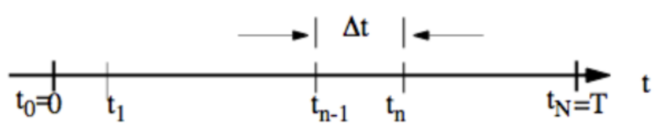
NE 255, Fa16
Equation Discretization
September 22 and 27, 2016

Start from the general time-dependent NTE without delayed neutrons, with 7 independent variables. We need to discretize each variable.

$$\begin{aligned}
\frac{1}{v}\frac{\partial \psi}{\partial t}(\vec{r}, E, \hat{\Omega}, t) + \hat{\Omega}\cdot\nabla\psi(\vec{r}, E, \hat{\Omega}, t) + \Sigma_t(\vec{r}, E)\psi(\vec{r}, E, \hat{\Omega}, t) \\
= \int_0^\infty \int_{4\pi} \Sigma_s(\vec{r}, E' \to E, \hat{\Omega}' \to \hat{\Omega})\psi(\vec{r}, E', \hat{\Omega}', t) d\hat{\Omega}' dE' \\
+ \frac{\chi_p(E)}{4\pi}\int_0^\infty \int_{4\pi} \nu(E')\Sigma_f(\vec{r}, E')\psi(\vec{r}, E', \hat{\Omega}', t) d\hat{\Omega}' dE' \\
+ S(\vec{r}, E, \hat{\Omega}, t).
\end{aligned} \tag{1}$$

Time

Discretize the time interval $[0, T]$ into N timesteps: Integrate the equation from $t = t_{n-1}$ to $t = t_n$,



where we will use the following definitions:

$$\psi(\vec{r}, E, \hat{\Omega}, t_n) = \psi_n(\vec{r}, E, \hat{\Omega})$$
$$\Delta t = t_n - t_{n-1}$$
$$\bar{\psi}(\vec{r}, E, \hat{\Omega}) = \frac{1}{\Delta t}\int_{t_{n-1}}^{t_n} dt\, \psi(\vec{r}, E, \hat{\Omega}, t)$$

(Note: we're not specifying what actually happens in the integration; we're generically defining a time-averaged angular flux).

We also need to handle the time derivative term so that we can approximate it on a time grid. We will use *First Order Backward Difference* (more on that later):

$$\frac{1}{v}\frac{\partial \psi}{\partial t}(\vec{r}, E, \hat{\Omega}, t) = \frac{1}{v}\frac{\psi_n(\vec{r}, E, \hat{\Omega}) - \psi_{n-1}(\vec{r}, E, \hat{\Omega})}{\Delta t}$$

To get the time behavior of the solution, we integrate the entire transport equation over each time step

$$\int_{t_{n-1}}^{t_n} dt\, [\cdot]$$

noting

$$\int_{t_{n-1}}^{t_n} dt\, \big(\frac{1}{v}\frac{\psi_n(\vec{r},E,\hat{\Omega})-\psi_{n-1}(\vec{r},E,\hat{\Omega})}{\Delta t}\big) = \frac{1}{v}\frac{\psi_n(\vec{r},E,\hat{\Omega})-\psi_{n-1}(\vec{r},E,\hat{\Omega})}{\Delta t}$$

which gives

$$\begin{aligned}
&\frac{1}{v}\frac{\psi_n(\vec{r},E,\hat{\Omega})-\psi_{n-1}(\vec{r},E,\hat{\Omega})}{\Delta t} + \hat{\Omega}\cdot\nabla\bar{\psi}(\vec{r},E,\hat{\Omega}) + \Sigma_t(\vec{r},E)\bar{\psi}(\vec{r},E,\hat{\Omega}) = \\
&\quad \int_0^\infty dE' \int_{4\pi} d\hat{\Omega}'\, \Sigma_s(\vec{r},E'\to E,\hat{\Omega}'\to\hat{\Omega})\bar{\psi}(\vec{r},E',\hat{\Omega}') \\
&\quad + \frac{\chi_p(E)}{4\pi}\int_0^\infty dE'\, \nu(E')\Sigma_f(\vec{r},E')\int_{4\pi} d\hat{\Omega}'\, \bar{\psi}(\vec{r},E',\hat{\Omega}') + \bar{S}(\vec{r},E,\hat{\Omega})
\end{aligned}$$

Note(!): we now have two unknowns (ψ_n and $\bar{\psi}$). We need to relate them; we choose a linear combination with a weighting parameter, β:

$$\bar{\psi} = \beta\psi_n + (1-\beta)\psi_{n-1}$$

We substitute this in to get

$$\begin{aligned}
\hat{\Omega}\cdot\nabla\bar{\psi}(\vec{r},E,\hat{\Omega}) + \big(\Sigma_t + \frac{1}{v\beta\Delta t}\big)\bar{\psi}(\vec{r},E,\hat{\Omega}) &= \frac{1}{v\beta\Delta t}\psi_{n-1}(\vec{r},E,\hat{\Omega}) \\
&+ \int_0^\infty dE' \int_{4\pi} d\hat{\Omega}'\, \Sigma_s(\vec{r},E'\to E,\hat{\Omega}'\to\hat{\Omega})\bar{\psi}(\vec{r},E',\hat{\Omega}') \\
&+ \frac{\chi_p(E)}{4\pi}\int_0^\infty dE'\, \nu(E')\Sigma_f(\vec{r},E')\int_{4\pi} d\hat{\Omega}'\, \bar{\psi}(\vec{r},E',\hat{\Omega}') + \bar{S}(\vec{r},E,\hat{\Omega})
\end{aligned}$$

We solve this for $n = 1,\ldots,N$ and ψ_0 is given (initial value problem!).

Aside about Finite Difference

Finite difference is a common way to numerically approximate derivatives. **Example** Given f is $C^2 \in [a,b]$ and $x_0 \in [a,b]$, find an approximation to $f'(x_0)$ and or $f''(x_0)$, etc.

We're going to come at this from **Taylor's theorem**, which gives an approximation of a k-times differentiable function around a given point by a k-th order Taylor polynomial.

$$f(x) = \sum_{0}^{k} \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n$$

To approximate any type of derivative to a specified order of accuracy, we Taylor expand several points in our collection. Then, we choose how many points to combine and in what ways.

$$\begin{aligned} f(x_0) &= f(x_0) \\ f(x_0 \pm h) &= f(x_0) \pm hf'(x_0) + h^2\frac{f''(x_0)}{2} \pm h^3\frac{f'''(x_0)}{6} + f^{(4)}(c_1)\frac{h^4}{24} \\ f(x_0 \pm 2h) &= f(x_0) \pm 2hf'(x_0) + 2h^2f''(x_0) \pm \frac{4}{3}h^3f'''(x_0) + \frac{2}{3}h^4f^{(4)}(c_2) \end{aligned}$$

We combine the expanded expressions, rearrange to group terms, and solve for what we want:

For $\underline{O(h)\text{ Backwards Difference}}$: combine the point and the next point backward:

$$\begin{aligned} f(x_0) &= f(x_0) \\ f(x_0 - h) &= f(x_0) - hf'(x_0) + h^2\frac{f''(c)}{2} \\ af(x_0) + bf(x_0 - h) &= f'(x_0) \\ af(x_0) + b\big(f(x_0) - hf'(x_0) + h^2\frac{f''(c)}{2}\big) &= f'(x_0) \\ (a+b)f(x_0) - bhf'(x_0) + bh^2\frac{f''(c)}{2} &= f'(x_0) \end{aligned}$$

Now, we solve for the coefficients to get what we want

$$\begin{aligned} a + b = 0 \quad &- bh = 1 \\ b = -\frac{1}{h} \quad &a = \frac{1}{h} \end{aligned}$$

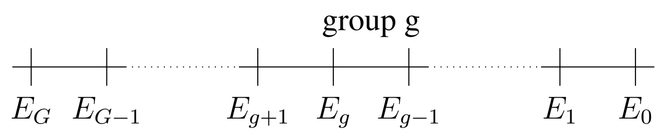
We now sub in a and b. This gives the first order ($O(h)$) Backwards Difference approximation, which is what we used for the time derivative.

$$\begin{aligned} \text{error } &= -\frac{1}{h}h^2\frac{f''(c)}{2} \\ f'(x_0) &= \frac{f(x_0) - f(x_0 - h)}{h} + \frac{1}{2}hf''(\mu) \end{aligned}$$

A note about what points to choose: you want to think about how your equations transmit information. A perturbation of the initial (or boundary) data of an *elliptic or parabolic* equation is felt at once by essentially all points in the domain. The solutions of hyperbolic equations are "wave-like." If a disturbance is made in the initial data of a hyperbolic differential equation, then not every point of space feels the disturbance at once.

Energy Discretization

We'd also like to handle the energy dimension by breaking continuous energy into groups:



We will use the following definitions:

$$\psi_g(\vec{r},\hat{\Omega}) \equiv \int_{E_g}^{E_{g-1}} dE\, \psi(\vec{r},\hat{\Omega},E) \qquad \phi_g(\vec{r}) \equiv \int_{E_g}^{E_{g-1}} dE\, \phi(\vec{r},E)$$
$$S_g(\vec{r},\hat{\Omega}) \equiv \int_{E_g}^{E_{g-1}} dE\, S(\vec{r},\hat{\Omega},E) \qquad \chi_g \equiv \int_{E_g}^{E_{g-1}} dE\, \chi(E)$$

To perform these integrals, we need to introduce approximations. We *assume the each item is separable in energy*. For example:

$$\psi(\vec{r},\hat{\Omega},E) \approx f(E)\psi_g(\vec{r},\hat{\Omega})\ , \quad E_g < E \leq E_{g-1}\ ,$$

where $f(E)$ is normalized such that $\int_g dE\, f(E) = 1$.

Before we can integrate the whole transport equation over energy, we will need a way to create multigroup cross sections. Options for how to do that in more detail are covered in NE250, so we will do the most common/generic here: weight with the angular flux,

$$\Sigma_{tg}(\vec{r}) \equiv \frac{\int_{E_g}^{E_{g-1}} dE\, \Sigma_t(\vec{r}, E) f(E)}{\int_{E_g}^{E_{g-1}} dE\, f(E)} = \frac{\int_{E_g}^{E_{g-1}} dE\, \Sigma_t(\vec{r}, E)\psi(\vec{r}, \hat{\Omega}, E)}{\int_{E_g}^{E_{g-1}} dE\, \psi(\vec{r}, \hat{\Omega}, E)}$$

similarly for fission

$$\Sigma_{s,gg'}(\hat{\Omega}' \cdot \hat{\Omega}) \equiv \frac{\int_{E_g}^{E_{g-1}} dE \int_{E'_g}^{E_{g'-1}} dE'\, \Sigma_s(E' \to E, \hat{\Omega}' \cdot \hat{\Omega}) f(E')}{\int_{E'_g}^{E_{g'-1}} dE'\, f(E')}$$
$$\equiv \frac{\int_{E_g}^{E_{g-1}} dE \int_{E'_g}^{E_{g'-1}} dE'\, \Sigma_s(E' \to E, \hat{\Omega}' \cdot \hat{\Omega}) \psi(\vec{r}, \hat{\Omega}', E')}{\int_{E'_g}^{E_{g'-1}} dE'\, \psi(\vec{r}, \hat{\Omega}', E')}$$

If we use all of those definitions and integrate the TE over energy, we get $g = 0, \ldots, G$:

$$[\hat{\Omega} \cdot \nabla + \Sigma_{tg}(\vec{r})]\psi_g(\vec{r}, \hat{\Omega}) = \sum_{g'=1}^{G} \int_{4\pi} d\hat{\Omega}'\, \Sigma_{s,gg'}(\vec{r}, \hat{\Omega}' \cdot \hat{\Omega}) \psi_{g'}(\vec{r}, \hat{\Omega}')$$
$$+ \frac{\chi_g}{4\pi} \sum_{g'=1}^{G} \nu\Sigma_{fg'}(\vec{r})\phi_{g'}(\vec{r}) + q_g(\vec{r}, \hat{\Omega})$$

Giving $G + 1$ coupled equations.

These equations are **exact** in the magical case where (1) the separability in energy holds and (2) the cross sections are constant within each energy group.

Angular Discretization

And the complicated one: angle. We have two main approaches, **Discrete Ordinates** and **Spherical Harmonics** (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 ($\hat{\Omega} \to \hat{\Omega}_a; n = 1, \ldots, n$) 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 contains scattering and external):

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

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, the most common 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).

Spherical Harmonics

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

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

where the Y_{lm} are

$$Y_{lm}(\theta, \varphi) = (-1)^m \sqrt{\frac{2l + 1}{4\pi} \frac{(l - m)!}{(l + m)!}}\, P_{lm}(\cos\theta) \mathrm{e}^{im\varphi} \,, \tag{3}$$

and the P_{lm} 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. [before we had called l n and negleced m. 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. First, the expansion is split into positive and negative components of m,

$$P_l(\hat{\Omega}'\cdot\hat{\Omega}) = \frac{4\pi}{2l+1}\Big[Y_{l0}(\hat{\Omega})Y_{l0}(\hat{\Omega}') + \sum_{m=1}^{l}\big(Y_{lm}(\hat{\Omega})Y_{lm}^*(\hat{\Omega}') + Y_{l-m}(\hat{\Omega})Y_{l-m}^*(\hat{\Omega}')\big)\Big]\,. \tag{4}$$

Examining the $m=0$ term gives the following result

$$Y_{l0} = \sqrt{\frac{2l+1}{4\pi}}\,P_{l0} = Y_{l0}^e\,, \tag{5}$$

where

$$Y_{lm}^e = D_{lm}P_{lm}\cos(m\varphi)\,, \tag{6}$$

$$Y_{lm}^o = D_{lm}P_{lm}\sin(m\varphi)\,, \tag{7}$$

$$D_{lm} = (-1)^m\sqrt{(2-\delta_{m0})\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\,. \tag{8}$$

Expanding the Spherical Harmonics into real and imaginary components, the sum over $m > 0$ becomes

$$\sum_{m=1}^{l}\Big(\hat{Y}_{lm}^e(\hat{\Omega})\hat{Y}_{lm}^e(\hat{\Omega}') + \hat{Y}_{lm}^o(\hat{\Omega})\hat{Y}_{lm}^o(\hat{\Omega}') + \hat{Y}_{l-m}^e(\hat{\Omega})\hat{Y}_{l-m}^e(\hat{\Omega}') + \hat{Y}_{l-m}^o(\hat{\Omega})\hat{Y}_{l-m}^o(\hat{\Omega}')\Big)\,, \tag{9}$$

where the imaginary terms have been set to zero because our values must be real. Using (derivation skipped for brevity)

$$\hat{Y}^e_{l-m} = (-1)^{-m}\hat{Y}^e_{lm} \equiv (-1)^m\hat{Y}^e_{lm} \text{ and} \tag{10}$$

$$\hat{Y}^o_{l-m} = -(-1)^m\hat{Y}^o_{lm} \,, \tag{11}$$

the summation becomes

$$\sum_{m=1}^{l}\Big(2\hat{Y}^e_{lm}(\hat{\Omega})\hat{Y}^e_{lm}(\hat{\Omega}') + 2\hat{Y}^o_{lm}(\hat{\Omega})\hat{Y}^o_{lm}(\hat{\Omega}')\Big) \tag{12}$$

Skipping some steps, we also have the following relationships,

$$\hat{Y}^e_{lm} = \frac{1}{\sqrt{2}}Y^e_{lm} \,, \quad \hat{Y}^o_{lm} = \frac{1}{\sqrt{2}}Y^o_{lm} \,. \tag{13}$$

After applying these equations in the $m > 0$ terms and combining with the $m = 0$ term described above, the expression for $P_l(\hat{\Omega} \cdot \hat{\Omega}')$ is

$$P_l(\hat{\Omega}' \cdot \hat{\Omega}) = \frac{4\pi}{2l+1}\Big[Y^e_{l0}(\hat{\Omega})Y^e_{l0}(\hat{\Omega}') + \sum_{m=1}^{l}\big(Y^e_{lm}(\hat{\Omega})Y^e_{lm}(\hat{\Omega}') + Y^o_{lm}(\hat{\Omega})Y^o_{lm}(\hat{\Omega}')\big)\Big] \,, \tag{14}$$

Sources

We can use these terms to expand our scattering and external sources (adding energy indexing back in) for multi-D and any degree of anisotropy. The **scattering source**:

$$q^g_s(\mathbf{r}, \hat{\Omega}) = \sum_{g'=1}^{G}\sum_{l=0}^{N}\frac{2l+1}{4\pi}\Sigma^{gg'}_{sl}(\vec{r})\int_{-1}^{1} d\mu' \; P_l(\hat{\Omega} \cdot \hat{\Omega}')\psi(\vec{r}, \hat{\Omega}') \tag{15}$$

$$q^g_s(\vec{r}, \hat{\Omega}) = \sum_{g'=0}^{G}\sum_{l=0}^{N}\Sigma^{gg'}_{s\,l}(\vec{r})\Big[Y^e_{l0}(\hat{\Omega})\phi^{g'}_{l0}(\vec{r}) + \sum_{m=1}^{l}\big(Y^e_{lm}(\hat{\Omega})\phi^{g'}_{lm}(\vec{r}) + Y^o_{lm}(\hat{\Omega})\vartheta^{g'}_{lm}(\vec{r})\big)\Big] \,, \tag{16}$$

where

$$\phi^g_{lm} = \int_{4\pi} Y^e_{lm}(\hat{\Omega})\psi^g(\hat{\Omega})\, d\hat{\Omega} \,, \quad m \geq 0 \,, \tag{17}$$

$$\vartheta^g_{lm} = \int_{4\pi} Y^o_{lm}(\hat{\Omega})\psi^g(\hat{\Omega})\, d\hat{\Omega} \,, \quad m > 0 \,. \tag{18}$$

Equation (16) is the multigroup anisotropic scattering source that is defined by the order of the Legendre expansion, P_N, of the scattering. For a given P_N order, $(N+1)^2$ moments are required to integrate the scattering operator. The moments in Eqs. (17) and (18) are the *angular flux moments* or, simply, flux moments.

Applying the same methodology gives the expansion of the **external source**

$$q_e^g((\vec{r}), \hat{\Omega}) = \sum_{l=0}^{N} \Big[Y_{l0}^e(\hat{\Omega}) q_{l0}^g(\vec{r}) + \sum_{m=1}^{l} \big(Y_{lm}^e(\hat{\Omega}) q_{lm}^g(\vec{r}) + Y_{lm}^o(\hat{\Omega}) s_{lm}^g(\vec{r}) \big) \Big] , \tag{19}$$

where the spatial dependence has been suppressed. The even and odd source moments are defined

$$q_{lm}^g = \int_{4\pi} Y_{lm}^e(\hat{\Omega}) q_e^g(\hat{\Omega}) \, d\hat{\Omega} , \quad m \geq 0 , \tag{20}$$

$$s_{lm}^g = \int_{4\pi} Y_{lm}^o(\hat{\Omega}) q_e^g(\hat{\Omega}) \, d\hat{\Omega} , \quad m > 0 . \tag{21}$$

We put alllll of that together to get

$$\begin{aligned}
&\hat{\Omega}_a \cdot \nabla \psi_a^g(\vec{r}) + \Sigma_t^g(\vec{r}) \psi_a^g(\vec{r}) = \\
&\qquad \sum_{g'=0}^{G} \sum_{l=0}^{N} \Sigma_{s\,l}^{gg'}(\vec{r}) \Big[Y_{l0}^e(\hat{\Omega}) \phi_{l0}^{g'}(\vec{r}) + \sum_{m=1}^{l} \big(Y_{lm}^e(\hat{\Omega}) \phi_{lm}^{g'}(\vec{r}) + Y_{lm}^o(\hat{\Omega}) \vartheta_{lm}^{g'}(\vec{r}) \big) \Big] \\
&\qquad + \sum_{l=0}^{N} \Big[Y_{l0}^e(\hat{\Omega}) q_{l0}^g(\vec{r}) + \sum_{m=1}^{l} \big(Y_{lm}^e(\hat{\Omega}) q_{lm}^g(\vec{r}) + Y_{lm}^o(\hat{\Omega}) s_{lm}^g(\vec{r}) \big) \Big]
\end{aligned}$$

The S_N method will be conservative if the quadrature set effectively integrates the even and odd Spherical Harmonics.

The thing that you solve for is the flux moments, and then you reconstruct that flux at the end.

Azimuthal Symmetry

This all gets simpler if we have azimuthal symmetry. In that case, $m = 0$ and

$$Y_{l0}(\theta, \varphi) = (-1)^0 \sqrt{\frac{2l+1}{4\pi} \frac{(l-0)!}{(l+0)!}} \, P_{l0}(\cos\theta) \mathrm{e}^{i0\varphi} = \frac{2l+1}{4\pi} P_l(\cos\theta),$$

then

$$
\begin{aligned}
&\hat{\Omega}_a \cdot \nabla \psi_a^g(\vec{r}) + \Sigma_t^g(\vec{r})\psi_a^g(\vec{r}) \\
&\qquad\qquad\qquad = \sum_{g'=0}^{G}\sum_{l=0}^{N} \Sigma_{s\,l}^{gg'}(\vec{r})\big(Y_l^e(\hat{\Omega})\phi_l^{g'}(\vec{r})\big) + \sum_{l=0}^{N}\big(Y_l^e(\hat{\Omega})q_l^g(\vec{r})\big) \\
&\qquad\qquad\qquad = \sum_{g'=0}^{G}\sum_{l=0}^{N} \Sigma_{s\,l}^{gg'}(\vec{r})\big(\frac{2l+1}{4\pi}P_l(\cos\theta)\phi_l^{g'}(\vec{r})\big) + \sum_{l=0}^{N}\big(\frac{2l+1}{4\pi}P_l(\cos\theta)q_l^g(\vec{r})\big)
\end{aligned}
$$

which is equivalent to what we did in the simplification class.