Physics 571 - Lecture # 6

Multipole Expansions II

General Cartesian Multipole Expansion

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

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

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

$$\frac{1}{|\vec{x}-\vec{x}'|} = \sum_{\ell=0}^{\infty}\frac{1}{\ell!}(-\vec{x}'\cdot\vec{\nabla})^\ell \frac{1}{r} = \frac{1}{r} - x_i'\partial_i\frac{1}{r} + \frac{1}{2}(x_i'x_j'\partial_i\partial_j)\frac{1}{r}$$

$$+ \cdots + \frac{(-1)^\ell}{\ell!}\underbrace{(x_{i_1}'x_{i_2}'\cdots x_{i_\ell}')}_{P_{i_1 i_2\cdots i_\ell}}\underbrace{\left(\partial_{i_1}\partial_{i_2}\cdots\partial_{i_\ell}\frac{1}{r}\right)}_{T_{i_1\cdots i_\ell}}$$

ℓ^{th} rank tensor outer product $\vec{x}'\vec{x}'\cdots\vec{x}'$ $\longrightarrow P_{i_1 i_2\cdots i_\ell}$

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

Note $T_{ij} = T_{ji}$ $\quad$ $\mathrm{Trace}(T_{ij}) = 0$ $\Rightarrow T_{ij}$ are <u>irreducible</u>

Generally $T_{i_1\cdots i_\ell}$ is a rank ℓ irreducible tensor

Trace over <u>any</u> two indicies (say $i_1 = i_2$) $\quad \frac{\partial}{\partial x_{i_3}}\cdots\frac{\partial}{\partial x_{i_\ell}}\nabla^2\frac{1}{r} = 0$

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

$\Rightarrow \mathrm{Tr}(T_{i_1\cdots i_\ell}) = 0$

Now $\frac{1}{|\vec{x}-\vec{x}'|} = \sum_{\ell}' \frac{(-1)^\ell}{\ell!} \mathrm{Tr}(\underset{\approx}{P}\,\underset{\approx}{T})$

But since $\underset{\approx}{T}$ is irreducible need only keep <u>irreducible</u> part of $\underset{\approx}{P}$

$$P_{ij}^{(2)} = P_{ij} - \frac{\delta_{ij}}{3}\mathrm{Tr}(P_{ij}) = x_i' x_j' - \frac{1}{3} r'^2 \, \delta_{ij}$$

etc.

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

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

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

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

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

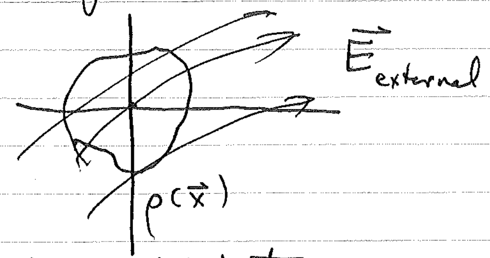
$$= \sum_\ell \frac{1}{\ell!} Q^{(\ell)}_{i_1 \cdots i_\ell} \frac{x_{i_1} x_{i_2} \cdots x_{i_\ell}}{r^{2\ell+1}}$$

$(2^{\ell})^{th}$-pole tensor $\boxed{Q^{(\ell)}_{i_1 i_2 \cdots i_\ell} = (2\ell-1)!! \int d^3x \, \rho(\vec{x}) \, [x_{i_1} x_{i_2} \cdots x_{i_\ell}]^{(\ell)}}$

General Cartesian expansion

Multipole expansion of the interaction energy

Charge distribution in an external field



Charge distribution localized at origin

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

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

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

$$\Phi(\vec{x}) = \Phi(0) + \vec{x}\cdot\vec{\nabla}\phi\Big|_0 + \cdots \frac{1}{\ell!}(x_{i_1}\cdots x_{i_\ell})\underbrace{\left(\partial_{i_1}\cdots\partial_{i_\ell}\Phi\right)}_{\text{irreducible}}\Big|_0$$

$$= \sum_{\ell=0}^{\infty} \frac{1}{\ell!}\,[x_{i_1}\cdots x_{i_\ell}]^{(\ell)}\left(\partial_{i_1}\partial_{i_2}\cdots\partial_{i_\ell}\Phi\right)\Big|_0$$

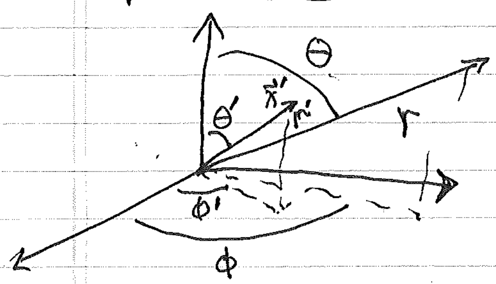
$$\Rightarrow U = \sum_\ell \frac{1}{\ell!}\underbrace{\left(\int \rho(\vec{x})\,[x_{i_1}\cdots x_{i_\ell}]^{(\ell)}\,d^3x\right)}_{\frac{1}{(2\ell-1)!!}Q^{(\ell)}_{i_1\cdots i_\ell}}\left(\partial_{i_1}\cdots\partial_{i_\ell}\Phi\right)\Big|_0$$

$$\Rightarrow U = \sum_\ell \frac{1}{\ell!\,(2\ell-1)!!}\,Q^{(\ell)}_{i_1\cdots i_\ell}\left(\partial_{i_1}\cdots\partial_{i_\ell}\Phi\right)\Big|_0$$

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

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

Spherical multipoles



"Addition theorem"
(Jackson 3.70)

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

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

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

$$\phi(r,\theta,\phi) = R_\ell(r)\, Y_{\ell,m}(\theta,\phi)$$

$$\nabla^2 = -\Big(\underbrace{\hat{p}_r^2}_{\text{radial derivative}} + \frac{\hat{L}^2}{r^2}\Big) \quad \leftarrow \text{angular derivative}$$

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

Angular momentum operator

$$\boxed{\begin{aligned} \hat{L}^2\, Y_{\ell,m}(\theta,\phi) &= \ell(\ell+1)\, Y_{\ell,m}(\theta,\phi) \\ \hat{L}_z\, Y_{\ell,m}(\theta,\phi) &= m\, Y_{\ell,m}(\theta,\phi) \end{aligned}}$$

$Y_{\ell,m}$'s are eigenstates of rotation about z-axis

$-\ell \le m \le \ell \Rightarrow 2\ell+1$

$$\hat{R}_z(\phi_0)\, Y_{\ell,m}(\theta,\phi) = e^{-im\phi_0}\, Y_{\ell,m}(\theta,\phi)$$

Orthogonality:

$$\int d\Omega\, Y^*_{\ell',m'}(\theta,\phi)\, Y_{\ell,m}(\theta,\phi) = \delta_{\ell,\ell'}\, \delta_{mm'}$$

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

$-\pi \le \theta \le \pi \qquad 0 \le \phi \le 2\pi \qquad -1 \le \cos\theta < 1$

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

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

$$Y_{\ell,m}(\theta,\phi) = \begin{pmatrix}\text{norm.}\\ \text{const.}\end{pmatrix} P_\ell^m(\cos\theta)\, e^{im\phi}$$

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

$m=0$ $\quad P_\ell(\mu)$: Legendre polymial (Jackson 3.15)

Examples of $Y_{\ell,m}$'s

$m \backslash \ell$	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

$$\boxed{\begin{gathered}\phi(\vec{x}) = \int \frac{\rho(\vec{x}')\,d^3x'}{|\vec{x}-\vec{x}'|} = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} \frac{4\pi}{2\ell+1}\, q_{\ell,m}\, \frac{Y_{\ell,m}(\theta,\phi)}{r^{\ell+1}} \\[2em] q_{\ell,m} = \int r'^2\,dr'\,d\Omega'\,\rho(r',\theta',\phi')\, r'^{\ell}\, Y^*_{\ell,m}(\theta',\phi')\end{gathered}}$$

2^ℓ-pole potential $\quad \boxed{\phi_{\ell,m}(\theta,\phi) = \frac{4\pi}{2\ell+1}\frac{Y_{\ell,m}(\theta,\phi)}{r^{\ell+1}}}$

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

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

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

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

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

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

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

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

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

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

$$\text{Generally} \quad Q^{(\ell)} = \frac{1}{\ell!} Q_{33\ldots3}$$

General relationship between Cartesian + Spherical moments

- Cartesian: $$\frac{1}{|\vec{x}-\vec{x}'|} = \sum_{\ell=0}^{\infty}{}' \frac{(2\ell-1)!!}{\ell!} \sum_{i_1 i_2 \cdots i_\ell}{}' \frac{[x'_{i_1} x'_{i_2} \cdots x'_{i_\ell}]^{(\ell)} [x_{i_1} \cdots x_{i_\ell}]^{(\ell)}}{r^{2\ell+1}}$$

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

Define: "Solid Harmonic" $\mathcal{Y}_{\ell m}(r,\theta,\phi) = r^{\ell}\, Y_{\ell,m}(\theta,\phi)$

Polynomial in x, y, z of order ℓ

invariant (up to a phase) under rotations about z

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

Spherical basis $\left\{ \begin{array}{l} \vec{e}_{\pm} = \mp(\vec{e}_x \pm i\vec{e}_y)/\sqrt{2}, \quad \vec{e}_0 = \vec{e}_z \\ x+iy \equiv x_+, \quad x-iy \equiv x_-, \quad z \equiv x_0 \end{array} \right\}$

Under rotation about z-axis $R_{\phi_0}\, x_q = e^{-iq\phi_0} x_q$

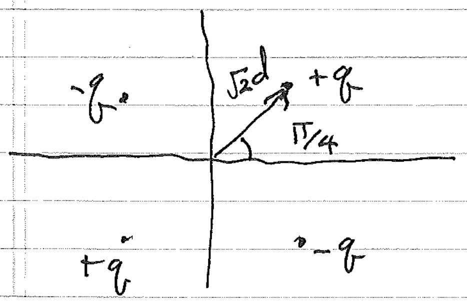
Solid Harmonics $r^{\ell}\, Y_{\ell,m}(\theta,\phi) = \Sigma\, (x+iy)^{m_1} (x-iy)^{m_2} z^{m_3}\, a(m_1,m_2,m_3)$

$$m_1 - m_2 = m, \quad m_1 + m_2 + m_3 = \ell$$

Example:

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

Example: Calculating Spherical multipoles



$$q_{00} = 0$$

$$q_{1,\pm1} \cong \sum_\alpha q_\alpha r_\alpha \sin\theta_\alpha e^{\pm i\phi_\alpha} = 0$$

$$q_{1,0} \cong \sum_\alpha q_\alpha r_\alpha \underset{\theta_\alpha = \pi/2}{\cos\theta_\alpha} = 0$$

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

$$q_{2,2} = \sum_\alpha q_\alpha r_\alpha^2 Y^*_{2,2}(\theta_\alpha, \phi_\alpha) = \sqrt{\frac{15}{32\pi}} \sum_\alpha q_\alpha (x_\alpha - i y_\alpha)^2$$

$$= \sqrt{\frac{15}{32\pi}} \sum_\alpha q_\alpha \underbrace{r_\alpha^2 \sin^2\theta_\alpha}_{2d^2 \text{ for all charges}} e^{-2i\phi_\alpha}$$

$$= \sqrt{\frac{15}{32\pi}}\, 2qd^2 \left(e^{-i\pi/2} - e^{+i\pi/2} - e^{-i3\pi/2} + e^{+i3\pi/2} \right)$$

$$(-i) - (+i) - (-i) + (-i)$$

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

$$q_{2,1} = \sum_\alpha q_\alpha r_\alpha^2 Y^*_{2,1}(\theta,\phi) \propto \sum_\alpha q_\alpha (x_\alpha + i y_\alpha)^* \overset{0}{z_\alpha} = 0$$

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

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

$$= \frac{4\pi}{5} \cdot 2\mathrm{Re}(q_{22} Y_{2,2}(\theta,\phi)) = \frac{8\pi}{5} \sqrt{\frac{15}{32\pi}}\, 4q\; \mathrm{Re}(-i Y_{22}(\theta,\phi))$$

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

L#6.9

Relationships between
Cartesian and spherical Multipoles:

$$q_{\ell m} = \int d^3x\ \rho(\vec{x})\ Y^*_{\ell m}(\vec{x})$$

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

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

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

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

$$Y_{2,\pm 1}(\vec{x}) = \mp\sqrt{\frac{15}{8\pi}}\ (x \pm iy)z = \mp\sqrt{\frac{15}{8\pi}}\left(xz \pm iyz\right)$$

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

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

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

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

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

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