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Angular Discretization
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Angular Discretization

We have two main approaches to angular disrectization, the **Discrete Ordinates** method and the **Spherical Harmonics** method (which we often simplify to Legendre polynomials and thus call P_N, not to be confused with the scattering expansion).

Discrete Ordinates

The discrete ordinates approximation is a collocation method in angle. A collocation method is a solution method for ODEs, PDEs, and integral equations. Choose a finite-dimensional space of candidate solutions, such as polynomials up to a certain degree, and a number of points within the domain, called collocation points. Select the solution that satisfies the equation at those points within that space.

For us, the collocation points are the discrete angles that we choose ($\hat{\Omega} \to \hat{\Omega}_a; a = 1, \ldots, n$) and the solution space is the flux. The TE is only valid along the selected set of angles $\hat{\Omega}_a$. We apply a compatible quadrature (integration approximation) to the integral term. We write one equation for each angle in the set (dropping energy dependence and fission for simplicity; the source term contains scattering and external sources):

$$\hat{\Omega}_a \cdot \nabla \psi_a(\vec{r}) + \Sigma_t(\vec{r})\psi_a(\vec{r}) = Q_a(\vec{r})$$
$$\psi_a(\vec{r}) \equiv \psi(\vec{r}, \hat{\Omega}_a) \qquad Q_a(\vec{r}) \equiv Q(\vec{r}, \hat{\Omega}_a)$$
$$\int_{4\pi} d\hat{\Omega} = \sum_{a=1}^{n} w_a = 4\pi$$
$$\phi(\vec{r}) = \int_{4\pi} d\hat{\Omega}\, \psi(\vec{r}, \hat{\Omega}) = \sum_{a=1}^{n} w_a \psi_a(\vec{r})$$

The collection $(\hat{\Omega}_a, w_a)$ is known as the angular quadrature set. The w_a are the integration weights that go with the angles to create an integration. The angle-weight combination + number of angles dictates the accuracy of the integration. The quadrature we choose also dictates the number of unknowns. For level-symmetric quadratures, the most common types and what people usually mean by S_N, we get $n = N(N+2)$ unknowns.

However, we still need to explain what's going on in the sources. To do that, we're going to look at *Spherical Harmonics* and how they relate to Legendre Polynomials. This will allow us to do angular expansions in three dimensions (derived from the Exnihilo manual and Wikipedia).

About Spherical Harmonics

The addition theorem of Spherical Harmonics can be used to evaluate the Legendre function $P_\ell(\hat{\Omega}' \cdot \hat{\Omega})$,

$$P_\ell(\hat{\Omega}' \cdot \hat{\Omega}) = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} Y_{\ell m}(\hat{\Omega}) Y_{\ell m}^*(\hat{\Omega}') \,, \tag{1}$$

where the spherical harmonics $Y_{\ell m}$ are

$$Y_{\ell m}(\theta, \varphi) = (-1)^m \sqrt{\frac{2\ell+1}{4\pi} \frac{(\ell-m)!}{(\ell+m)!}} \, P_{\ell m}(\cos\theta) \mathrm{e}^{im\varphi} \,, \tag{2}$$

and the $P_{\ell m}$ are the *associated Legendre Polynomials*. These are the solutions to

$$(1-x^2)\frac{d^2}{dx^2}P_\ell^m(x) - 2x\frac{d}{dx}P_\ell^m(x) + \left[\ell(\ell+1) - \frac{m^2}{1-x^2}\right] P_\ell^m(x) = 0 \,,$$

where the indices ℓ and m are referred to as the degree and order of the associated Legendre polynomial, respectively. When m is zero, these functions are identical to the Legendre polynomials.

We're going to use Spherical Harmonics to expand our scattering and external source. Everything in our equations must be real; therefore, we can follow a methodology that shows expands a real-valued function using complex Spherical Harmonics (Y^* indicates complex conjugate). First, the expansion is split into positive and negative components of m:

$$P_\ell(\hat{\Omega}' \cdot \hat{\Omega}) = \frac{4\pi}{2\ell+1} \left[Y_{\ell 0}(\hat{\Omega}) Y_{\ell 0}(\hat{\Omega}') + \sum_{m=1}^{l} \big(Y_{\ell m}(\hat{\Omega}) Y_{\ell m}^*(\hat{\Omega}') + Y_{\ell -m}(\hat{\Omega}) Y_{\ell -m}^*(\hat{\Omega}') \big) \right] . \tag{3}$$

Next, we're going to go through a bunch of mathematical maneuvers to get rid of the negative m components and the complex conjugate values. The motivation is ease of analysis and handling.

First, we'll simplify the $m = 0$ term:

$$Y_{\ell 0} = \sqrt{\frac{2\ell + 1}{4\pi}}\, P_{\ell 0} = Y_{\ell 0}^{e} \,, \tag{4}$$

where we have used the idea that we can separate a spherical harmonic into even and odd components using the e^{ix} identity,

$$Y_{\ell m}^{e} = D_{\ell m} P_{\ell m} \cos(m\varphi) \,, \tag{5}$$

$$Y_{\ell m}^{o} = D_{\ell m} P_{\ell m} \sin(m\varphi) \,, \tag{6}$$

$$D_{\ell m} = (-1)^{m} \sqrt{(2 - \delta_{m0}) \frac{2\ell + 1}{4\pi} \frac{(\ell - m)!}{(\ell + m)!}} \,. \tag{7}$$

The $\sqrt{(2 - \delta_{m0})}$ term appears as an orthogonality requirement. When we expand a function in an entirely *real* basis (as opposed to the complex basis of the general spherical harmonics), the basis functions for the real basis must be orthogonal. The spherical harmonics basis functions are orthogonal, but they also contain complex components that we don't need for real physical quantities such as the scattering source. Hence, the basis functions for the real basis need to be orthogonal, which means that the integral of $\hat{Y}_{\ell m}^{e} \hat{Y}_{\ell' m'}^{e}$ over the unit sphere must give unity (with some Kronecker Deltas hanging around as well). We likewise require this orthogonality condition for the odd components. These two orthogonality statements do not give values of 1 unless the definitions contain an extra factor of $\sqrt{(2 - \delta_{m0})}$ (the δ_{m0} term appears from the orthogonality of cosines in the definition of $\hat{Y}_{lm}^{e}$).

We will make this substitution in order to satisfy the orthogonality requirement:

$$\hat{Y}_{lm}^{e} = \frac{1}{\sqrt{2 - \delta_{m0}}} Y_{lm}^{e} \,, \quad \hat{Y}_{lm}^{o} = \frac{1}{\sqrt{2 - \delta_{m0}}} Y_{lm}^{o} \,. \tag{8}$$

Because $\hat{Y}_{\ell 0}^{o} = 0$ based on the inclusion of $\sin(m\varphi)$ in its definition, the above sometimes neglects the δ_{m0} term in the odd function since it is implied that $m = 0$ leads to an identically zero function anyways.