Lecture 3
The Boltzmann Scattering Operator

The purpose of this lecture is to discuss transformations between the scattering frame and the laboratory frame that are useful for constructing the inscatter integral, and to demonstrate that spherical-harmonic functions are eigenfunctions of the Boltzmann scattering operator. Finally, we use this eigenfunction property to construct a useful expression for the scattering source.

1 Transformations Between Frames

We next discuss transformations between the laboratory-frame and the scattering-frame. The initial direction for a particle undergoing a scattering interaction, $\overrightarrow{\Omega}_i$, is shown in the laboratory-frame in Fig. 1. The scattering frame is obtained from the lab frame via two rotations, which have the effect of aligning the z-axis of the laboratory frame with $\overrightarrow{\Omega}_i$. The first rotation consist of a rotation about the laboratory-frame z-axis through an angle ω_i, as illustrated in Fig. 2. We refer to the intermediate frame obtained after this rotation as the "0" frame. The rotation matrix that maps the "0"-frame cosines to the lab-frame

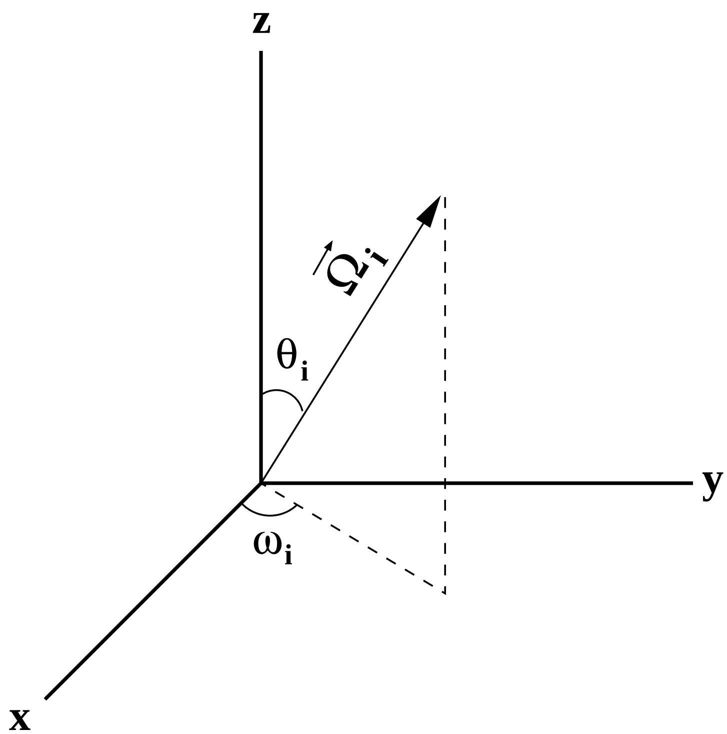

Figure 1: The initial scattering direction, $\overrightarrow{\Omega}_i$, in the laboratory frame.

cosines is

$$\begin{pmatrix} \mu \\ \eta \\ \xi \end{pmatrix} = \begin{bmatrix} \cos(\omega_i) & -\sin(\omega_i) & 0 \\ \sin(\omega_i) & \cos(\omega_i) & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{pmatrix} \mu_0 \\ \eta_0 \\ \xi_0 \end{pmatrix} . \tag{1}$$

The second rotation consists of a rotation about the y_0 axis through an angle of θ_i. This rotation is illustrated in Fig. 3. The rotation matrix that maps the scattering-frame cosines to the "0"-frame cosines is

$$\begin{pmatrix} \mu_0 \\ \eta_0 \\ \xi_0 \end{pmatrix} = \begin{bmatrix} \cos(\theta_i) & 0 & \sin(\theta_i) \\ 0 & 1 & 0 \\ -\sin(\theta_i) & 0 & \cos(\theta_i) \end{bmatrix} \begin{pmatrix} \mu_s \\ \eta_s \\ \xi_s \end{pmatrix} . \tag{2}$$

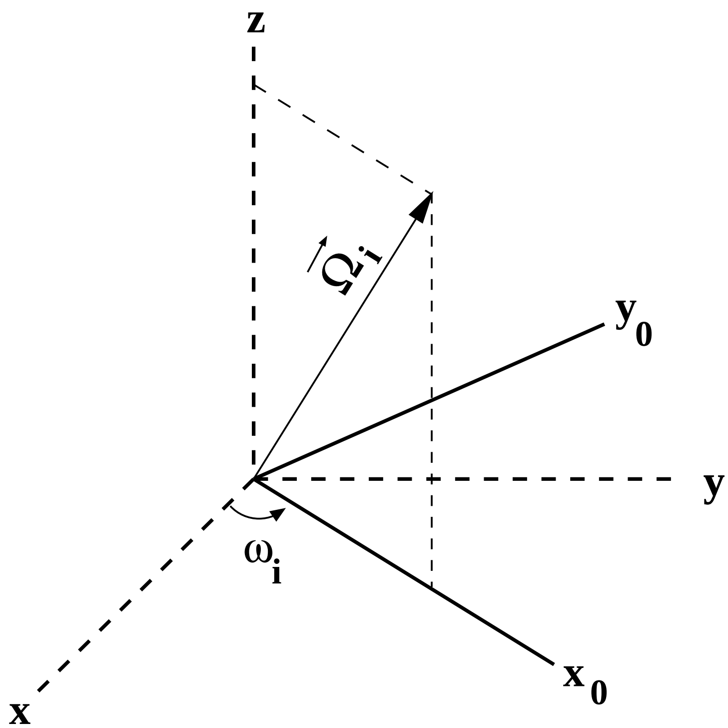

Figure 2: Rotation about the z-axis to obtain the intermediate "0" frame.

The "0"-frame cosines can be eliminated from Eq. (1) via substitution from Eq. (2) to obtain a matrix that maps the scattering-frame cosines to the lab-frame cosines:

$$\begin{pmatrix} \mu \\ \eta \\ \xi \end{pmatrix} = \begin{bmatrix} \cos(\theta_i)\cos(\omega_i) & -\sin(\omega_i) & \sin(\theta_i)\cos(\omega_i) \\ \cos(\theta_i)\sin(\omega_i) & \cos(\omega_i) & \sin(\theta_i)\sin(\omega_i) \\ -\sin(\theta_i) & 0 & \cos(\theta_i) \end{bmatrix} \begin{pmatrix} \mu_s \\ \eta_s \\ \xi_s \end{pmatrix} . \tag{3}$$

Equation (3) is useful in Monte Carlo transport simulations. It can also be used to derive relationships needed for certain non-standard forms of the inscatter source that are useful in deriving certain asymptotic transport limits.

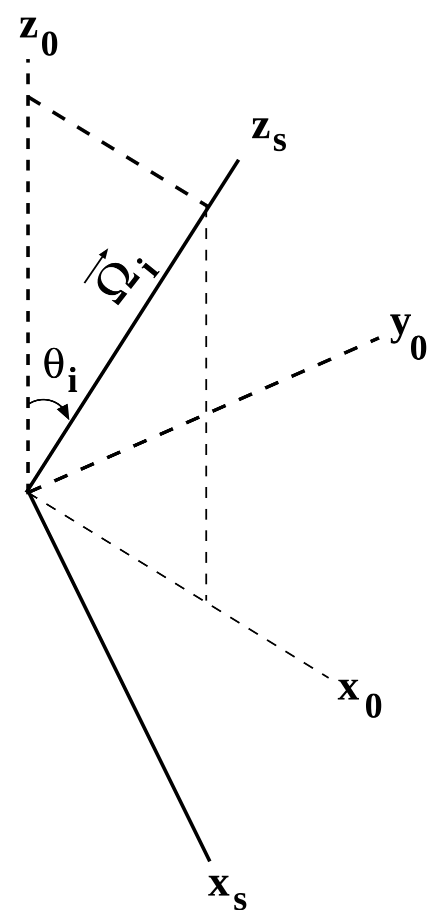

Figure 3: Rotation about the y_0-axis to obtain the scattering frame.

Because the matrix appearing in Eq. (3) is a rotation matrix, it's inverse is its transpose:

$$\begin{pmatrix} \mu_s \\ \eta_s \\ \xi_s \end{pmatrix} = \begin{bmatrix} \cos(\theta_i)\cos(\omega_i) & \cos(\theta_i)\sin(\omega_i) & -\sin(\theta_i) \\ -\sin(\omega_i) & \cos(\omega_i) & 0 \\ \sin(\theta_i)\cos(\omega_i) & \sin(\theta_i)\sin(\omega_i) & \cos(\theta_i) \end{bmatrix} \begin{pmatrix} \mu \\ \eta \\ \xi \end{pmatrix} . \tag{4}$$

Equation (4) can be used to derive $\xi_s \equiv \overrightarrow{\Omega}' \cdot \overrightarrow{\Omega}$ in terms of the ξ-cosines and azimuthal angles of any two directions, $\overrightarrow{\Omega}$ and $\overrightarrow{\Omega}'$:

$$\xi_s = \xi\xi' + \sqrt{(1-\xi)\left(1-\xi'^2\right)}\cos\left(\omega' - \omega\right) . \tag{5}$$

This expression is needed to construct the inscatter source in standard form:

$$\mathbf{S}\psi = \int_0^\infty \int_0^{2\pi} \int_{-1}^{+1} \sigma_s \left(E' \to E, \xi_s\right) \psi \left(\xi', \omega'\right) \, d\xi' \, d\omega' \, . \tag{6}$$

2 Spherical-Harmonic Eigenfunctions

We next show that the spherical-harmonic functions are the eigenfunctions of the Boltzmann scattering operator, and the composite (removal minus scattering) Boltzmann operator. We begin by defining the spherical-harmonic function of degree ℓ and order m:

$$\begin{aligned} Y_\ell^m(\overrightarrow{\Omega}) &= \sqrt{C_\ell^m} P_\ell^m(\xi) \cos(m\,\omega) \qquad , 0 \le m \le \ell, \\ &= \sqrt{C_\ell^m} P_\ell^{|m|}(\mu) \sin(|m|\,\omega) \quad , -\ell \le m < 0, \end{aligned} \tag{7}$$

where $P_\ell^m(x)$ is the associated Legendre function, ξ is the cosine of the polar angle, ω is the azimuthal angle, and

$$C_\ell^m = (2 - \delta_{m,0}) \frac{(\ell - |m|)!}{(\ell + |m|)!} \, . \tag{8}$$

The spherical-harmonic functions are orthogonal:

$$\int_0^{2\pi} \int Y_\ell^m \, Y_k^j \, d\xi d\omega = \delta_{\ell,k} \delta_{m,j} \frac{4\pi}{2\ell + 1} \, . \tag{9}$$

Furthermore, the space spanned by the harmonics of degree L, where L is any positive integer, is rotationally invariant. This means that any arbitrarily rotated harmonic of degree L can be expressed as a linear combination of harmonics of degree L. This property is unique to the spherical harmonics. There exists no other function spaces defined over the unit sphere that are rotationally invariant.

To demonstrate that the spherical harmonics are eigenfunctions of the composite Boltzmann operator, we first apply the monoenergetic version of this operator to an arbitrary spherical-harmonic function, Y_k^j:

$$\begin{aligned}(\sigma_t - \mathbf{S})\, Y_k^j &= \sigma_t Y_k^j - \mathbf{S} Y_k^j \\ &= \sigma_t Y_k^j - \int_{4\pi} \sigma_s \left(\overrightarrow{\Omega}' \cdot \overrightarrow{\Omega} \right) \, Y_k^j \left(\overrightarrow{\Omega}' \right) d\Omega' \,. \end{aligned} \tag{10}$$

Next we expand the scattering cross-section in the spherical harmonic functions of order 0, which are more commonly known as the Legendre polynomials:

$$\mathbf{S} Y_k^j = \int_{4\pi} \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} \sigma_\ell P_\ell^0 \left(\overrightarrow{\Omega}' \cdot \overrightarrow{\Omega} \right) \, Y_k^j \left(\overrightarrow{\Omega}' \right) d\Omega' \,, \tag{11}$$

where

$$\sigma_\ell = 2\pi \int_{-1}^{+1} \sigma_s \left(\xi_s \right) \, P_\ell^0 \left(\xi_s \right) \, d\xi_s \,. \tag{12}$$

Using the addition theorem to re-express $P_\ell^0 \left(\overrightarrow{\Omega}' \cdot \overrightarrow{\Omega} \right)$, we obtain:

$$P_\ell^0 \left(\overrightarrow{\Omega}' \cdot \overrightarrow{\Omega} \right) = \sum_{m=0}^{\ell} C_\ell^m P_\ell^m \left(\xi \right) P_\ell^m \left(\xi' \right) \cos \left[m \left(\omega - \omega' \right) \right] \,. \tag{13}$$

Applying the formula for the cosine of the difference of two angles to Eq. (13), we obtain

$$\begin{aligned} P_\ell^0 \left(\overrightarrow{\Omega}' \cdot \overrightarrow{\Omega} \right) &= \textstyle\sum_{m=0}^{\ell} C_\ell^m P_\ell^m \left(\xi \right) P_\ell^m \left(\xi' \right) \left[\cos(m\,\omega) \cos(m\,\omega') + \sin(m\,\omega) \sin(m\,\omega') \right] \,, \\ &= \textstyle\sum_{m=-\ell}^{\ell} Y_\ell^m \left(\overrightarrow{\Omega} \right) Y_\ell^m \left(\overrightarrow{\Omega}' \right) \,. \end{aligned} \tag{14}$$

Substituting from Eq. (14) into Eq. (11), we obtain

$$\mathbf{S}Y_k^j = \int_{4\pi} \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi}\sigma_\ell \sum_{m=-\ell}^{\ell} Y_\ell^m\left(\overrightarrow{\Omega}\right) Y_\ell^m\left(\overrightarrow{\Omega}'\right) Y_k^j\left(\overrightarrow{\Omega}'\right) d\Omega' \,. \tag{15}$$

Using the orthogonality condition expressed by Eq. (9), we find that Eq. (15) reduces to:

$$\mathbf{S}Y_k^j = \sigma_k Y_k^j\left(\overrightarrow{\Omega}\right) \,, \tag{16}$$

Equation (16) demonstrates that the spherical-harmonic function Y_k^j is an eigenfunction of the inscatter operator with eigenvalue, σ_k. Substituting from Eq. (16) into Eq. (10), we obtain the final result:

$$\left(\sigma_t - \mathbf{S}\right) Y_k^j = \left(\sigma_t - \sigma_k\right) Y_k^j \,. \tag{17}$$

Equation (17) shows that the spherical-harmonic function Y_k^j is an eigenfunction of the composite Boltzmann scattering operator with eigenvalue $\sigma_t - \sigma_k$.

3 Scattering Source Representation

The eigenfunction property of the spherical-harmonics can be exploited to construct a general expression for the inscatter source that is useful both theoretically and numerically. To derive this expression, we first expand the angular flux in spherical harmonics as follows:

$$\psi(\overrightarrow{\Omega}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} \frac{2\ell+1}{4\pi} \phi_\ell^m Y_\ell^m\left(\overrightarrow{\Omega}\right) \,. \tag{18}$$

Multiplying Eq. (18) by an arbitrary spherical harmonic, integrating over all directions, and using the orthogonality of the harmonics, we find that the expansion coefficients are angular flux moments defined as follows:

$$\phi_\ell^m = \int_{4\pi} \psi\left(\overrightarrow{\Omega}\right) Y_\ell^m\left(\overrightarrow{\Omega}\right)\, d\Omega\,. \tag{19}$$

It is tedious but straightforward to show that ϕ_0^0 is the scalar flux, ϕ_1^{-1} is the η-component of the current, ϕ_1^0 is the ξ-component of the current, and ϕ_1^1 is the μ-component of the current. Applying the inscatter operator to Eq. (18), and using Eq. (16), we obtain the desired expression for the inscatter source:

$$\mathbf{S}\psi = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell}\frac{2\ell+1}{4\pi}\sigma_\ell\phi_\ell^m Y_\ell^m\left(\overrightarrow{\Omega}\right)\,. \tag{20}$$

Although we have only considered the monoenergetic case in our derivation of the eigenvalue properties, these properties carry through in the energy-dependent case as well. In particular, in this case Eq. (18) becomes

$$\psi(\overrightarrow{\Omega},E) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell}\frac{2\ell+1}{4\pi}\phi_\ell^m(E) Y_\ell^m\left(\overrightarrow{\Omega}\right)\,, \tag{21}$$

Eq. (19) becomes

$$\phi_\ell^m(E) = \int_{4\pi} \psi\left(\overrightarrow{\Omega},E\right) Y_\ell^m\left(\overrightarrow{\Omega}\right)\, d\Omega\,, \tag{22}$$

and Eq. (20) becomes

$$\mathbf{S}\psi = \int_0^\infty \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell}\frac{2\ell+1}{4\pi}\sigma_\ell\left(E'\to E\right)\phi_\ell^m Y_\ell^m\left(\overrightarrow{\Omega}\right)\, dE', \tag{23}$$

where

$$\sigma_\ell \left(E' \rightarrow E\right) = 2\pi \int_{-1}^{+1} \sigma_s \left(E' \rightarrow E, \xi_s\right)\ P_\ell^0 \left(\xi_s\right)\ d\xi_s\,. \tag{24}$$