LECTURE # 17

Note Title 11/5/2007

FRI NOV 9 MAKEUP

NOV 14 MIDTERM II

ELECTRONIC STATES IN SOLIDS

→ Chapt 8 (All except proofs)

→ Chapt 9 Nearly-free electron 152-162 (No Brillouin Zones)

→ Chap 10 Tight-binding 176-183

→ $\boxed{\text{Chap 22}}$ Theory of Harmonic Crystal

① RESISTIVITY

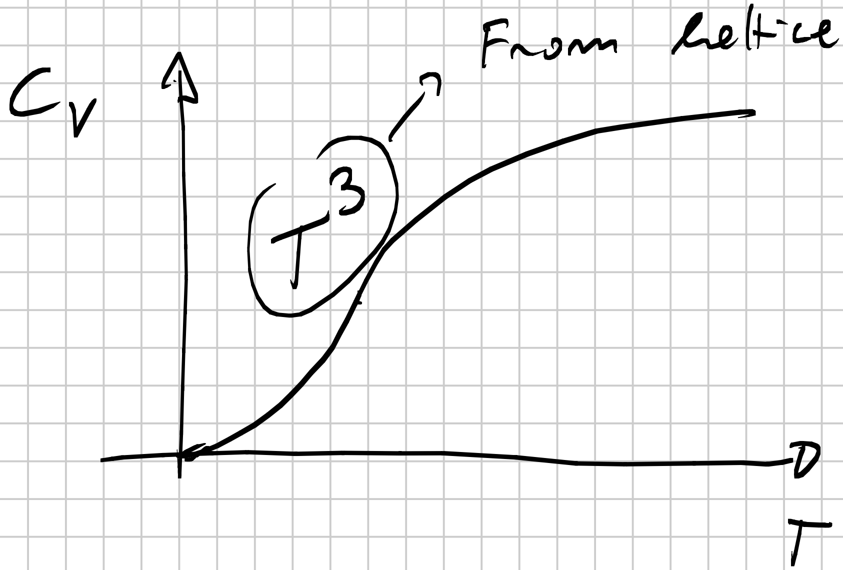
Electronic state

with $v_g = \dfrac{1}{\hbar}\dfrac{dE(k)}{dk}$ Group velocity

RESISTVITY = 0 FOR A

BLOCH ELECTRON

② Specific Heat



③ Transmission of sounds, melting ....

(Chp 21)

Fermions

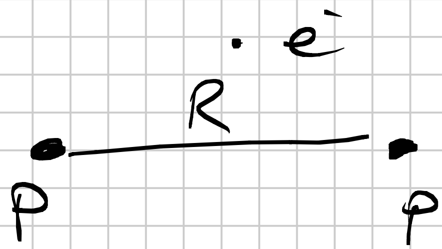
$$U \sim K_B T \left(\frac{K_B T}{\varepsilon_F} \right)$$

e^- at Fermi surface

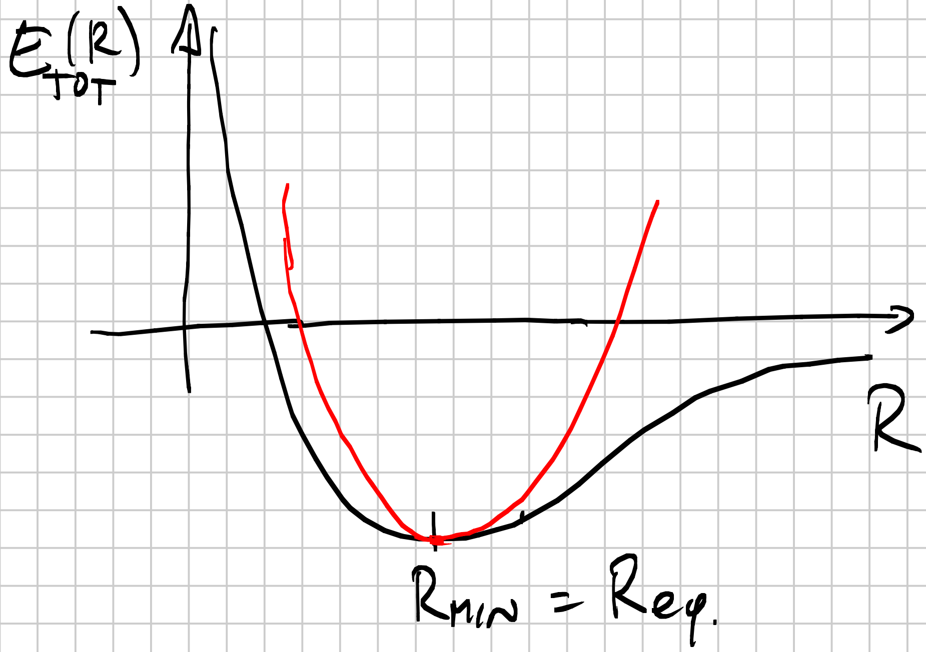
$$U \propto T^2 \qquad C_V = \frac{\partial U}{\partial T}$$

$$C_V \sim T$$

Go back to Molecule: H_2^+



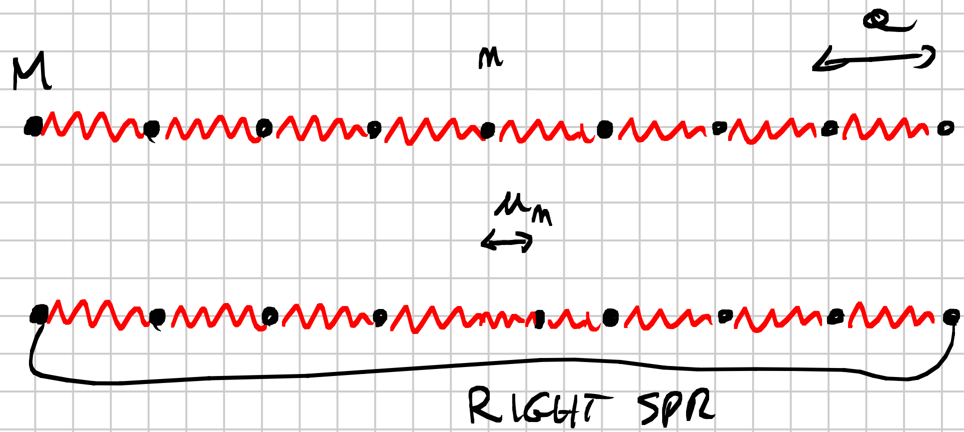
BORN - OPPENHEIMER APPROX



$$E_{TOT}(R) \sim \frac{1}{2} K (R - R_e)^2$$

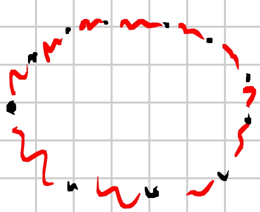
$$K = \frac{d^2 E_{TOT}}{d R^2}$$

$$\hbar = 0$$



$$M \ddot{u}_n = -K\,(u_n - u_{n+1}) - K\,(u_n - u_{n-1})$$

BORN VON KARMANN BOUNDARY CONDITIONS



$$\boxed{u_n(q) = e^{i(qna - \omega t)}} \rightarrow \text{WAVE} \qquad q = \frac{2\pi}{\lambda}$$

$\frac{\omega(q)}{2\pi}$ FREQUENCY OF OSCILLATION

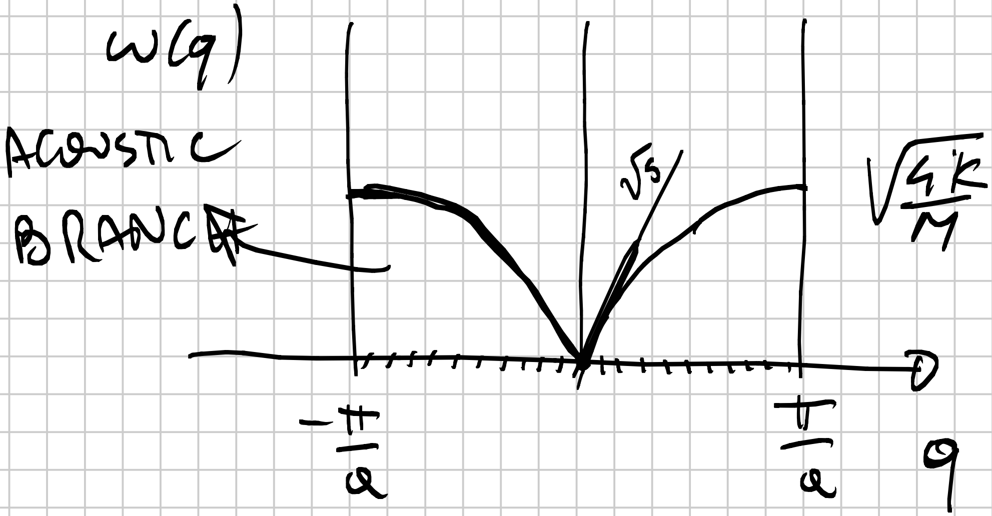
$\omega(q)$ $\qquad u_{n+1}(q) = e^{iqa} u_n(q)$

$$-M\omega^2 \cancel{u_n(q)} = -K\left(2 - e^{iqa} - e^{-iqa}\right) \cancel{u_n(q)}$$

$$\omega^2(q) = \frac{2K}{M}\left(1 - \cos qa\right) = \frac{4K}{M} \sin^2 \frac{qa}{2}$$

$$\omega(q + K_1) = \omega(q) \qquad u_n(q + K_1) = u_n(q)$$

$\Downarrow$ PLOT $\omega(q)$ in the 1° Brillouin Zone



$$\omega(q) = \sqrt{\frac{4K}{M}}\,\sin\frac{qa}{2}$$

N atoms

$$e^{iqNa} = 1$$

$$q = \frac{2\pi}{a}\frac{n}{N}$$

For small q = $(\lambda \to \infty)$

$\lambda \gg a$

$$\omega(q) \sim \sqrt{\frac{4K}{M}}\,\frac{qa}{2}$$

$$v_s = \frac{d\,\omega(q)}{dq} = \sqrt{\frac{K}{M}}\,a$$

Speed of sound in crystal

Crystal with a basis

1 2

same mass

u_{1n}

u_{2n}

$$\begin{cases} M\ddot{u}_{1m} = -K(u_{1m} - u_{2m}) - G(u_{1m} - u_{2m-1}) \\ M\ddot{u}_{2m} = -G(u_{2m} - u_{1m+1}) - K(u_{2m} - u_{1m}) \end{cases}$$

$$\begin{cases} u_{1m}(q) = \varepsilon_1 \, e^{i(qma - \omega t)} \\ u_{2m}(q) = \varepsilon_2 \, e^{i(qma - \omega t)} \end{cases}$$

$$\left[M\omega^2 - (K+G)\right]\varepsilon_1 + \left(K + G e^{-iqa}\right)\varepsilon_2 = 0$$

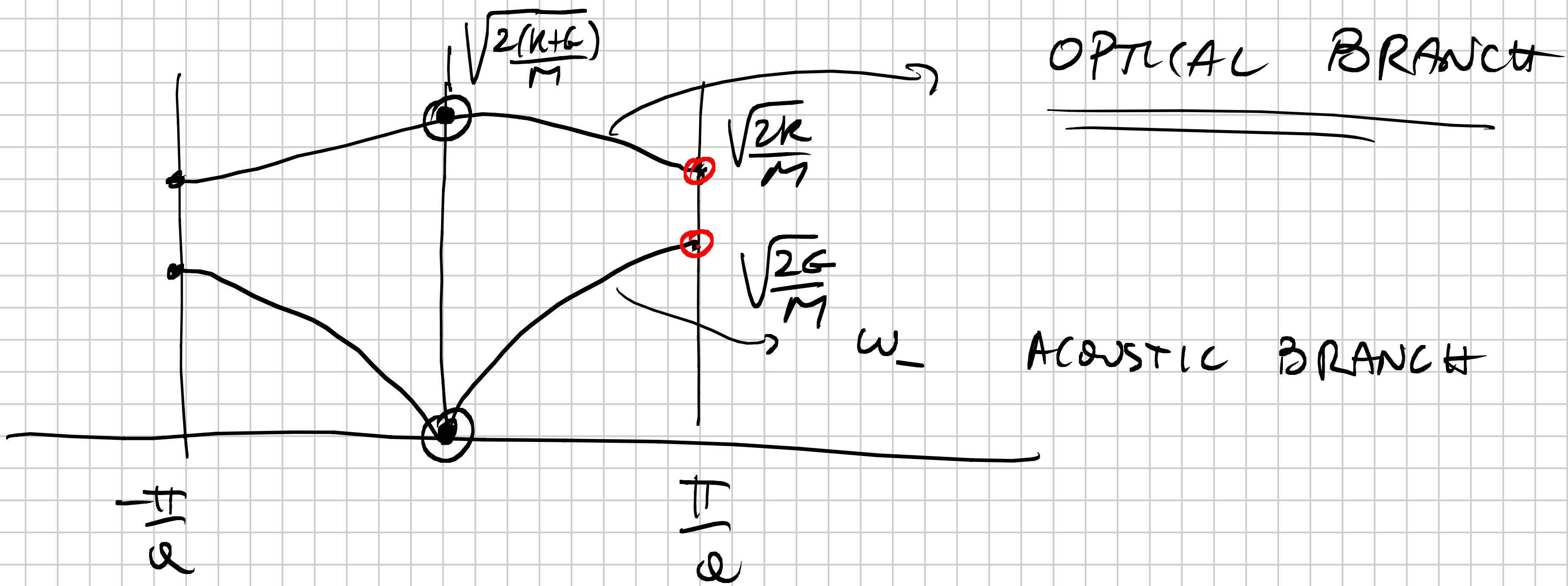
$$\left(K + G e^{iqa}\right)\varepsilon_1 + \left[M\omega^2 - (K+G)\right]\varepsilon_2 = 0$$

$$A(\omega)\begin{pmatrix}\varepsilon_1 \\ \varepsilon_2\end{pmatrix} = 0$$

$\Rightarrow$ Solutions only if $\boxed{\operatorname{Det} A(\omega) = 0}$

$$\left[M \omega^2 - (K+G)\right]^2 - \left(K^2 + G^2 + 2KG\cos qa\right) = 0$$

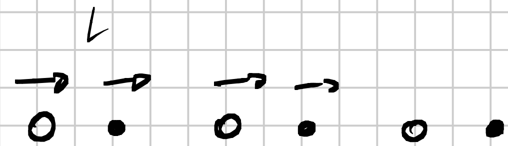
$$\omega_\pm^2(q) = \frac{K+G}{M} \pm \frac{1}{M}\sqrt{K^2+G^2+2KG\cos qa}$$



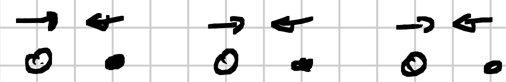
$$\omega_\pm \longrightarrow \frac{\varepsilon_1}{\varepsilon_2} = \mp \frac{K+Ge^{iqa}}{|K+Ge^{iqa}|}$$

FOR $q \to 0$

ACOUSTIC $\to$ $\varepsilon_1 = \varepsilon_2$



OPTICAL MODE $\varepsilon_1 = -\varepsilon_2$



FOR $q = \frac{\pi}{a}$

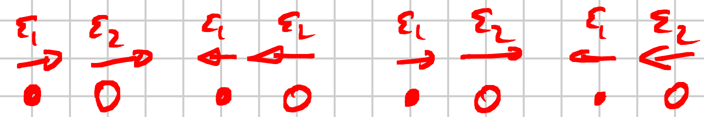
ACOUSTIC BRANCH

ε_1 ε_2 SAME DIRECTION

$$u_n e^{iqna} = e^{in\pi}$$

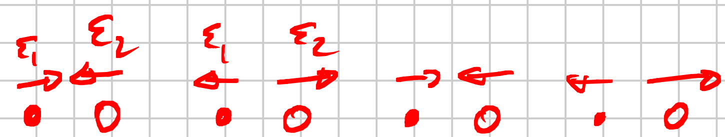
$$\downarrow$$

$$1 \quad -1$$



OPTICAL BRANCH

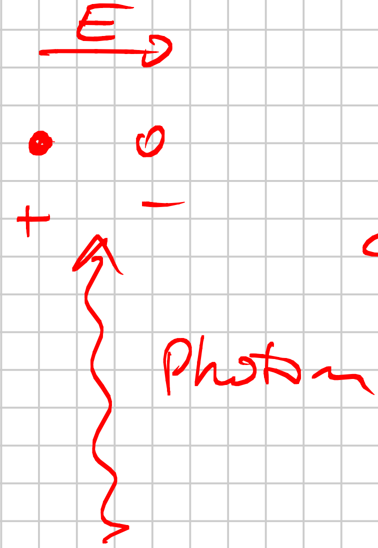
$\boxed{\varepsilon_1 \ \varepsilon_2 \text{ OPPOSITE}}$



LONGITUDINAL

$\vec{q} \parallel u$

1D



Optical Modes coupled to em waves

2D

1 LONGITUDINAL

1 TRANSVERSAL

3D

1 LONG

2 TRANSV