SET- 25

Spherical harmonics

(1) Starting from Maxwell's equations for electrostatics we have

$$\vec{\nabla} \cdot \epsilon_0 \vec{E} = \rho(\vec{r})$$

$$\vec{\nabla} \times \vec{E} = 0 \quad \Rightarrow \quad \vec{E} = -\vec{\nabla}\phi$$

$$-\epsilon_0 \nabla^2 \phi = \rho \qquad\qquad (-\epsilon_0 \nabla^2)\, G = 1$$

$$G = (-\epsilon_0 \nabla^2)^{-1}$$

$$\phi = (-\epsilon_0 \nabla^2)^{-1} \rho = G \rho$$

$$G(\vec{r}, \vec{r}') = \frac{1}{4\pi\epsilon_0} \frac{1}{|\vec{r} - \vec{r}'|}$$

$$\phi(\vec{r}) = \int d^3r'\, G(\vec{r}, \vec{r}')\, \rho(\vec{r}')$$

$$= \frac{1}{4\pi\epsilon_0} \int d^3r' \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|}$$

(2) Observe that

$$f(x+a) = f(x) + a\frac{d}{dx} f(x) + \frac{1}{2!}\left(a\frac{d}{dx}\right)^2 f(x) + \cdots$$

$$= \left[1 + a\frac{d}{dx} + \frac{1}{2!}\left(a\frac{d}{dx}\right)^2 + \cdots\right] f(x)$$

$$e^A = 1 + A + \frac{1}{2!}A^2 + \cdots$$

$$= \sum_{l=0}^{\infty} \frac{1}{l!}\left(a\frac{d}{dx}\right)^l f(x)$$

$$= e^{a\frac{d}{dx}} f(x)$$

In the same spirit we have.

$$\frac{1}{|\vec{r} - \vec{r}'|} = e^{(-\vec{r}' \cdot \vec{\nabla})} \frac{1}{r} = \sum_{l=0}^{\infty} \frac{1}{l!} (-\vec{r}' \cdot \vec{\nabla})^l \frac{1}{r}$$

(3) $\underline{\underline{l=0}}$ : $\frac{1}{r}$

(4) $\underline{\underline{l=1}}$ : $\frac{1}{1!}(-\vec{r}'\cdot\vec{\nabla})\frac{1}{r} = \frac{\vec{r}'\cdot\vec{r}}{r^3}$

$\vec{\nabla}\vec{r} = \overleftrightarrow{1}$

$\vec{\nabla} r = \hat{r}$

(5) $\underline{\underline{l=2}}$ : $\frac{1}{2!}(-\vec{r}'\cdot\vec{\nabla})^2\frac{1}{r} = \frac{1}{2}(-\vec{r}'\cdot\vec{\nabla})\frac{\vec{r}'\cdot\vec{r}}{r^3}$

$$= -\frac{1}{2}r_i'\nabla_i\frac{r_j' r_j}{r^3}$$

$$= -\frac{1}{2}r_i' r_j'\left[\frac{\delta_{ij}}{r^3} - 3\frac{r_i r_j}{r^5}\right]$$

$$= \frac{1}{2}\left[\frac{3(\vec{r}'\cdot\vec{r})(\vec{r}'\cdot\vec{r})}{r^5} - \frac{r'^2}{r^3}\right]$$

$$= \frac{1}{2}\frac{1}{r^5}\vec{r}\cdot\left[3\vec{r}'\vec{r}' - \overleftrightarrow{1}r'^2\right]\cdot\vec{r}$$

(6) Using (3) to (5) in (2)

$$\frac{1}{|\vec{r}-\vec{r}'|} = \underbrace{\frac{1}{r}}_{l=0} + \underbrace{\frac{1}{1!}(-\vec{r}'\cdot\vec{\nabla})\frac{1}{r}}_{l=1} + \underbrace{\frac{1}{2!}(-\vec{r}'\cdot\vec{\nabla})^2\frac{1}{r}}_{l=2} + \cdots$$

$$= \frac{1}{r} + \frac{\vec{r}'\cdot\vec{r}}{r^3} + \frac{1}{2}\frac{1}{r^5}\vec{r}\cdot\left[3\vec{r}'\vec{r}' - \overleftrightarrow{1}r'^2\right]\cdot\vec{r} + \cdots$$

7 Using 6 in 1 we have the multipole expansion

$$\phi(\vec{r}) = \frac{1}{4\pi\epsilon_0}\left[\frac{1}{r}\int d^3r'\,\rho(\vec{r}) + \frac{\vec{r}}{r^3}\cdot\int d^3r'\,\rho(\vec{r}\,')\,\vec{r}\,' + \frac{1}{2}\frac{1}{r^5}\,\vec{r}\cdot\left(\int d^3r'\,\rho(\vec{r}\,')\left[3\vec{r}\,'\vec{r}\,' - \overleftrightarrow{1}\,r'^2\right]\right)\cdot\vec{r} + \dots\right]$$

$$= \frac{1}{4\pi\epsilon_0}\left[\frac{e}{r} + \frac{\vec{r}}{r^3}\cdot\vec{d} + \frac{1}{2}\frac{1}{r^5}\,\vec{r}\cdot\overleftrightarrow{q}\cdot\vec{r} + \dots\right]$$

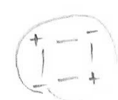
where

total charge $\quad e = \int d^3r'\,\rho(\vec{r}\,')$

dipole moment $\quad \vec{d} = \int d^3r'\,\rho(\vec{r}\,')\,\vec{r}\,'$

quadrapole moment. $\quad \overleftrightarrow{q} = \int d^3r'\,\rho(\vec{r}\,')\left[3\vec{r}\,'\vec{r}\,' - \overleftrightarrow{1}\,r'^2\right]$


dipole.
(3 independent ones)




quadrapole
(5 independent ones)

→ moments are mean, variance, etc.

8 One observes that, for $\vec{r} \neq 0$

$\underline{l=0}$ $\quad -\nabla^2 \frac{1}{r} = 0$

$\underline{l=1}$ $\quad -\nabla^2 (-\vec{a}\cdot\vec{\nabla}) \frac{1}{r} \xrightarrow{HW} -\nabla^2 \left(\frac{\vec{a}\cdot\vec{r}}{r^3}\right) = 0$

$\underline{l=2}$ $\quad -\nabla^2 (-\vec{a}_1\cdot\vec{\nabla})(-\vec{a}_2\cdot\vec{\nabla}) \frac{1}{r} \xrightarrow{HW} -\nabla^2\left(\frac{1}{r^5}\left[3(\vec{a}_1\cdot\vec{r})(\vec{a}_2\cdot\vec{r}) - (\vec{a}_1\cdot\vec{a}_2)r^2\right]\right) = 0$

$\vdots$

$\underline{l=l}$ $\quad -\nabla^2 (-\vec{a}_1\cdot\vec{\nabla}) \cdots (-\vec{a}_l\cdot\vec{\nabla}) \frac{1}{r} = -\nabla^2\left(\frac{1}{r} Y_l\left(\frac{\vec{r}}{r^2}\right)\right) = 0$

The left hand side in each case is easily verified to be zero because $\nabla^2$ passes through. The second equality in each case can be explicitly verified.

$Y_l\left(\frac{\vec{r}}{r^2}\right) \to$ solid harmonics

$Y_l\left(\frac{\vec{r}}{r}\right) \to$ spherical harmonics.

9 Inversion theorem:

true both ways.

If $\quad -\nabla^2 \phi(\vec{r}) = 0,$

then $\quad -\nabla^2\left[\frac{1}{r}\phi\left(\frac{\vec{r}}{r^2}\right)\right] = 0.$

10 Using 9 in 8 we have.

$$-\nabla^2\left[\frac{1}{r} Y_l\left(\frac{\vec{r}}{r^2}\right)\right] = -\nabla^2\left[\frac{1}{r^{2l+1}} Y_l(\vec{r})\right] = 0$$

$$\Rightarrow \quad -\nabla^2 Y_l(\vec{r}) = 0$$

11 Dipole has 3 independent solutions, quadrapole has 5 independent solutions, how many independent solutions are there in the $l$-th multipole moment?

12 $\underline{l=2}$ $\rightarrow$ An arbitrary symmetric dyadic or a homogeneous polynomial of degree 2 has 9 independent components before symmetrization.

$\rightarrow$ $\overleftrightarrow{q}$ is symmetric. Takes away 3 components

$\rightarrow$ $\nabla^2 Y_2(\vec{r}) = 0 \Rightarrow 1$ constraint

$$\begin{pmatrix} xx & xy & xz \\ yx & yy & yz \\ zx & zy & zz \end{pmatrix}$$

$\rightarrow$ terms in a homogeneous polynomial of degree 2.

Thus $9-3-1 = 5$ independent solutions.

13 In general

$\rightarrow$ A homogeneous polynomial of degree $l$ has

$$\frac{1}{2}(l+1)(l+2)$$

terms. $\rightarrow$ refer following page.

$\rightarrow$ $\nabla^2 Y_l(\vec{r}) = 0$ is a homogeneous polynomial of degree $l-2$. Thus it has

$$\frac{1}{2}(l-1)\,l$$

contraints.

$$\Rightarrow \text{Total independent solutions} = \frac{1}{2}(l+1)(l+2) - \frac{1}{2}l(l-1)$$
$$= \frac{1}{2}\left[l^2+3l+2-l^2+l\right]$$
$$= 2l+1.$$

14 Let us find the number of terms in a homogeneous polynomial of degree $l$ constructed out of $x, y, z$.

$x_1 = x$
$x_2 = y$
$x_3 = z$

$$x_1^{k_1} x_2^{k_2} x_3^{k_3} \qquad k_1 + k_2 + k_3 = l.$$

15 Keep $k_3$ fixed, eg: if $k_3 = 0$, then we have $l+1$ terms.

$$x_1^{k_1} x_2^{k_2} \qquad k_1 + k_2 = l - k_3.$$

has $k_1 + k_2 + 1$ terms. Thus, for all possible $k_3$ we have.

$$\sum_{k_3=0}^{l} (k_1 + k_2 + 1) = \sum_{k_3=0}^{l} (l - k_3 + 1)$$

$$= l(l+1) - \frac{l(l+1)}{2} + (l+1)$$

$$= (l+1)\left[ l - \frac{l}{2} + 1 \right]$$

$$= \frac{1}{2}(l+1)(l+2)$$

which is what we used in 13 to show that the $l$-th multipole moment has $(2l+1)$ independent solutions.

(16) We consider structures of the form

$$(\vec{a}\cdot\vec{r})^l$$

and ask for what conditions is it a solution of the Laplacian,

$$\nabla^2 (\vec{a}\cdot\vec{r})^l = 0 \quad ?$$

(17)
$$\begin{aligned}
\nabla^2 (\vec{a}\cdot\vec{r})^l &= \vec{\nabla}\cdot\left[\, l\,(\vec{a}\cdot\vec{r})^{l-1}\,\vec{a}\,\right] \\
&= l\;\vec{a}\cdot\vec{\nabla}\,(\vec{a}\cdot\vec{r})^{l-1} \\
&= l(l-1)\,(\vec{a}\cdot\vec{r})^{l-2}\;\vec{a}\cdot\vec{a}
\end{aligned}$$

Thus, $\nabla^2 (\vec{a}\cdot\vec{r})^l = 0$

$$\Rightarrow \quad \vec{a}\cdot\vec{a} = 0$$

(18) This is possible only for complex components. Let

$$\vec{a} = (a_1, a_2, a_3)$$

$a_i$ are complex

$Y_\pm$ are complex

$$\begin{aligned}
a_1 + i a_2 &= Y_-^2 \\
a_1 - i a_2 &= -\,Y_+^2 \\
a_3 &= Y_+ Y_-
\end{aligned}
\quad\Rightarrow\quad
\begin{aligned}
a_1 &= \tfrac{1}{2}\left(Y_-^2 - Y_+^2\right) \\
a_2 &= \tfrac{1}{2i}\left(Y_-^2 + Y_+^2\right) \\
a_3 &= Y_+ Y_-
\end{aligned}$$

$$\begin{aligned}
a_1^2 + a_2^2 + a_3^2 &= (a_1 + i a_2)(a_1 - i a_2) + a_3^2 \\
&= -\,Y_-^2 Y_+^2 + (Y_+ Y_-)^2 \\
&= 0 .
\end{aligned}$$

(19)
$$\vec{a} = \frac{1}{2}\left( y_-^2 - y_+^2 \,,\; -i\,y_-^2 - i\,y_+^2 \,,\; 2\,y_+\,y_- \right)$$
$$\vec{r} = r\left( \sin\theta\cos\phi \,,\; \sin\theta\sin\phi \,,\; \cos\theta \right)$$

(20) The spherical harmonics, $Y_{lm}(\theta,\phi)$, are defined by the generating function
$$\frac{1}{l!}\left(\frac{\vec{a}\cdot\vec{r}}{r}\right)^l = \sum_{m=-l}^{l} \frac{y_+^{\,l+m}}{\sqrt{(l+m)!}}\;\frac{y_-^{\,l-m}}{\sqrt{(l-m)!}}\;\sqrt{\frac{4\pi}{2l+1}}\;\;Y_{lm}(\theta,\phi)$$

(21) Using (19) we can write
$$\frac{1}{l!}\left(\frac{\vec{a}\cdot\vec{r}}{r}\right)^l = \frac{1}{l!\,2^l}\Big[\left(y_-^2 - y_+^2\right)\sin\theta\cos\phi - i\left(y_-^2 + y_+^2\right)\sin\theta\sin\phi + 2\,y_+\,y_-\cos\theta\Big]^l$$
$$= \frac{1}{l!\,2^l}\Big[\, y_-^2\sin\theta\, e^{-i\phi} - y_+^2\sin\theta\, e^{i\phi} + 2\,y_+\,y_-\cos\theta\Big]^l$$
$$= \frac{1}{l!}\left(\frac{y_+^2\, e^{i\phi}}{2^l\sin\theta}\right)^l \Big[\frac{y_-^2}{y_+^2}\sin^2\theta\, e^{-2i\phi} - \overset{(1-\cos^2\theta)}{\sin^2\theta} + 2\,\frac{y_-}{y_+}\sin\theta\, e^{-i\phi}\cos\theta\Big]^l$$
$$= \frac{1}{l!}\left(\frac{y_+^2\, e^{i\phi}}{2^l\sin\theta}\right)^l \Big[\left(\frac{y_-}{y_+}\sin\theta\, e^{-i\phi} + \cos\theta\right)^2 - 1\Big]^l$$

(22)
$$I_l(x+a) = \left[(x+a)^2-1\right]^l$$
$$= e^{a\frac{d}{dx}} I_l(x)$$
$$= \sum_{n=0}^{\infty} \frac{1}{n!} a^n \frac{d^n}{dx^n}(x^2-1)^l$$
$$= \sum_{n=0}^{2l} \frac{1}{n!} a^n \frac{d^n}{dx^n}(x^2-1)^l \qquad \begin{array}{l} n = l-m \\ m = l-n \end{array}$$
$$= \sum_{m=+l}^{-l} \frac{1}{(l-m)!} a^{l-m}\left(\frac{d}{dx}\right)^{l-m}(x^2-1)^l$$
$$= \sum_{m=-l}^{l} \frac{1}{(l-m)!} a^{l-m}\left(\frac{d}{dx}\right)^{l-m}(x^2-1)^l$$

(23) Using (22) in (21)

$$\frac{1}{l!}\left(\frac{\vec{a}\cdot\vec{r}}{r}\right)^l = \frac{1}{l!}\left(\frac{Y_+ e^{i\phi}}{2^l \sin\theta}\right)^l \sum_{m=-l}^{l} \frac{1}{(l-m)!}\left(\frac{Y_-}{Y_+}\sin\theta\, e^{-i\phi}\right)^{l-m}\left(\frac{d}{dt}\right)^{l-m}(t^2-1)^l \Bigg|_{t=\cos\theta}$$
$$= \sum_{m=-l}^{l} \frac{Y_+^{l+m}}{\sqrt{(l+m)!}} \frac{Y_-^{l-m}}{\sqrt{(l-m)!}} \sqrt{\frac{(l+m)!}{(l-m)!}} \left(\frac{e^{i\phi}}{\sin\theta}\right)^m \left(\frac{d}{dt}\right)^{l-m} \frac{(t^2-1)^l}{2^l\, l!} \Bigg|_{t=\cos\theta}$$

(24) Comparing (20) and (23) we have.

$$Y_{lm}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}} \sqrt{\frac{(l+m)!}{(l-m)!}} \left(\frac{e^{i\phi}}{\sin\theta}\right)^m \left(\frac{d}{dt}\right)^{l-m} \frac{(t^2-1)^l}{2^l\, l!} \Bigg|_{t=\cos\theta}$$

25
$$Y_{00}(\theta,\phi) = \sqrt{\frac{1}{4\pi}}\sqrt{\frac{0!}{0!}}\left(\frac{e^{i\phi}}{\sin\theta}\right)^0\left(\frac{d}{dt}\right)^0\frac{(t^2-1)^0}{1\cdot 1}$$
$$= \frac{1}{\sqrt{4\pi}}$$

$$Y_{21}(\theta,\phi) = \sqrt{\frac{5}{4\pi}}\sqrt{\frac{3!}{1!}}\left(\frac{e^{i\phi}}{\sin\theta}\right)^1\left(\frac{d}{dt}\right)\frac{(t^2-1)^2}{2^2\,2!}\Bigg|_{t=\cos\theta}$$
$$= \sqrt{\frac{5}{4\pi}}\sqrt{6}\,\frac{e^{i\phi}}{\sin\theta}\,\frac{1}{8}\,\frac{d}{dt}\left(t^4-2t^2+1\right)\Big|_{t=\cos\theta}$$
$$= \sqrt{\frac{30}{4\pi}}\,\frac{1}{8}\,\frac{e^{i\phi}}{\sin\theta}\left(4t^3-4t\right)\Big|_{t=\cos\theta}$$
$$= \sqrt{\frac{30}{4\pi}}\,\frac{1}{2}\,\frac{e^{i\phi}}{\sin\theta}\left(\cos^3\theta-\cos\theta\right)$$
$$= \sqrt{\frac{30}{16\pi}}\,\frac{e^{i\phi}}{\sin\theta}\cos\theta\,\underbrace{\left(\cos^2\theta-1\right)}_{-\sin^2\theta}$$
$$= \sqrt{\frac{15}{8\pi}}\,e^{i\phi}\cos\theta\sin\theta$$

26 Legendre polynomials: Set $m=0$.
$$Y_{l0}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}}\left(\frac{d}{dt}\right)^l\frac{(t^2-1)^l}{2^l\,l!}\Bigg|_{t=\cos\theta}$$
$$= \sqrt{\frac{2l+1}{4\pi}}\,P_l(\cos\theta)$$

$P_l(t) \rightarrow$ Legendre polynomials.

where
$$P_l(t) = \left(\frac{d}{dt}\right)^l\frac{(t^2-1)^l}{2^l\,l!}$$

27

$$Y_{22}(\theta,\phi) = \sqrt{\frac{15}{32\pi}} \left(\frac{x+iy}{r}\right)^2 = \sqrt{\frac{15}{32\pi}} \sin^2\theta \, e^{2i\phi}$$

$$Y_{21}(\theta,\phi) = -\sqrt{\frac{15}{8\pi}} \left(\frac{x+iy}{r}\right)\frac{z}{r} = -\sqrt{\frac{15}{8\pi}} \sin\theta \cos\theta \, e^{i\phi}$$

$$Y_{20}(\theta,\phi) = \sqrt{\frac{5}{16\pi}} \left(3\frac{z^2}{r^2} - 1\right) = \sqrt{\frac{5}{16\pi}} \left(3\cos^2\theta - 1\right)$$

Plotting these with Mathematica helps. Use.
SphericalHarmonicY[l, m, θ, φ].
Spherical Density Plot and