Chpt. 27 - Dielectric Properties of Insulators

Overview: 1. Micro vs. macro. (Fig. 27. 2)

$$\nabla \cdot E = -\underbrace{4\pi}_{\text{units}} \nabla \cdot P \quad , \quad P(r) = \frac{p(r)}{\text{vol.}} \leftarrow \text{unit cell}$$

2. $$E^{loc} = E(r) + E^{loc}_{near} - E^{macro}_{near}$$

$$= E(r) + \underbrace{E^{loc'}_{near}}_{0} + \frac{4\pi P}{3}$$

Lorentz relation (cubic symmetry)

$$D(r) = \varepsilon E(r)$$

$$\rightarrow E^{loc}(r) = \frac{\varepsilon + 2}{3} E(r)$$

$$p = \alpha E$$

$$\rightarrow \frac{\varepsilon - 1}{\varepsilon + 2} = \frac{4\pi\alpha}{3v} \quad \text{Clausius-Mossotti}$$

3. Polarizability

Atomic: $\alpha = \dfrac{Z_i e^2}{m(\omega_0^2 - \omega^2)}$

Displacement: $\alpha^{dis} = \dfrac{e^2}{M(\bar{\omega}^2 - \omega^2)} = \alpha^+ + \alpha^-$

4. Long-Wavelength optical modes:

$$\omega_L^2 = \frac{\varepsilon_0}{\varepsilon_\infty} \omega_T^2$$

5. Materials

Macroscopic Maxwell Eqs.

(MKS units)
(Chpt. 4 Jackson)

$$\nabla \cdot E = \frac{\rho}{\varepsilon_0}$$

$$D = \varepsilon_0 E + P$$

$$\boxed{\nabla \cdot E = \frac{\rho}{\varepsilon_0} - \frac{1}{\varepsilon_0} \nabla \cdot P}$$

$$\rho = 0 \rightarrow \nabla \cdot E = -\frac{1}{\varepsilon_0} \nabla \cdot P$$

$$E(r) = \int d^3 r' \, E^{micro}(r - r') f(r')$$

$$\nabla \cdot E(r) = \int d^3 r' \, \frac{\rho^{micro}(r - r')}{\varepsilon_0} f(r')$$

$$\rho^{micro}(r) = \sum_j \rho_j (r - r_j)$$ ion, atom, molecule location

$$\rho_0^{micro}(r) = \sum_j \rho_j^{\circ} (r - r_j^{\circ})$$ o means equilibrium

$$\nabla \cdot E(r) = \sum_j \int d^3 r' \, \frac{\rho^{micro}(r - r_j - r')}{\varepsilon_0} f(r')$$

$$\bar{r} = r - r_j - r'$$

$$r' = r - r_j - \bar{r}$$

$$= r - r_j^{\circ} - (\bar{r} + \underbrace{r_j - r_j^{\circ}}_{\Delta_j})$$

$$= \sum_j \int d^3 \bar{r} \, \rho^{micro}(\bar{r}) f(r - r_j^{\circ} - (\bar{r} + \Delta_j))$$

$$f(r - r_j^{\circ}) - (\bar{r} + \Delta_j) \cdot \nabla f(r - r_j^{\circ}) \cdots$$

$$\nabla \cdot E(r) = \sum_j \int d^3 \bar{r} \, \frac{\rho^{micro}(\bar{r})}{\varepsilon_0} f(r - r_j^{\circ}) \rightarrow \sum_j e_j f(r - r_j^{\circ}) \rightarrow 0$$

$$- \sum_j \int d^3 \bar{r} \, \frac{\rho^{micro}(\bar{r})}{\varepsilon_0} (\bar{r} + \Delta_j) \cdot \nabla f(r - r_j^{\circ})$$

$$e_j = \int d^3\bar{r}\, \rho_j(\bar{r})$$

$$p_j = \int d^3\bar{r}\, \rho_j(\bar{r})\, \bar{r}$$

$$\nabla \cdot E(r) = -\nabla \sum_j \left(\frac{p_j}{\varepsilon_0} f(r - r_j^\circ) + \frac{e_j}{\varepsilon_0} \Delta_j f(r - r_j^\circ) \right)$$

$$\boxed{\begin{aligned} p(R) &= \sum_{\substack{d \\ \text{basis}}} \left[e(d)\, u(R,d) + p(R,d) \right] \\ P(r) &= \sum_R f(r-R)\, p(R) \end{aligned}}$$

$$= \frac{1}{v} \sum_R v f(r-R)\, p(R)$$

$$\approx \frac{1}{v} \int d\bar{r}\, f(r-\bar{r})\, p(\bar{r}) \approx \frac{p(r)}{v} \approx P(r)$$

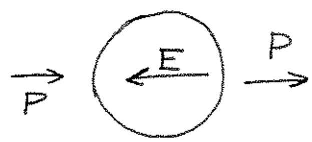
Local field:

$$E^{loc} = E^{loc}_{near} + E^{micro}_{far} = E^{loc}_{near} + E^{macro}_{far}$$

$$E = E^{macro}_{far} + E^{macro}_{near}$$

$$E^{loc} = E - E^{macro}_{near} + E^{loc}_{near}$$

$$\hookrightarrow E = -\frac{P}{3\varepsilon_0}$$



sphere

$$E^{loc} = E + E^{loc}_{near} + \frac{P}{3\varepsilon_0}$$

Approximation: $e(d)u(R+d) + p(R+d)$

cubic $\rightarrow E^{loc}_{near} = 0$

$$\boxed{E^{loc}_{(r)} = E(r) + \frac{P(r)}{3\varepsilon_0}}$$

(27.29)

$$D = \varepsilon E = \varepsilon_0 E + P \longrightarrow P = (\varepsilon - \varepsilon_0) E = \varepsilon_0 \left(\frac{\varepsilon}{\varepsilon_0} - 1\right) E$$

$$E^{loc} = \left(1 + \frac{\varepsilon - \varepsilon_0}{3\varepsilon_0}\right) E = \frac{2\varepsilon_0 + \varepsilon}{3\varepsilon_0} E$$

$$E^{loc} = \frac{\varepsilon/\varepsilon_0 + 2}{3} E$$

$$\text{If } p = \alpha E^{loc} \rightarrow P = \frac{\alpha}{V} E^{loc} = \varepsilon_0 \left(\frac{\varepsilon}{\varepsilon_0} - 1\right) E = \frac{\alpha}{V} \frac{\varepsilon/\varepsilon_0 + 2}{3} E$$

$$\rightarrow \boxed{\frac{\alpha}{3\varepsilon_0 V} = \frac{(\varepsilon/\varepsilon_0 - 1)}{(\varepsilon/\varepsilon_0 + 2)}}$$

Clausius-Mossotti relation $\frac{\varepsilon}{\varepsilon_0}$ to get α

Atomic Polarizability: (driven s.h.o.)

$$E^{loc} = Re\{E_0 e^{-i\omega t}\}$$

$$r = Re\{r_0 e^{-i\omega t}\} \qquad p = Re\{p_0 e^{-i\omega t}\} = -Z_i e r$$

$$Z_i m\ddot{r} = -Kr - Z_i e E^{loc}$$

$$-Z_i \omega^2 m r_0 = -K r_0 - Z_i e E_0$$

$$(Z_i m \omega^2 - K) r_0 = Z_i e E_0$$

$$r_0 = \frac{Z_i e E_0}{Z_i m \omega^2 - K} = \frac{e E_0/m}{\omega^2 - \underbrace{K/m Z_i}_{\omega_0^2}} = \frac{-e E_0/m}{\omega_0^2 - \omega^2}$$

$$p_0 = \frac{Z_i e^2 E_0/m}{\omega_0^2 - \omega^2}$$

$$\boxed{\alpha^{at} = \frac{Z_i e^2}{m(\omega_0^2 - \omega^2)}}$$

Simple model; $\omega \ll \omega_0$ $\quad \alpha^{at} = \dfrac{Z_i e^2}{m\omega_0^2}$

$\hbar\omega_0 \sim eV$ (atomic excitation)

not see until ultraviolet

Displacement polarizability

$$\vec{P} = e\vec{w} \qquad \vec{w} = \vec{u}^+ - \vec{u}^-$$

$$M_+ \ddot{u}^+ = -k(u^+ - u^-) + eE^{loc}$$

$$M_- \ddot{u}^- = -k(u^- - u^+) - eE^{loc}$$

$$\ddot{w} = -\frac{k}{M_+} w - \frac{k}{M_-} w + \frac{e}{M_+} E^{loc} + \frac{e}{M_-} E^{loc}$$

$$M^{-1} \equiv \frac{1}{M_+} + \frac{1}{M_-}$$

$$\ddot{w} = \frac{e}{M} E^{loc} - \underbrace{\frac{k}{M}}_{\bar{\omega}^2} w$$

$$(\bar{\omega}^2 - \omega^2)\, w = \frac{e}{M} E^{loc}$$

$$\boxed{\alpha = \frac{e^2}{M(\bar{\omega}^2 - \omega^2)}}$$

Same structure

$$\alpha = \alpha^+ + \alpha^- + \frac{e^2}{M(\bar{\omega}^2 - \omega^2)}$$

Apply CM rel:

$$\frac{\varepsilon/\varepsilon_0 - 1}{\varepsilon/\varepsilon_0 + 2} = \frac{\alpha}{3\varepsilon_0 V} = \frac{1}{3\varepsilon_0 V}\left(\alpha^+ + \alpha^- + \frac{e^2}{M(\bar{\omega}^2 - \omega^2)}\right)$$

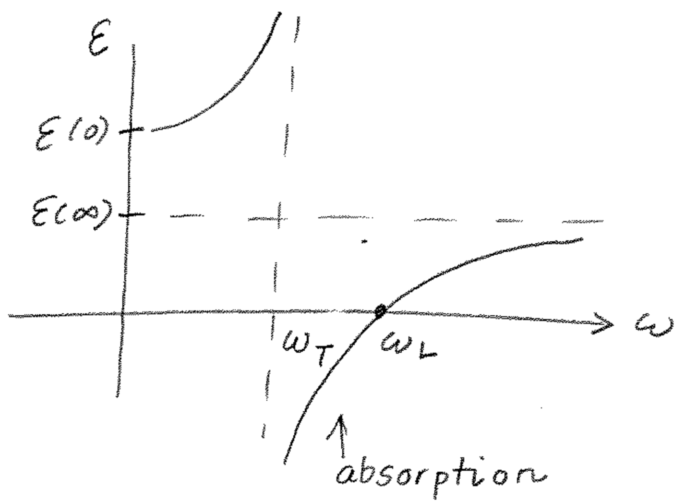
$$\frac{\varepsilon(0)/\varepsilon_0 - 1}{\varepsilon(0)/\varepsilon_0 + 2} = \frac{1}{3\varepsilon_0 V}\left(\alpha^+ + \alpha^- + \frac{e^2}{M\bar{\omega}^2}\right) \qquad \omega \ll \bar{\omega}$$

$$\frac{\varepsilon(\infty)/\varepsilon_0 - 1}{\varepsilon(\infty)/\varepsilon_0 + 2} = \frac{1}{3\varepsilon_0 V}\left(\alpha^+ + \alpha^-\right) \qquad \bar{\omega} \ll \omega \ll \omega_0$$

$$\frac{\varepsilon(\omega)/\varepsilon_0 - 1}{\varepsilon(\omega)/\varepsilon_0 + 2} = \frac{\varepsilon(\infty)/\varepsilon_0 - 1}{\varepsilon(\infty)/\varepsilon_0 + 2} + \frac{1}{1-(\omega/\bar{\omega})^2}\left(\frac{\varepsilon(0)/\varepsilon_0 - 1}{\varepsilon(0)/\varepsilon_0 + 2} - \frac{\varepsilon(\infty)/\varepsilon_0 - 1}{\varepsilon(\infty)/\varepsilon_0 + 2}\right)$$

$$\longrightarrow \boxed{\frac{\varepsilon(\omega)}{\varepsilon_0} = \frac{\varepsilon(\infty)}{\varepsilon_0} + \frac{(\varepsilon(\infty) - \varepsilon(0))/\varepsilon_0}{(\omega/\omega_T)^2 - 1}}$$

$$\omega_T^2 = \bar{\omega}^2\left(\frac{\varepsilon(\infty)+2}{\varepsilon(0)+2}\right) = \bar{\omega}^2\left(1 - \frac{\varepsilon(0) - \varepsilon(\infty)}{\varepsilon(0)+2}\right)$$



Optical Modes

no free charge $\rightarrow \nabla \cdot D = 0$

cubic $\rightarrow E \parallel D$

$\nabla \times E = 0$ (wait)

$E = 0$, $\varepsilon = \infty$
transverse
$D, E, P \perp k$

$D, E, P \parallel k$
longitudinal
D vanishes
$\varepsilon = 0 \quad E = -\frac{P}{\varepsilon_0}$

$$\omega_L^2 = \frac{\varepsilon_0}{\varepsilon_\infty} \omega_T^2$$

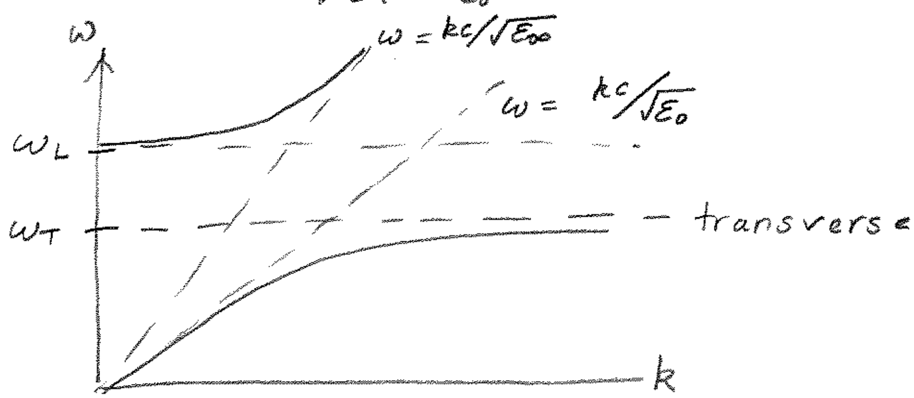
Lyddane-Sachs-Teller

More accurate: $\nabla \times E = -\frac{\partial B}{\partial t}$

$$\frac{\varepsilon(\omega)}{\varepsilon_0} = \frac{k^2 c^2}{\omega^2}$$

$kc \gg \omega$, $\varepsilon(\omega) = \infty$ ok

$$\omega = \frac{kc}{\sqrt{\varepsilon(\omega)/\varepsilon_0}}$$



no free currents & charges

$$\nabla \times H = \frac{\partial D}{\partial t} \qquad \nabla \cdot D = 0$$

$$\nabla \times E + \frac{\partial B}{\partial t} = 0 \qquad \nabla \cdot B = 0$$

$$\nabla \times (\nabla \times a) = \nabla(\nabla \cdot a) - \nabla^2 a$$

$$-\nabla^2 B = \varepsilon \frac{\partial}{\partial t} \nabla \times E = -\frac{\partial^2}{\partial t^2} \varepsilon B$$

$$-\nabla^2 E = -\frac{\partial}{\partial t} \nabla \times B = -\frac{\partial^2}{\partial t^2} \varepsilon E$$

$$\boxed{\cancel{\omega^2 = c^2 \frac{\varepsilon}{\varepsilon_0} k^2}} \qquad \omega = c\sqrt{\frac{\varepsilon_0}{\varepsilon}}\, k$$