Class 9 (2/8/2024)

Multipole Expansion

Summary of Solutions to Laplace Equation in Spherical Coordinates

For boundary value problems in electrostatics which are conveniently described in spherical coordinates and exhibit azimuthal symmetry:

$$\vec{\nabla}^2 V(r,\theta) = 0$$

Solution $V(r,\theta) = R(r)\,\Theta(\theta)$

with $R(r) = A_n r^n + B_n \dfrac{1}{r^{n+1}}$ $\quad n = 0, 1, 2, 3, 4, \ldots$

$\Theta(\theta) = P_n(\cos\theta)$ $\quad$ Legendre Polynoms

for inside a spherical volume which includes $r = 0$

$$V_i(r,\theta) = \sum_{n=0}^{\infty} A_n r^n P_n(\cos\theta)$$

Because for r-> 0, V(r,θ)-> finite

for outside a spherical volume

$$V_o(r,\theta) = \sum_{n=0}^{\infty} B_n \frac{1}{r^{n+1}} P_n(\cos\theta)$$

Because for r-> ∞, V(r,θ)-> 0

If the surface is charged (surface charge σ) the electrical potential is continuous: $V(r=R,\theta) = V_0(r=R,\theta)$
at boundary.
gradient of the el. potential is discontinuous:
at boundary

$$\vec{\nabla} V_0 - \vec{\nabla}_i V = -\frac{\sigma}{\varepsilon_0}$$

Determine A_n, B_n by exploiting the orthogonality relation for Legendre Polynoms

$$\int_0^\pi P_n(\cos\theta)\, P_{n'}(\cos\theta) \sin\theta \, d\theta = \frac{2}{2n+1}\, \delta_{nn'}$$

and [in PHYS4210] try to express $V(R,\theta)$ as a linear combination of Legendre Polynoms.

Methods for solving Laplace's & Poisson's equations

cylindrical coordinates
(Bessel function)

multipole
expansion

Green's
function

separation
of variables

spherical
coordinates
(Legendre Polynoms)

image
charges

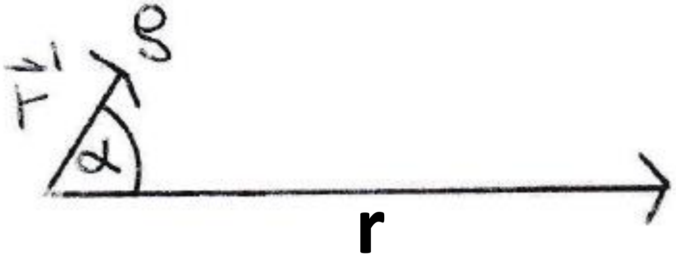
$$\nabla^2 V = 0 \Leftarrow \nabla^2 V = -\frac{\rho}{\varepsilon_0}$$

cartesian coordinates
(Fourier series)

direct integration of the 1-dimensional
Laplace's and Poisson's equations

When do we apply multipole expansion to solve Poisson's equation?

Multipole Expansion is an approach to describe localized charge distribution at point $\vec{r}$ far away from the location of the charge at $\vec{r}'$.



$V(\vec{r})$, $\cos\alpha = \vec{r}' \cdot \vec{r}$, $\vec{r} \gg \vec{r}'$

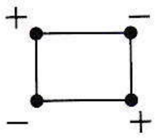
$$\vec{\nabla}^2 V = -\frac{\rho}{\varepsilon_0}, \quad \vec{E} = -\vec{\nabla} V, \quad \vec{F} = q\vec{E}$$

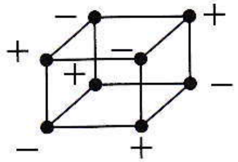
Multipole expansion is useful for e.g. molecular physics (e.g. long range molecular forces). The method is used to describe electric potentials (potential energies U(**r**)=qV(**r**)) originating from electric charge distributions within atoms & molecules. Conceptually, potential energies U(**r**) are inserted into the Schroedinger equation $H\Psi=[(\mathbf{p}^2/2m)+U(\mathbf{r})]\Psi=E\Psi$. Calculated energy levels are compared to experimental observation (spectra).

Basic (electrostatic) models of molecules can be constructed from e.g. point charges:

Atomic physics H^+: 

CO: 





Multipole Expansion is an approach to describe localized charge distribution at point $\vec{r}$ far away from the location of the charge at $\vec{r}'$.

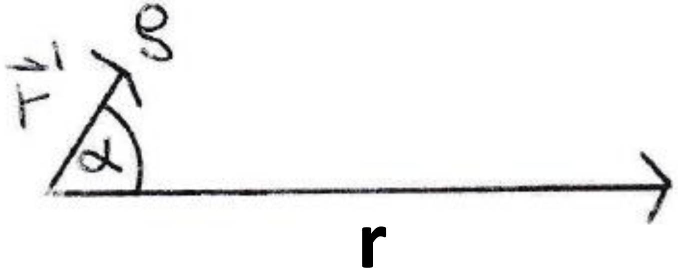
Basically, we take the general description of the electrical potential:

$$V(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\int_{V'} \frac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|}\, dV' = V_0+V_1+V_2+V_3+\ldots.$$

Let's look at $\frac{1}{|\vec{r}-\vec{r}'|}$ and rewrite as $\frac{1}{|r\hat{r} - r'\hat{r}'|}$

and $\frac{1}{r|\hat{r}-\frac{r'}{r}\hat{r}'|}$. Now if $\frac{r'}{r} < 1$, $\frac{1}{r|\hat{r}-\frac{r'}{r}\hat{r}'|}$

can be expanded into a binominal series.



$V(\vec r)$, $\cos\alpha = \vec r' \cdot \vec r$, $\vec r \gg \vec r'$

Consider $|\vec r - \vec r'|^2 = r^2 + r'^2 - 2rr'\cos\alpha$

$$= r^2\left(1 + \frac{r'^2}{r^2} - \frac{2r'}{r}\cos\alpha\right)$$

$$= r^2\Big(1 + \underbrace{\frac{r'}{r}\left(\frac{r'}{r} - 2\cos\alpha\right)}_{\text{small because } \frac{r'}{r} \text{ is small}}\Big)$$

Expand $\dfrac{1}{|\vec r - \vec r'|} = \dfrac{1}{r}(1+\varepsilon)^{-1/2}$ look up in table

result $\dfrac{1}{|\vec r - \vec r'|} = \dfrac{1}{r}\displaystyle\sum_{n=0}^{\infty}\left(\frac{r'}{r}\right)^n P_n(\cos\alpha)$

$$V(\vec{r}) = \frac{1}{4\pi\varepsilon_0} \int_{V'} \frac{\rho(\vec{r}\,')}{|\vec{r} - \vec{r}\,'|} \, dV' .$$

$$\frac{1}{|\vec{r} - \vec{r}\,'|} = \frac{1}{r} \sum_{n=0}^{\infty} \left(\frac{r'}{r} \right)^n P_n(\cos\alpha)$$

$$V(\vec{r}) = V_0 + V_1 + V_2 +$$

$$V_0 = \frac{1}{4\pi\varepsilon_0} \frac{1}{r} \int_{V'} \rho(\vec{r}\,') \, dV'$$ electric monopole

$$V_1 = \frac{1}{4\pi\varepsilon_0} \frac{1}{r^2} \int_{V'} r' \cos\alpha \; \rho(\vec{r}\,') \, dV'$$ electric dipole

$$V_2 = \frac{1}{4\pi\varepsilon_0} \frac{1}{r^3} \int_{V'} r'^2 \left(\frac{3}{2} \cos^2\alpha - \frac{1}{2} \right) \rho(\vec{r}\,') \, dV'$$ electric quadrupol

$\cos\alpha = \hat{r} \cdot \hat{r}\,'$

$$dV' = 2\pi r^2 dr \sin\alpha \, d\alpha = r^2 \sin\alpha \, dr \, d\alpha \, d\phi$$

The First Three Terms of the **Multipole** Expansion

$$V_0 = \frac{1}{4\pi\varepsilon_0}\frac{1}{r}\int_{V'} \rho(\vec{r}\,')\, dV' \quad \text{electric monopole}$$

$$V_1 = \frac{1}{4\pi\varepsilon_0}\frac{1}{r^2}\int_{V'} r'\cos\alpha\, \rho(\vec{r}\,')\, dV' \quad \text{electric dipole}$$

$$V_2 = \frac{1}{4\pi\varepsilon_0}\frac{1}{r^3}\int_{V'} r'^2\left(\frac{3}{2}\cos^2\alpha - \frac{1}{2}\right) \rho(\vec{r}\,')\, dV' \quad \text{electric quadrupol}$$

$$dV' = 2\pi r^2 dr \sin\alpha\, d\alpha = r^2 \sin\alpha\, dr\, d\alpha\, d\phi$$

useful for point charges $\delta^3(\vec{r}) = \frac{1}{r^2 \sin\alpha}\delta(r)\,\delta(\alpha)\,\delta(\phi)$

Good to remember: α is angle between **r** and **r’** , i.e. **r·r’ =** r r’ cosα. However, sometimes the geometry of the problem permits to orient **r** or **r’** along z-axis, then $\alpha=\theta$ with θ the spherical coordinate.

Visualization of the power of expressing electric potentials using multipole expansion $V=V_0+V_1+V_2+V_3+\ldots$: