

Physics 511 - Lecture #6

Multipole Expansions II

General Cartesian Multipole Expansion

Taylor series 1D: $f(x+a) = f(x) + a \frac{df}{dx} + \dots + \frac{1}{l!} a^l \frac{d^l}{dx^l} f(x)$

3D $f(\vec{x}+\vec{a}) = \sum_{l=0}^{\infty} \frac{1}{l!} (\vec{a} \cdot \vec{\nabla})^l f(\vec{x})$

Let $f(\vec{x}) = \frac{1}{|\vec{x}-\vec{x}'|}$, seek Taylor series about $|\vec{x}'|=0$

$$\frac{1}{|\vec{x}-\vec{x}'|} = \sum_{l=0}^{\infty} \frac{1}{l!} (-\vec{x}' \cdot \vec{\nabla})^l \frac{1}{r} = \frac{1}{r} - x'_i \partial_i \frac{1}{r} + \frac{1}{2} (x'_i x'_j \partial_i \partial_j) \frac{1}{r} + \dots + \frac{(-1)^l}{l!} \underbrace{(x'_{i_1} x'_{i_2} \dots x'_{i_l})}_{\substack{l^{\text{th}} \text{ rank tensor} \\ \text{outer product } \vec{x}' \vec{x}' \dots \vec{x}'}} \underbrace{(\partial_{i_1} \partial_{i_2} \dots \partial_{i_l} \frac{1}{r})}_{T_{i_1 \dots i_l}}$$

Eg. $T_{ij} = \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} \frac{1}{r} = \frac{\partial}{\partial x_i} \left(\frac{-x_j}{r^3} \right) = \frac{3x_i x_j - \delta_{ij} r^2}{r^5}$

Note $T_{ij} = T_{ji}$ $\text{Trace}(T_{ij}) = 0 \Rightarrow T_{ij}$ are irreducible

Generally $T_{i_1 \dots i_l}$ is a rank l irreducible tensor

Trace over any two indices say $i_1 = i_2$ $\frac{\partial}{\partial x_{i_3}} \dots \frac{\partial}{\partial x_{i_l}} \nabla^2 \frac{1}{r} = 0$

But $\nabla^2 \frac{1}{r} = 0$ away from charge distribution

$$\Rightarrow \text{Tr}(T_{i_1 \dots i_l}) = 0$$

$$\text{Now } \frac{1}{|\vec{x} - \vec{x}'|} = \sum_{\ell} \frac{(-1)^{\ell}}{\ell!} \text{Tr}(\underline{P} \underline{T})$$

But since \underline{T} is irreducible need only keep irreducible part of \underline{P}

$$P_{ij}^{(2)} = P_{ij} - \frac{\delta_{ij}}{3} \text{Tr}(P_{ij}) = x'_i x'_j - \frac{1}{3} r'^2 \delta_{ij}$$

etc.

Generally $P_{i_1 \dots i_{\ell}}^{(\ell)} = [x'_{i_1} \dots x'_{i_{\ell}}]^{(\ell)}$ (ℓ^{th} irreducible part)

Also, one can show: $T_{i_1 \dots i_{\ell}}^{(\ell)} = \frac{(-1)^{\ell} (2\ell-1)!! [x_{i_1} \dots x_{i_{\ell}}]^{(\ell)}}{r^{2\ell+1}}$

$$(\ell!! \equiv \ell(\ell-2)\dots 1)$$

$$\Rightarrow \frac{1}{|\vec{x} - \vec{x}'|} = \sum_{\ell} \frac{(2\ell-1)!!}{\ell!} \frac{[x'_{i_1} \dots x'_{i_{\ell}}]^{(\ell)} [x_{i_1} \dots x_{i_{\ell}}]^{(\ell)}}{r^{2\ell+1}}$$

$$\Rightarrow \phi(\vec{x}) = \sum_{\ell} \frac{1}{\ell!} \frac{Q_{i_1 \dots i_{\ell}}^{(\ell)} [x_{i_1} \dots x_{i_{\ell}}]^{(\ell)}}{r^{2\ell+1}}$$

$$= \sum_{\ell} \frac{1}{\ell!} Q_{i_1 \dots i_{\ell}}^{(\ell)} \frac{x_{i_1} x_{i_2} \dots x_{i_{\ell}}}{r^{2\ell+1}}$$

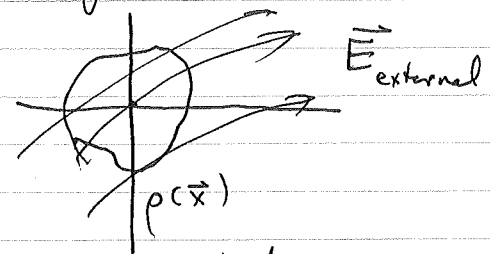
$\binom{2\ell}{\ell}$ -pole tensor

$$Q_{i_1 i_2 \dots i_{\ell}}^{(\ell)} = (2\ell-1)!! \int d^3x \rho(\vec{x}) [x_{i_1} x_{i_2} \dots x_{i_{\ell}}]^{(\ell)}$$

General Cartesian expansion

Multipole expansion of the interaction energy

Charge distribution in an external field



$$U = \int \rho(\vec{x}) \Phi(\vec{x}) d^3x$$

$$\nabla^2 \Phi(\vec{x}) = 0 \text{ external}$$

Charge distribution localized at origin

⇒ Expand $\Phi(\vec{x})$ as a Taylor series at origin

$$\Phi(\vec{x}) = \Phi(0) + \vec{x} \cdot \vec{\nabla} \Phi|_0 + \dots + \frac{1}{l!} (x_{i_1} \dots x_{i_l}) \underbrace{(\partial_{i_1} \dots \partial_{i_l} \Phi)|_0}_{\text{irreducible}}$$

$$= \sum_{l=0}^{\infty} \frac{1}{l!} [x_{i_1} \dots x_{i_l}]^{(l)} (\partial_{i_1} \partial_{i_2} \dots \partial_{i_l} \Phi)|_0$$

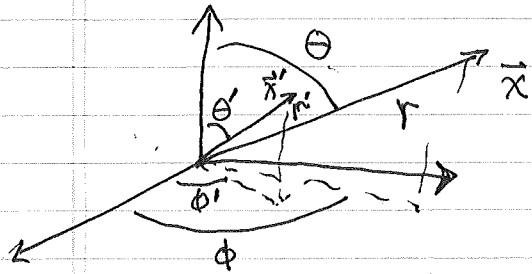
$$\Rightarrow U = \sum_l \frac{1}{l!} \left(\int \rho(\vec{x}) [x_{i_1} \dots x_{i_l}]^{(l)} d^3x \right) (\partial_{i_1} \dots \partial_{i_l} \Phi)|_0$$

$\underbrace{\hspace{10em}}_{\frac{1}{(2l-1)!!} Q_{i_1 \dots i_l}^{(l)}}$

$$\Rightarrow U = \sum_l \frac{1}{l! (2l-1)!!} Q_{i_1 \dots i_l}^{(l)} (\partial_{i_1} \dots \partial_{i_l} \Phi)|_0$$

$$= q_{\text{net}} \Phi(0) + Q_i^{(1)} \underbrace{\partial_i \Phi|_0}_{-\vec{E}(0)} + \frac{1}{6} Q_{ij} \partial_i \partial_j \Phi|_0$$

$$U = q_{\text{net}} \Phi(0) - \vec{p} \cdot \vec{E}(0) - \frac{1}{6} Q_{ij} \frac{\partial E_i}{\partial x_j}|_0 + \dots$$

Spherical multipoles

"Addition theorem"
(Jackson 3.70)

$$\frac{1}{|\vec{x} - \vec{x}'|} = \sum_{l=0}^{\infty} \frac{4\pi}{2l+1} \frac{r'^l}{r^{l+1}} \sum_{m=-l}^l Y_{l,m}^*(\theta', \phi') Y_{l,m}(\theta, \phi)$$

$r > r'$

$Y_{l,m}(\theta, \phi)$: "Spherical Harmonics"

Angular part of a "harmonic function" $\nabla^2 \phi = 0$

$$\phi(r, \theta, \phi) = R_l(r) Y_{l,m}(\theta, \phi)$$

$$\nabla^2 = - \left(\hat{p}_r^2 + \frac{\hat{L}^2}{r^2} \right)$$

\hat{p}_r → radial derivative
 \hat{L}^2 ← angular derivative

$$\hat{L} = \frac{1}{i} \vec{r} \times \vec{\nabla}$$

Angular momentum operator

$$\hat{L}^2 Y_{l,m}(\theta, \phi) = l(l+1) Y_{l,m}(\theta, \phi)$$

$$\hat{L}_z Y_{l,m}(\theta, \phi) = m Y_{l,m}(\theta, \phi)$$

$Y_{l,m}$'s are eigenstates
of rotation about z-axis
 $-l \leq m \leq l \Rightarrow 2l+1$

$$\hat{R}_z(\phi_0) Y_{l,m}(\theta, \phi) = e^{i m \phi_0} Y_{l,m}(\theta, \phi)$$

Orthogonality:

$$\int d\Omega Y_{l',m'}^*(\theta, \phi) Y_{l,m}(\theta, \phi) = \delta_{l,l'} \delta_{m,m'}$$

$$d\Omega = \sin\theta d\theta d\phi = d(\cos\theta) d\phi$$

$-\pi \leq \theta \leq \pi \quad 0 \leq \phi \leq 2\pi \quad -1 \leq \cos\theta \leq 1$

$Y_{l,m}(\theta, \phi)$ for a "complete" set

General expression for $Y_{l,m}(\theta, \phi)$

$$Y_{l,m}(\theta, \phi) = \left(\begin{smallmatrix} \text{norm.} \\ \text{const.} \end{smallmatrix} \right) P_l^m(\cos\theta) e^{im\phi}$$

$P_l^m(\cos\theta)$: Associated Legendre polynomials

$m=0$ $P_l(\mu)$: Legendre polynomial (Jackson ~~3.15~~ ^{3.15})

Examples of $Y_{l,m}$'s

$m \setminus l$	0	1	2
2			$\sqrt{\frac{15}{32\pi}} \sin^2\theta e^{2i\phi}$
1		$-\sqrt{\frac{3}{8\pi}} \sin\theta e^{i\phi}$	$\sqrt{\frac{15}{2\pi}} \sin 2\theta e^{i\phi}$
0	$\frac{1}{\sqrt{4\pi}}$	$\sqrt{\frac{3}{4\pi}} \cos\theta$	$\sqrt{\frac{5}{16\pi}} (3\cos^2\theta - 1)$

Spherical moments

$$\phi(\vec{x}) = \int \frac{\rho(\vec{x}') d^3x'}{|\vec{x} - \vec{x}'|} = \sum_{l=0}^{\infty} \sum_{m=-l}^l \frac{4\pi}{2l+1} q_{l,m} \frac{Y_{l,m}(\theta, \phi)}{r^{l+1}}$$

$$q_{l,m} = \int r'^2 dr' d\Omega' \rho(r', \theta', \phi') r'^l Y_{l,m}^*(\theta', \phi')$$

2^l -pole potential

$$\phi_{l,m}(\theta, \phi) = \frac{4\pi}{2l+1} \frac{Y_{l,m}(\theta, \phi)}{r^{l+1}}$$

Special case: Azimuthal symmetry $\rho(r, \theta)$ independent of ϕ

$$\Rightarrow g_{\ell, m} = 0 \text{ unless } m = 0$$

$$\phi(\vec{x}) = \sum_{\ell=0}^{\infty} \frac{4\pi}{2\ell+1} g_{\ell, 0} \frac{Y_{\ell, 0}(\theta, \phi)}{r^{\ell+1}}$$

$$Y_{\ell, 0}(\theta, \phi) = \sqrt{\frac{2\ell+1}{4\pi}} P_{\ell}(\cos\theta) \quad g_{\ell, 0} = \sqrt{\frac{2\ell+1}{4\pi}} \int r^2 dr d\Omega \rho(r, \theta) r^{\ell} P_{\ell}(\cos\theta)$$

$$\Rightarrow \phi(\vec{x}) = \sum_{\ell=0}^{\infty} Q^{(\ell)} \frac{P_{\ell}(\cos\theta)}{r^{\ell+1}}$$

One number for (2ℓ) th pole: $Q^{(\ell)} = 2\pi \int r^2 dr d\phi \rho(r, \theta) r^{\ell} P_{\ell}(\cos\theta)$

Example: Quadrupole moment for azimuthal symmetry

$$\phi^{(2)}(\vec{x}) = Q^{(2)} \frac{P_2(\cos\theta)}{r^3} = Q^{(2)} \left(\frac{3\cos^2\theta - 1}{2r^3} \right)$$

In Cartesian expansion: $\phi^{(2)}(\vec{x}) = \frac{1}{2} Q_{ij} \frac{x_i x_j}{r^5}$

$$Q_{ij} = Q_{zz} \begin{bmatrix} -\frac{1}{2} & 0 & 0 \\ 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{One number}$$

$$\Rightarrow \phi^{(2)}(\vec{x}) = \frac{Q_{zz}}{2r^5} (-x^2 - y^2 + z^2) = \frac{1}{2} \frac{Q_{zz}}{r^3} \left(\frac{3\cos^2\theta - 1}{2} \right)$$

$$\text{So } Q^{(\ell)} = \frac{1}{2} Q_{zzz}$$

$$\text{Generally } Q^{(\ell)} = \frac{1}{\ell!} Q_{\ell 3 3 \dots 3}$$

General relationship between Cartesian & Spherical moments

• Cartesian: $\frac{1}{|\vec{x} - \vec{x}'|} = \sum_{l=0}^{\infty} \frac{(2l-1)!!}{l!} \frac{[x'_1 x'_2 \dots x'_{il}]^{(l)}}{r^{2l+1}} [x_{i_1} \dots x_{i_l}]^{(l)}$

• Spherical: $\frac{1}{|\vec{x} - \vec{x}'|} = \sum_{l=0}^{\infty} \frac{4\pi}{2l+1} \sum_{m=-l}^l \frac{(r'^l Y_{l,m}^*(\theta', \phi')) (r^l Y_{l,m}(\theta, \phi))}{r^{2l+1}}$

Define: "Solid Harmonic" $y_{lm}(r, \theta, \phi) = r^l Y_{l,m}(\theta, \phi)$

Polynomial in x, y, z of order l
 invariant (up to a phase) under rotations about z

The $2l+1$ independent elements of irreducible tensor $[x_{i_1} x_{i_2} \dots x_{i_l}]^{(l)}$ are linear combinations of the $Y_{l,m}$ s!

Spherical basis $\left\{ \begin{aligned} \bar{e}_+ &\equiv \frac{1}{\sqrt{2}}(\bar{e}_x + i\bar{e}_y), & \bar{e}_0 &\equiv \bar{e}_z \\ x + iy &\equiv x_+, & x - iy &\equiv x_-, & z &\equiv x_0 \end{aligned} \right\}$

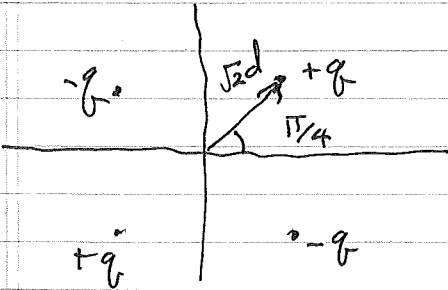
Under rotation about z -axis $R_\phi x_q = e^{-iq\phi} x_q$

Solid Harmonics $r^l Y_{l,m}(\theta, \phi) = \sum (x+iy)^{m_1} (x-iy)^{m_2} z^{m_3} a_{(m_1, m_2, m_3)}$
 $m_1 - m_2 = m, \quad m_1 + m_2 + m_3 = l$

Example:

$$x + iy = r \sin\theta (\cos\phi + i \sin\phi) \approx r \sin\theta e^{i\phi} \approx r Y_{1,1}(\theta, \phi)$$

Example: Calculating Spherical multipoles



$$q_{00} = 0$$

$$q_{1,\pm 1} \approx \sum_{\alpha} q_{\alpha} r_{\alpha} \sin \theta_{\alpha} e^{\pm i \phi_{\alpha}} = 0$$

$$q_{1,0} \approx \sum_{\alpha} q_{\alpha} r_{\alpha} \cos \theta_{\alpha} = 0$$

$\theta_{\alpha} = \pi/2$

First non-vanishing multipole: $q_{l,m}$ $l=2$

$$\begin{aligned} q_{2,2} &= \sum_{\alpha} q_{\alpha} r_{\alpha}^2 Y_{2,2}^*(\theta_{\alpha}, \phi_{\alpha}) = \sqrt{\frac{15}{32\pi}} \sum_{\alpha} q_{\alpha} (x_{\alpha} - iy_{\alpha})^2 \\ &= \sqrt{\frac{15}{32\pi}} \sum_{\alpha} q_{\alpha} \frac{r_{\alpha}^2 \sin^2 \theta_{\alpha}}{2d^2} e^{-2i\phi_{\alpha}} \end{aligned}$$

$\hookrightarrow (2d^2 \text{ for all charges})$

$$= \sqrt{\frac{15}{32\pi}} 2qd^2 \begin{pmatrix} e^{-i\pi/2} & e^{+i\pi/2} & -e^{-i3\pi/2} & +e^{+i3\pi/2} \\ (-i) & (+i) & -(-i) & +(-i) \end{pmatrix}$$

$$\Rightarrow q_{2,2} = \sqrt{\frac{15}{32\pi}} -4iqd^2 = q_{2,-2}^*$$

$$q_{2,1} = \sum_{\alpha} q_{\alpha} r_{\alpha}^2 Y_{2,1}^*(\theta, \phi) \approx \sum_{\alpha} q_{\alpha} (x_{\alpha} + iy_{\alpha})^* z_{\alpha} = 0$$

$$q_{2,0} = \sum_{\alpha} q_{\alpha} r_{\alpha}^2 Y_{2,0}^*(\theta, \phi) = \sqrt{\frac{5}{16\pi}} \sum_{\alpha} q_{\alpha} r_{\alpha}^2 (3\cos^2 \theta_{\alpha} - 1) = 0$$

$$\therefore \phi(\vec{x}) = \frac{4\pi}{2(1+1)} \left(q_{2,2} \frac{Y_{2,2}(\theta, \phi)}{r^3} + q_{2,-2} \frac{Y_{2,-2}(\theta, \phi)}{r^3} \right)$$

$$= \frac{4\pi}{5} \cdot 2\text{Re}(q_{2,2} Y_{2,2}(\theta, \phi)) = \frac{8\pi}{5} \sqrt{\frac{15}{32\pi}} 4q \text{Re}(-i Y_{2,2}(\theta, \phi))$$

$$= 6qd^2 \frac{\sin^2 \theta \sin 2\phi}{r^3} = 12qd^2 \frac{xy}{r^5} \quad \checkmark$$

(#6.9)

Relationships between
Cartesian and spherical Multipoles:

$$q_{lm} = \int d^3x \rho(\vec{x}) y_{lm}^*(\vec{x})$$

$$y_{0,0}(\vec{x}) = \frac{1}{\sqrt{4\pi}}$$

$$y_{1,\pm 1}(\vec{x}) = \mp \sqrt{\frac{3}{8\pi}} (x \pm iy)$$

$$y_{1,0}(\vec{x}) = \sqrt{\frac{3}{4\pi}} z$$

$$y_{2,\pm 2}(\vec{x}) = \sqrt{\frac{15}{32\pi}} (x \pm iy)^2 = \sqrt{\frac{15}{32\pi}} (x^2 - y^2 \pm 2ixy)$$

$$y_{2,\pm 1}(\vec{x}) = \mp \sqrt{\frac{15}{8\pi}} (x \pm iy)z = \mp \sqrt{\frac{15}{8\pi}} (xz \pm iy_z)$$

$$y_{2,0}(\vec{x}) = \sqrt{\frac{5}{16\pi}} (3z^2 - r^2)$$

$$\therefore q_{00} = \frac{1}{\sqrt{4\pi}} q$$

$$q_{1,\pm 1} = \mp \sqrt{\frac{3}{8\pi}} (p_x \pm ip_y), \quad q_{1,0} = \sqrt{\frac{3}{4\pi}} p_z$$

$$q_{2,\pm 2} = \frac{1}{3} \sqrt{\frac{15}{32\pi}} (Q_{xx} - Q_{yy} \pm 2i Q_{xy})$$

$$q_{2,\pm 1} = \mp \frac{1}{3} \sqrt{\frac{15}{8\pi}} (Q_{xz} - i Q_{yz})$$

$$q_{2,0} = \sqrt{\frac{5}{16\pi}} Q_{zz}$$