandrasekhar polynomials of the first and second kinds are defined as

\[ z h_i g_i(z) - (l + 1) g_{i+1}(z) - l g_{i-1}(z) = 0, \quad g_0(z) = 1, \quad g_1(z) = z(1 - \omega), \]

and

\[ z h_i \rho_i(z) - (l + 1) \rho_{i+1}(z) - l \rho_{i-1}(z) = 0, \quad \rho_0(z) = 0, \quad \rho_1(z) = z. \]

We can express \( \tilde{\psi}_l \) as

\[ \tilde{\psi}_l = a(z) g_i(z) + b(z) \rho_i(z) + (1 - \delta_{i0}) z \sum_{j=1}^{l} \alpha_{i,j}(z) S_j. \] (16)

By setting \( l = 0 \) in Equation (16), we first notice that

\[ a(z) = \tilde{\psi}_0. \]

By plugging Equation (16) into Equation (15), we have

\[ - [b(z) \rho_1(z) + z \alpha_{1,1}(z) S_1] = z. \]

Suppose \( l > 0 \). Let us impose

\[ z h_i \alpha_{i,j} - (l + 1) \alpha_{i+1,j} - l \alpha_{i-1,j} = 0. \] (17)

By substituting Equation (16) for \( \tilde{\psi}_l \) in Equation (15), we obtain

\[ z h_i \alpha_{i,j} S_l - (l + 1) \left( \alpha_{i+1,j} S_l + \alpha_{i+1,j+1} S_{l+1} \right) = S_l. \]

The left-hand side of the above equation can be rewritten as

\[ \text{LHS} = -(l + 1) \alpha_{i+1,j+1} S_{l+1} + l \alpha_{i-1,j} S_l. \]

Hence, we can put

\[ \alpha_{i-1,l} = \frac{1}{l}, \quad \alpha_{i+1,l+1} = 0. \] (18)

Thus, we find

\[ b(z) = -1. \]

To find \( \alpha_{i,j}(z) \), let us plug the expression \( \alpha_{i,j} = u_j g_i + v_j \rho_i \) into \( \alpha_{i,l} = 0 \) and \( \alpha_{i-1,l} = 1/l \). We obtain

\[ u_j = \frac{\rho_i}{l[g_{i-1} \rho_i - g_i \rho_{i-1}]}, \quad v_j = \frac{-g_i}{l[g_{i-1} \rho_i - g_i \rho_{i-1}]} \]

We subtract \( \rho_i [z h_i g_i - (l + 1) g_{i+1} - l g_{i-1}] = 0 \) from \( g_i [z h_i \rho_i - (l + 1) \rho_{i+1} - l \rho_{i-1}] = 0 \), and obtain

\[ (l + 1) [g_i(z) \rho_{i+1}(z) - g_{i+1}(z) \rho_i(z)] = l [g_{i-1}(z) \rho_i(z) - g_i(z) \rho_{i-1}(z)] = (l - 1) [g_{i-2}(z) \rho_{i-1}(z) - g_{i-1}(z) \rho_{i-2}(z)] = g_0(z) \rho_1(z) - g_1(z) \rho_0(z) = z. \]
Thus, we obtain
\[ z\alpha_{i,j}(z) = \rho_j(z)g_l(z) - g_j(z)\rho_l(z). \]

Finally, Equation (16) becomes
\[ \tilde{\psi}_l = g_l(z)\tilde{\psi}_0 - \chi_l(k), \quad (19) \]
where
\[ \chi_l(k) = (1 - \delta_{l0}) \sum_{j=1}^{l} \left[ \rho_l(z)g_j(z) - g_l(z)\rho_j(z) \right] S_j(\hat{k}) + \rho_l(z) \]
\[ = \sum_{j=0}^{l} \left[ \rho_l(z)g_j(z) - g_l(z)\rho_j(z) \right] S_j(\hat{k}). \quad (20) \]

To find the initial term \( \tilde{\psi}_0 \), we return to Equation (13). We obtain
\[ \tilde{G}(k, \Omega; \hat{\Omega}_0) = \frac{\sigma}{4\pi} \tilde{\psi}_0(k) + \frac{1}{1 + i\Omega \cdot \hat{\Omega}_0} \delta(\Omega - \hat{\Omega}_0). \]

Thus, we have
\[ \tilde{\psi}_1(k) = \frac{\sigma}{2} \tilde{\psi}_0(k) \int_{-1}^{1} \frac{P_l(\mu)}{1 + ik\mu} d\mu + \frac{1}{1 + i\Omega \cdot \hat{\Omega}_0} P_l(\hat{k} \cdot \hat{\Omega}_0). \]

Setting \( l = 0 \), we have
\[ [1 - \sigma L_0(z)] \tilde{\psi}_0(k) = \frac{1}{1 + ik \cdot \hat{\Omega}_0}, \]
where
\[ L_l(z) = \frac{1}{2} \int_{-1}^{1} \frac{P_l(\mu)}{1 + ik\mu} d\mu = \frac{z}{2} \int_{-1}^{1} \frac{P_l(\mu)}{z - \mu} d\mu = zQ_l(z). \]

Here, \( Q_l(z) \) is the Legendre function of the second kind which has a branch cut on \([-1, 1]\]. We obtain
\[ \tilde{\psi}_0(k) = \frac{1}{\Lambda(z)} \frac{z}{z - \hat{k} \cdot \hat{\Omega}_0}, \quad (21) \]
where we used
\[ 1 - \sigma L_0(z) = 1 - \sigma zQ_0(z) = 1 - \frac{\sigma z}{2} \ln \frac{z + 1}{z} = 1 - \sigma z \tanh^{-1} \left( \frac{1}{z} \right) = \Lambda(z). \]

The function \( \Lambda(z) \) is defined in Equation (6). We can calculate \( \tilde{\psi}_1(k) \) using Equations (19) and (21).

Equation (14) implies that the Fourier transform of the angular flux is given by
\[ \tilde{\psi}(k, \Omega) = \sum_{l=0}^{\infty} \frac{2l + 1}{4\pi} \tilde{\psi}_l(k) R_k P_l(\mu). \quad (22) \]
When the above equation is rewritten using Equation (19), the dependence of $\tilde{\psi}_0$ becomes evident as

$$\tilde{\psi}(k, \hat{\Omega}) = \phi_k(z, \hat{\Omega})\tilde{\psi}_0(k) - T_k(z, \hat{\Omega}),$$

where

$$\phi_k(z, \hat{\Omega}) = \sum_{l=0}^{\infty} \frac{2l + 1}{4\pi} g_l(z) \mathcal{R}_k P_l(\mu),$$

$$T_k(z, \hat{\Omega}) = \sum_{l=0}^{\infty} \frac{2l + 1}{4\pi} \chi_l(k) \mathcal{R}_k P_l(\mu).$$

Now, we return to the real space from the Fourier space by inverting $\tilde{\psi}(k, \hat{\Omega})$.

From Equations (19), (21), and (22), we obtain

$$\psi(r, \hat{\Omega}) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} e^{ik \cdot r} \tilde{\psi}(k, \hat{\Omega}) \, dk = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} e^{ik \cdot r} \sum_{l=0}^{\infty} \sqrt{\frac{2l + 1}{4\pi}} \left[ \mathcal{R}_k Y_l(\hat{\Omega}) \right]$$

$$\times \left[ g_l(z)\tilde{\psi}_0(k) - \chi_l(k) \right] \, dk. \quad (23)$$

Moreover from (23), we have

$$\psi(r, \hat{\Omega}) = \frac{1}{(2\pi)^3} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sqrt{\frac{2l + 1}{4\pi}} Y_{lm}(\hat{\Omega})$$

$$\times \int_{\mathbb{R}^3} e^{ik \cdot r} e^{-im\hat{\psi}_0} d_m(\theta_k) \left[ g_l(z)\tilde{\psi}_0(k) - \chi_l(k) \right] \, dk$$

$$= \frac{1}{(2\pi)^3} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{lm}(\hat{\Omega}) \int_{\mathbb{R}^3} e^{ik \cdot r} e^{-im\hat{\psi}_0} \kappa_{lm}(k) \, dk, \quad (24)$$

where

$$\kappa_{lm}(k) = \sqrt{\frac{2l + 1}{4\pi}} d_m(\theta_k) \left[ g_l(z) \frac{z}{\Lambda(z) z - \hat{k} \cdot \hat{\Omega}_0} - \chi_l(k) \right].$$

We can obtain the Green’s function (24) with this approach also in the case of anisotropic scattering (Machida, 2016).

4. Concluding remarks

Using the simple case of isotropic scattering in a 3D infinite medium, we have seen how the angular flux is obtained with rotated reference frames. In one dimension, the solution by the singular-eigenfunction approach can be derived from the
Fourier-transform approach (Ganapol, 2000, 2015). It is an interesting future problem to show the equivalence of Equations (10) and (24).

References


