

$$U = \frac{e^2}{4\pi\epsilon_0 a} \sum_{m_x} \sum_{m_y} \sum_{m_z} \left[\frac{(-1)^{m_x+m_y+m_z}}{|\vec{m}|} \right]$$

electrostatic energy of ion at (0,0,0) $\neq (0,0,0)$

→ 270, 260

$$U_0 = \frac{2e^2}{4\pi\epsilon_0 a} \left[\underbrace{-\frac{1}{1} + \frac{(-1)^2}{2} - \frac{1}{3} + \frac{1}{4} - \dots}_{-\ln 2} \right]$$

$$\sum_{\vec{m}} \frac{1}{m} \quad D$$

$$\sum_{\vec{m}} \frac{1}{m^2} \quad C$$

$$U = U_0 + 4U_0 + \dots \approx \frac{-e^2}{4\pi\epsilon_0 a} (1.7476)$$

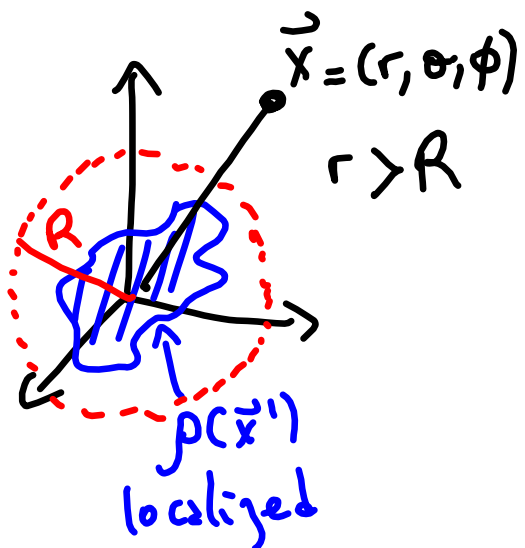
Madelung constants

- Energy needed to dissociate crystal into well separated ions
- "Madelung constant" wikipedia

— 0 —

Midterm

Given Feb. 12 ; returned Feb. 19
 No lecture Feb. 17 \rightarrow (office hours)

4.1 Multipole expansion

$$\Phi(r, \theta, \phi) = \sum_{l, m} \underbrace{B_{lm}}_{\rightarrow \frac{1}{4\pi\epsilon_0} \frac{4\pi}{2l+1} q_{lm}} r^{-l-1} Y_{lm}(\theta, \phi)$$

change of notation

$$\Phi(r, \theta, \phi) = \frac{1}{4\pi\epsilon_0} \int_R \frac{\rho(\vec{x}') d^3x'}{|\vec{x} - \vec{x}'|}$$

Compare both and find q_{lm} .

"Magic" formula (Eq (3.70)):

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

$$\Phi(r, \theta, \phi) = \frac{1}{4\pi\epsilon_0} \sum_{lm} \frac{4\pi}{2l+1} \left[\int d^3x' \rho(\vec{x}') r'^l Y_{lm}^*(\theta', \phi') \right] \frac{Y_{lm}(\theta, \phi)}{r^{l+1}}$$

q_{lm}

$$q_{00} = \int d^3x' \rho(\vec{x}') (r')^0 \underbrace{Y_{00}^*(\theta', \phi')}_{\frac{1}{\sqrt{4\pi}}} = \frac{1}{\sqrt{4\pi}} \underbrace{\int d^3x' \rho(\vec{x}')}_q = \frac{q}{\sqrt{4\pi}}$$

Charge

$$q_{11} = \int d^3x' \rho(\vec{x}') (r')^{-1} Y_{11}^*(\theta', \phi')$$

$x' = r' \sin\theta' \cos\phi'$
 $y' = r' \sin\theta' \sin\phi'$

$-\sqrt{\frac{3}{8\pi}} \sin\theta' e^{-i\phi'} \cos\phi' - i \sin\theta' \sin\phi'$

$$q_{11} = -\sqrt{\frac{3}{8\pi}} \int d^3x' \rho(\vec{x}') (x' - iy')$$

$$q_{11} = -\sqrt{\frac{3}{8\pi}} (p_x - ip_y)$$

$$q_{10} = \sqrt{\frac{3}{4\pi}} p_z$$

.....

electric dipole moment

$$\vec{p} \stackrel{\text{def}}{=} \int d^3x' \rho(\vec{x}') \vec{r}'$$

↑
(x', y', z')

$$q_{22} = \frac{1}{4} \sqrt{\frac{15}{2\pi}} \int d^3x' \rho(\vec{x}') (x'^2 - 2ix'y' - y'^2)$$

$$q_{21}, q_{20}, q_{2-1}, q_{2-2} \dots$$

Quadrupole moment tensor, 3x3 matrix, traceless

$$Q_{11} = \int d^3x' \rho(\vec{x}') (3x'^2 - \underbrace{r'^2}_{x'^2 + y'^2 + z'^2})$$

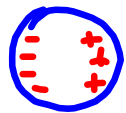
$$\boxed{Q_{ij} = \int d^3x' \rho(\vec{x}') (3x'_i x'_j - r'^2 \delta_{ij})}$$

$i, j = 1, 2, 3$

$$\boxed{\Phi(\vec{x}) = \frac{1}{4\pi\epsilon_0} \left[\frac{q}{r} + \frac{\vec{p} \cdot \vec{x}}{r^3} + \frac{1}{2} \sum_{ij} Q_{ij} \frac{x_i x_j}{r^5} + \dots \right]}$$

4.3 Electrostatic with ponderable media

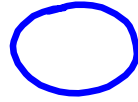
Previous example



electric dipole was induced

Atoms, molecules are like tiny metallic spheres

$$\vec{E}_0 = 0$$

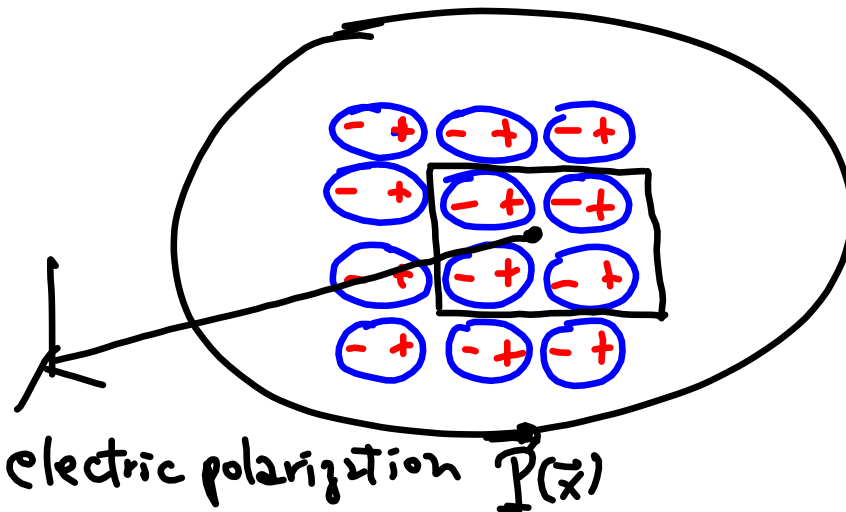


$$\vec{p} = 0$$

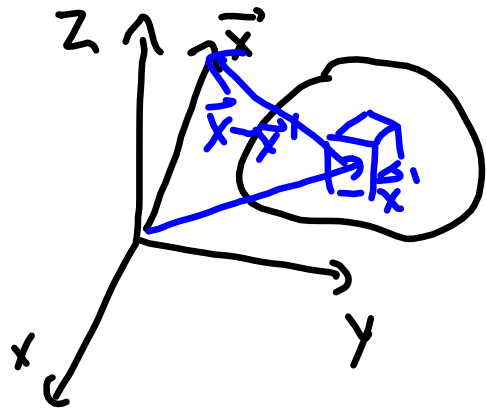
$$\vec{E}_0 \neq 0$$



$$\vec{p} \neq 0$$



electric polarization $\vec{P}(\vec{x})$



$$\Delta \Phi \text{ from } \Delta V \approx \frac{1}{4\pi\epsilon_0} \left[\frac{\rho(\vec{x}') \Delta V}{|\vec{x} - \vec{x}'|} + \frac{\vec{P}(\vec{x}') \cdot (\vec{x} - \vec{x}')}{|\vec{x} - \vec{x}'|^3} \Delta V \right]$$

$$\frac{1}{4\pi\epsilon_0} \left[\frac{q}{r} + \frac{\vec{p} \cdot \vec{r}}{r^3} + \dots \right]$$

$$\Phi(\vec{x}) = \frac{1}{4\pi\epsilon_0} \int d^3x' \left[\frac{\rho(\vec{x}')}{|\vec{x} - \vec{x}'|} + \frac{\vec{P}(\vec{x}') \cdot (\vec{x} - \vec{x}')}{|\vec{x} - \vec{x}'|^3} \right]$$

↳ $\nabla' \left(\frac{1}{|\vec{x} - \vec{x}'|} \right)$