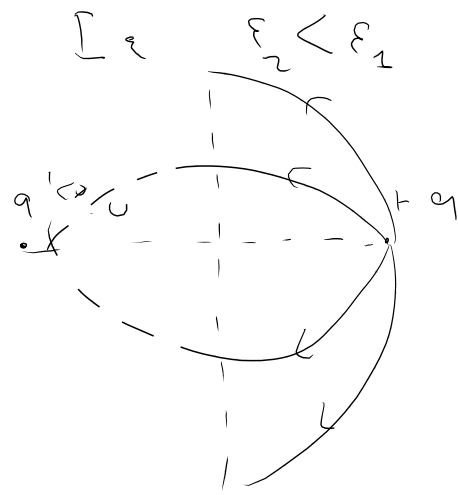
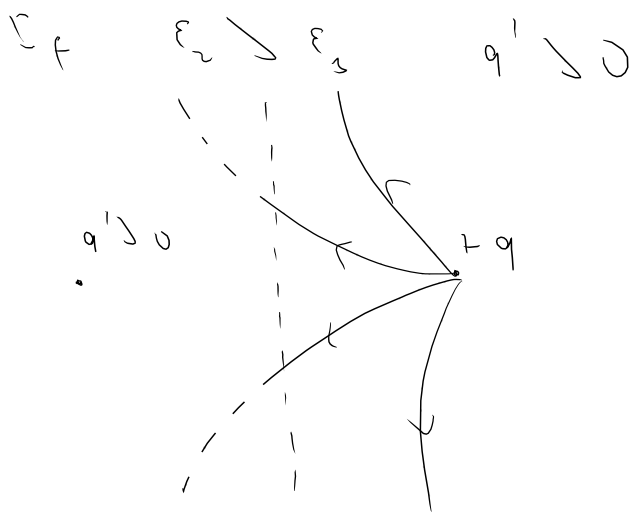


$\vec{E} \Rightarrow \parallel \hat{z}$

$$\frac{1}{\epsilon_1} \frac{q''}{\sqrt{q''^2 - z^2}}$$

$$q'' = \frac{2\epsilon_2}{\epsilon_1 + \epsilon_2}$$

$$q' = \frac{\epsilon_2 - \epsilon_1}{\epsilon_1 + \epsilon_2}$$



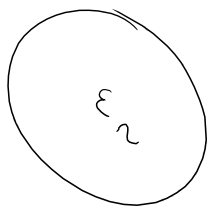
$$\vec{\nabla} \times \vec{E} = 0 \Rightarrow \Delta \vec{E}_{\parallel} = 0$$

$$\vec{\nabla} \cdot \vec{E} = 4\pi(\rho + \rho_b) \Rightarrow \Delta E_{\perp} = 4\pi(\sigma + \sigma_b)$$

$$\Delta E_{\perp} = 4\pi\sigma_b$$

E_x

ϵ_1



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$$\vec{D} = \vec{E} + 4\pi\vec{P}$$

$$\nabla \cdot \vec{D} = -\rho_b$$

$$\vec{\nabla} \cdot \vec{D} = \rho_b$$

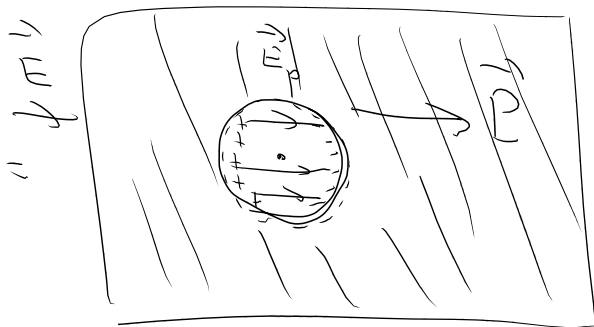
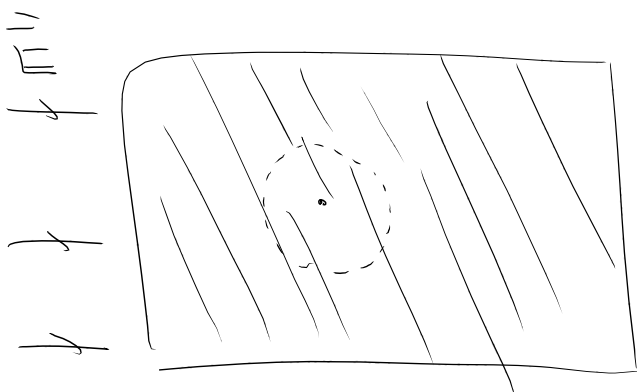
$$\vec{D} = \epsilon \vec{E}$$

$$\vec{D} = \chi_e \vec{E}$$

$$\epsilon = 1 + 4\pi\chi_e$$

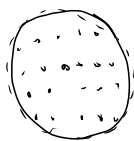
$$\vec{E} = \vec{E}_0 + \vec{E}_p + \vec{E}_i$$

$$\vec{E}_{loc} = \vec{E} + \vec{E}_p + \vec{E}_i$$



+

\vec{E}_i



\vec{E}_i

$$V(\vec{r}) = \sum_{lm} \frac{q_{lm}}{r^{l+1}} Y_{lm}(\Omega)$$

$$q_{lm} = \int d^3r \rho(\vec{r}) r^l Y_{lm}^*(\Omega)$$

$$V(\vec{r}) \approx \frac{q_0}{r} + \sum_{n=1}^{\infty} \frac{q_{1n}}{r^2} Y_{1n}(\Omega)$$

other terms are negligible if

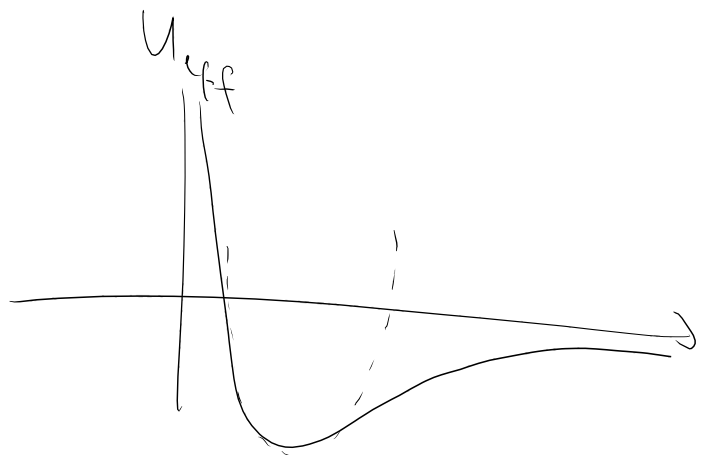
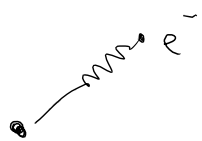
i) $\frac{d}{r} \ll 1$

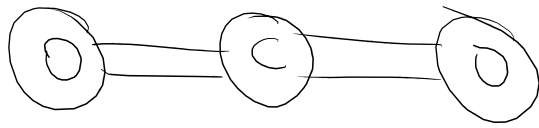
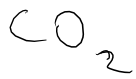


ii) $q_{lm} \approx 0$ for $l \gg 1$

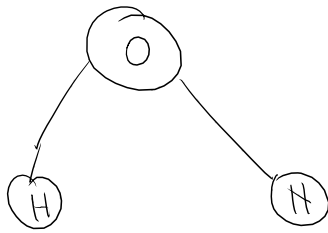
$$\vec{p}_{\text{pol}} = \gamma_{\text{pol}} \vec{E}_{\text{loc}}$$

$$\epsilon, \chi \rightarrow \gamma_{\text{pol}}$$





$\vec{p} = 0$



$\vec{p} \neq 0$



$\vec{p} \cdot \vec{e}_1 = \chi_{vol} \vec{e}_1$

$\Rightarrow V = -\vec{p} \cdot \vec{e}_1$

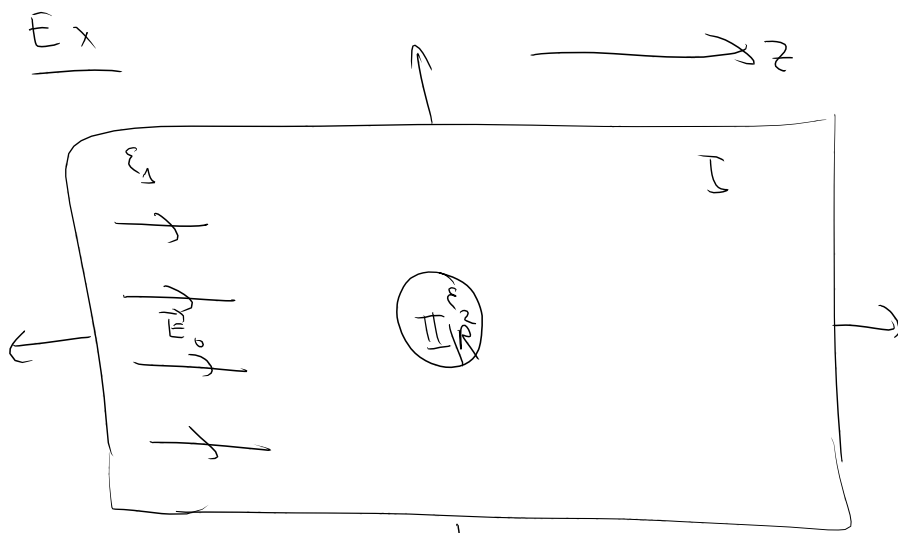
$[\vec{p}] = [q \ d] = [q] \ [d]$

$[\vec{e}_1] = \frac{[q]}{[d^2]}$

$[\chi_{vol}] = \frac{[\vec{p}]}{[\vec{e}_1]} = \frac{[q][d]}{\frac{[q]}{[d^2]}} = [d^3] = [\text{Volume}]$

$[\chi_{vol}] \approx v_0$

v_0 : volume of the molecule



$$\vec{D} = \vec{E} + 4\pi\vec{P}$$

$$\vec{\nabla} \cdot \vec{D} = \vec{\nabla} \cdot \vec{E} + 4\pi\vec{\nabla} \cdot \vec{P}$$

$$= 4\pi(\rho_{free} + \rho_b)$$

$$\vec{\nabla} \cdot \vec{D} = 0$$

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

$$\vec{\nabla} \cdot \vec{D} = 4\pi\rho_{free}$$

$$\vec{P} = (-\vec{E} + \vec{D}) \frac{1}{4\pi}$$

$$\epsilon = 1 + 4\pi\chi_e$$

$$\boxed{\vec{D} = \epsilon\vec{E}}$$

$$\vec{\nabla} \cdot (\epsilon\vec{E}) = 0$$

inside region I & II $\epsilon = \text{const}$

$$\epsilon\vec{\nabla} \cdot \vec{E} = 0 \Rightarrow \vec{\nabla} \cdot \vec{E} = 0 \Rightarrow \boxed{\nabla^2\phi = 0}$$

The boundaries: $r = R$
 $r = 0$

$$\nabla^2\phi = 0$$

$$\phi(\vec{r}) = \sum_{l,m} \left(A_{lm} r^l + B_{lm} \frac{1}{r^{l+1}} \right) Y_{lm}(\Omega)$$

$$\phi^{\text{II}}(\vec{r}) = \sum_{lm} \left(A_{lm}^{\text{II}} r^l + B_{lm}^{\text{II}} \frac{1}{r^{l+1}} \right) Y_{lm}(\Omega)$$

$(\vec{r} = 0) \in \text{Region II}$ ϕ^{II} should be finite

$$\Rightarrow \boxed{B_{lm}^{\text{II}} = 0}$$

$$\boxed{\phi^{\text{II}}(\vec{r}) = \sum_{lm} A_{lm}^{\text{II}} r^l Y_{lm}(\Omega)}$$

$$\phi^{\text{I}}(\vec{r}) = \sum_{lm} \left(A_{lm}^{\text{I}} r^l + B_{lm}^{\text{I}} \frac{1}{r^{l+1}} \right) Y_{lm}(\Omega)$$

as $r \rightarrow \infty$, $\vec{E}(\vec{r}) \rightarrow \vec{E}_0 = E_0 \hat{z}$

$$\begin{aligned} \phi^{\text{I}}(\vec{r}) &\xrightarrow{r \rightarrow \infty} -E_0 z = -E_0 r \cos\theta \\ &\Rightarrow E_0 r P_1(\cos\theta) \end{aligned}$$

$$P_0(x) = 1$$

$$P_1(x) = x$$

$$P_2(x) = \frac{1}{2}(x^2 - 1)$$

$$\phi^{\text{II}}(\vec{r}) = \sum_{lm} A_{lm}^{\text{II}} r^l Y_{lm}(\Omega)$$

$$\phi^{\text{I,II}}(\vec{r}) = \sum_{lm} \left(A_{lm}^{\text{I}} r^l + \frac{B_{lm}^{\text{I}}}{r^{l+1}} \right) Y_{lm}(\Omega)$$

$\phi^{\text{I,II}}(\vec{r})$ should be independent of φ coordinate.

$$Y_{lm}(\Omega) \propto P_l^m(\cos\theta) e^{im\varphi}$$

$$A_{lm}^{\text{II}}, A_{lm}^{\text{I}}, B_{lm}^{\text{I}} = 0 \quad \text{if } m \neq 0$$

$$\phi^{\text{I}}(\vec{r}) = \sum_l \left(a_l r^l + \frac{b_l}{r^{l+1}} \right) P_l(\cos\theta)$$

$$\phi^{\text{II}}(\vec{r}) = \sum_l c_l r^l P_l(\cos\theta)$$

$$\int_{-1}^1 d\theta \sin\theta P_l(\cos\theta) P_{l'}(\cos\theta) = \frac{2}{2l+1} \delta_{ll'}$$

$$\int_{-1}^1 dx P_l(x) P_{l'}(x) = \delta_{ll'} \frac{2}{2l+1}$$

$$\phi^{\text{I}}(\vec{r}) \xrightarrow{r \rightarrow \infty} \sum_l a_l r^l P_l(\cos\theta) = -E_0 r P_1(\cos\theta)$$

$$a_1 r = -E_0 r \Rightarrow a_1 = -E_0$$

$$l \neq 1 \quad a_l r^l = 0 \Rightarrow a_l = 0 \quad \text{if } l \neq 1$$

$$\Phi^{\text{II}}(r^{\text{II}}) = \sum_{l=0}^{\infty} c_l r^l P_l(\cos \theta)$$

$$\Phi^{\text{I}}(r^{\text{I}}) = -E_0 r \cos \theta + \sum_{l=0}^{\infty} \frac{b_l}{r^{l+1}} P_l(\cos \theta)$$

$$\vec{\nabla} \times \vec{E} = 0 \Rightarrow \Delta E_{\parallel} = 0 \Rightarrow \Phi \text{ is continuous}$$

$$\vec{\nabla} \cdot \vec{D} = 0 \Rightarrow \Delta \Phi_{\perp} = 0$$

$$\Phi^{\text{I}}(R) = \Phi^{\text{II}}(R) \quad \Leftarrow$$

$$\epsilon_1 \frac{\partial \Phi^{\text{I}}}{\partial r} \Big|_{r=R} = \epsilon_2 \frac{\partial \Phi^{\text{II}}}{\partial r} \Big|_{r=R} \quad \Leftarrow$$