① POLAR MATERIALS AND LO-TO SPLITTING

- WE DERIVED "DYNAMICAL MATRIX FORMALISM"
  (INTERATOMIC FORCE CONSTANT METHOD)

- LIMIT OF THIS APPROACH: NEGLECTING INTERACTION OF PHONONS WITH ELECTROMAGNETIC FIELD

FROM PREVIOUS LECTURE IN 3D WE HAVE:

$$\| D_{\nu\alpha,\nu'\alpha'}(q) - M_\nu \omega^2 \delta_{\alpha\alpha'} \delta_{\nu\nu'} \| = 0 \,;$$

$$D_{\nu\alpha,\nu'\alpha'}(q) = \sum_m D_{m\nu,\alpha,m\nu'\alpha'} \, e^{iq(t_m - t_{m'})}$$

DYNAMICAL MATRIX

$D_{m,m'} = D_{m,m'}$ IF $t_m - t_{m'} = t_m - t_{m'}$ — TRANS SYM

SOLUTION IN 3D

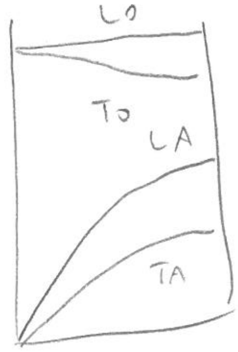
$$\vec{u}_{m\nu}(t) = \vec{A}_\nu(q,\omega) \, e^{i(q t_m - \omega t)}$$

$\vec{A}_\nu(q,\omega) \cdot \vec{q} = 0$ TRANSVERSAL PHONON $\times 2$

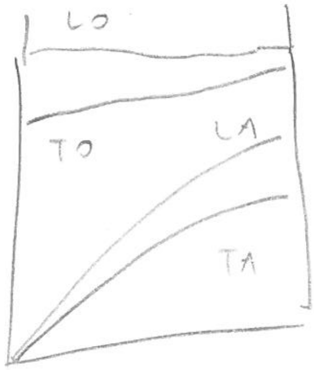
$\vec{A}_\nu(q,\omega) \cdot \vec{q} \neq 0$ LONGITUDINAL PHONON

IN NON POLAR MATERIALS $\omega_{LO}(q \to 0) = \omega_{TO}(q \to 0)$

IN POLAR MATERIALS $\omega_{LO}(q \to 0) \neq \omega_{TO}(q \to 0)$



VS



STRONG REFLECTION INFRARED LIGHT
BETWEEN $\omega_{TO} < \omega < \omega_{LO}$ & | RESTRAHLEN RADIATION

.) FURTHERMORE $\frac{\omega_{LO}^2}{\omega_{TO}^2} = \frac{\varepsilon_s}{\varepsilon_\infty}$

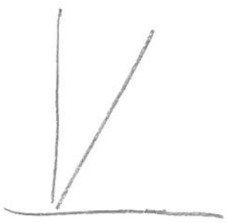
ε_s → DIELECTRIC CONSTANT INCLUDING PHONON

ε_∞ → DIELECTRIC CONSTANT WITHOUT PHONON CONTRIBUTION

.) DISPERSION OF LIGHT

$\omega(q) = \frac{cq}{\sqrt{\varepsilon_\infty}}$

WE EXPECT INTERACTION FOR $q_0 \simeq \sqrt{\varepsilon_\infty}\, \omega_{TO}/c$



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

SIMPLE HARMONIC OSCILLATOR

$\pm e^*$ M_1, M_2 M^*

$$\ddot{u}_n = -\omega_0^2 u_n + \frac{e^*}{M^*} E$$

$d = e^* u$

$$\ddot{d}_n = -\omega_0^2 d + \frac{e^{*2}}{M^*} E$$

(3) WE SEARCH FOR A STEADY-STATE SOLUTION

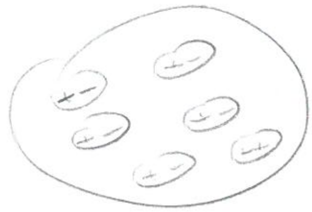
$$u = u_0 \, e^{i(kr - \omega t)}$$

RESPONSE PHIONS TO

$$E(r,t) = E_0 \, e^{i(kr - \omega t)}$$

$$u_0 = \frac{e^* E}{M(\omega_0^2 - \omega^2)}$$

$$P = \frac{N}{V} e^* \cdot u(r,t) \longrightarrow$$ THE MACROSCOPIC POLARIZATION



$$\frac{N}{V} = n \text{ (DENSITY)}$$

WE KNOW MAXWELL EQUATIONS IN SOLIDS

$$D = E + 4\pi P = \varepsilon E$$

$E \longrightarrow \nabla E = 4\pi \rho_{TOT}$

$D \longrightarrow \nabla D = 4\pi \rho_{EXT}$

FROM PREVIOUS EQUATION

$$\varepsilon = 1 + 4\pi \frac{N}{V} \frac{e^{*2}}{M(\omega_0^2 - \omega^2)}$$

$\Leftarrow$ ANOMALOUS DISPERSION IN THE REFRACTIVE INDEX

SELLMEIER EQ.

$\Downarrow$ INCLUDING ALSO ELECTRONS

$$\varepsilon(\omega) = \varepsilon_\infty + 4\pi \frac{N}{V} \frac{e^{*2}}{M(\omega_0^2 - \omega^2)}$$

FOR $\omega \gg \omega_T$ ATOMS CANNOT FOLLO ELECTRIC FIELD ONLY ELECTRON CONTRIBUTION

WE KNOW FROM GAUSS LAW THAT

$$\nabla D = 0 \qquad \nabla D = \nabla(\varepsilon \cdot E) \simeq \varepsilon \nabla E = \varepsilon (k \cdot E) = 0$$

CASE 1 (circled: C1)

$E_0 \perp k$

$(k \cdot E) = 0$

IF E_0 IS ZERO TRIVIAL CASE $u = P = D = 0$
NO ELECTRIC FIELD

OTHERWISE $\omega_i = \omega_T$

FOR TO PHONON $\varepsilon(\omega)$ HAS POLES AT $\omega = \omega_T$

CASE 2 $E_0 \parallel k \Rightarrow \varepsilon = 0$

$$\varepsilon(\omega_L) = 0 \qquad \omega_L^2 = \omega_T^2 + 4\pi \frac{N}{V} \frac{e^{*2}}{M \varepsilon_\infty}$$

WHEN $\varepsilon = 0$ $\quad D = 0 = E + 4\pi P$

$$\Rightarrow \quad E_L = -\frac{4\pi P}{\varepsilon_\infty} = -\frac{4\pi}{\varepsilon_\infty} \frac{N e^{*2}}{VM}$$

RESTORING
FORCE
PRODUCE
HIGHER FREQUENCY

IF YOU EXCITE A
LO PHONON THE
E CHANGE IS FREQUENCY

N, V, e^*, M^* DIFFICULT TO MEASURE LET DEFINE

① $$\varepsilon(0) = \varepsilon_\infty + \frac{4\pi}{M} \frac{N}{V} e^{*} \frac{1}{\omega_T^2}$$

② $$4\pi \frac{N}{V} \frac{e^{*2}}{M^*} = (\varepsilon_0 - \varepsilon_\infty)\, \omega_T^2$$

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$$\varepsilon(\omega) = \varepsilon_\infty + \omega_T^2 (\varepsilon_0 - \varepsilon_\infty) \frac{1}{\omega^2 - \omega_T^2}$$

$$\Downarrow$$

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

$$\Downarrow$$

$$\frac{\varepsilon(\omega)}{\varepsilon_\infty} = \frac{\omega_L^2 - \omega}{\omega_T^2 - \omega} \rightarrow \frac{\varepsilon_0}{\varepsilon_\infty} = \frac{\omega_L^2}{\omega_T^2} \ !!$$

LYDDANE - SACHS - TELLER RELATION

) MORE GENERAL CASE

FULL MAXWELL EQUATIONS

•) PROBLEMS WITH PREVIOUS RESULT

1) NOT FULL MAXWELL EQUATION

2) LO - TO SHOULD BE DEGENERATE AT $q = 0$ AT $q = 0$ NOT POSSIBLE TO DISTINGUISH LO AND TO !

FULL MAXWELL EQUATIONS REQUIRE

(6)

$$\begin{cases} \nabla D = 0 \\ \nabla B = 0 \\ \nabla \times H = \frac{1}{c}\frac{\partial D}{\partial t} \\ \nabla \times E = -\frac{1}{c}\frac{\partial B}{\partial t} \end{cases}$$

$B \to$ MAGNETIC INDUCTION

$H \to$ MAGNETIC FIELD

- SINCE EM WAVES ARE TRANSVERSE THEY COUPLE TO TO MODES

- FOR NON-MAGNETIC MATERIALS $B = H$

$$D = \varepsilon E = \varepsilon_\infty E + 4\pi P_{IND}$$

$$\nabla \times H = \frac{1}{c}\frac{\partial D}{\partial t} = \frac{\varepsilon_\infty}{c}\frac{\partial E}{\partial t} + \frac{4\pi}{c}\frac{\partial P}{\partial t}$$

$\Downarrow$

$$\nabla \times \nabla \times E = -\frac{1}{c}\frac{\partial \nabla \times B}{\partial t} = -\frac{1}{c^2}\frac{\partial^2 D}{\partial t^2}$$

$\Downarrow$

$$\nabla \times \nabla \times E = -\frac{\varepsilon_\infty}{c^2}\frac{\partial^2 E}{\partial t^2} - \frac{4\pi}{c^2}\frac{\partial P^2}{\partial t^2}$$

$\Downarrow$

$$\nabla \times \nabla \times = \vec{\nabla}(\nabla \ldots) - \nabla^2$$

$\Downarrow$

$$\begin{cases} -\nabla^2 E = -\frac{\varepsilon_\infty}{c^2}\ddot{E} - \frac{4\pi}{c^2}\ddot{P} \\ \ddot{P} = -\omega_T^2 P - \frac{N e^2 E}{M} = -\omega_T^2 P + (\varepsilon_0 - \varepsilon_\infty)\,\omega_T^2 \end{cases}$$

$$P = N e^* \vec{u}$$

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$$P = P_0\, e^{i(qr - \omega t)} \qquad E = E_0\, e^{i(qr - \omega t)}$$

IF WE SUBSTITUTE WE FIND:

$$\begin{cases} -\omega^2 P_0 = -\omega_0^2 P_0 + \omega_0 \dfrac{\varepsilon_0 - \varepsilon_\infty}{4\pi} E_0 \\ q^2 E_0 = \dfrac{\varepsilon_\infty}{c^2}\omega^2 E_0 + \dfrac{4\pi}{c^2}\omega^2 P_0 \end{cases}$$

$$\begin{vmatrix} \omega_0^2 - \omega^2 & -\omega_0^2 \dfrac{\varepsilon_s - \varepsilon_\infty}{4\pi} \\ -4\pi\omega^2 & c^2 q^2 - \varepsilon_\infty \omega^2 \end{vmatrix} = 0$$

SOLUTION

$$\omega^2 = \frac{1}{2\varepsilon_\infty}\left[\omega_0^2 \varepsilon_\infty + c^2 q^2 \pm \sqrt{(\omega_0^2 \varepsilon_s + c^2 q^2) - 4\omega_0^2 c^2 q^2 \varepsilon_\infty}\right.$$

TWO CASES $\quad (c/\sqrt{\varepsilon_\infty})\, q_0 = \omega_{TO} \qquad q \gg q_0$

$$\begin{cases} \omega^2 = \omega_0^2 = \omega_{TO}^2 & E_0 = 0 \quad P_0 \neq 0 \quad \text{PHONON} \\ \omega^2 = \dfrac{c^2}{\varepsilon_\infty} q^2 & E_0 \neq 0 \quad P = 0 \quad \text{light} \end{cases}$$

$q \ll q_0$

$$\begin{cases} \omega^2 = \omega_0^2 \dfrac{\varepsilon_s}{\varepsilon_\infty} = \omega_{LO}^2 & E_0 = -\dfrac{4\pi}{\varepsilon_\infty} P_0 \\ \omega^2 = \dfrac{c^2}{\varepsilon_s} q^2 & P_0 = \dfrac{\varepsilon_s - \varepsilon_\infty}{4\pi} E_0 \end{cases} \qquad q < q_0$$

MECANICAL - ELECTROMAGNETIC WAVE

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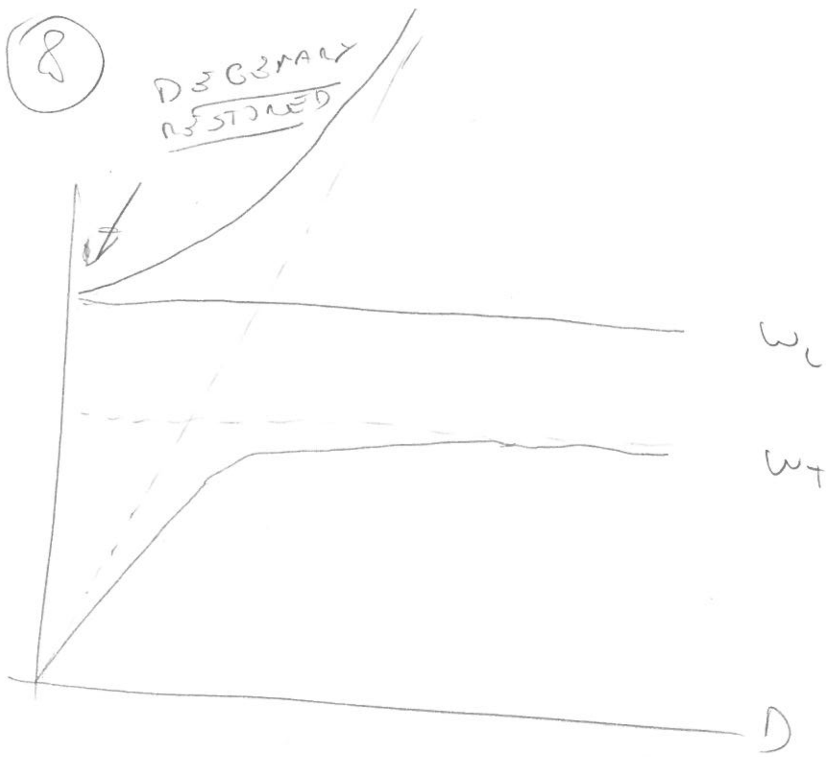

LEVEL

ANTI CROSSING

FOR $\omega \ll \omega_T$

TO CONTRIBUTE

TO THE DIELECTRIC

CONSTANT

CHANGE PHOTON

DISPERSION

ε_0 INSTEAD OF ε_∞