LECTURE #20

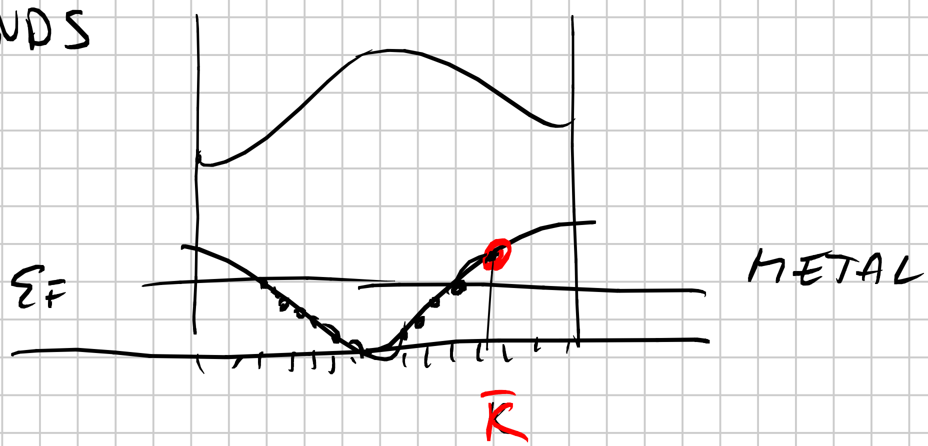
Note Title 11/17/2008

Chapt 10 176-183

Chapt 22 theory of harmonic crystal

ELECTRONIC STATES

BANDS



IF I HAVE A BLOCH ELECTRON WITH A GIVEN $\bar{K}$ THIS IS A STEADY-STATE SOLUTION

TRY TO CALCULATE RESISTIVITY $\Rightarrow$ NO RESISTIVITY AT ALL ...

WITHIN THE BLOCH ELECTRON PICTURE

SCATTERING OF ELECTRONS WITH FIXED IONS

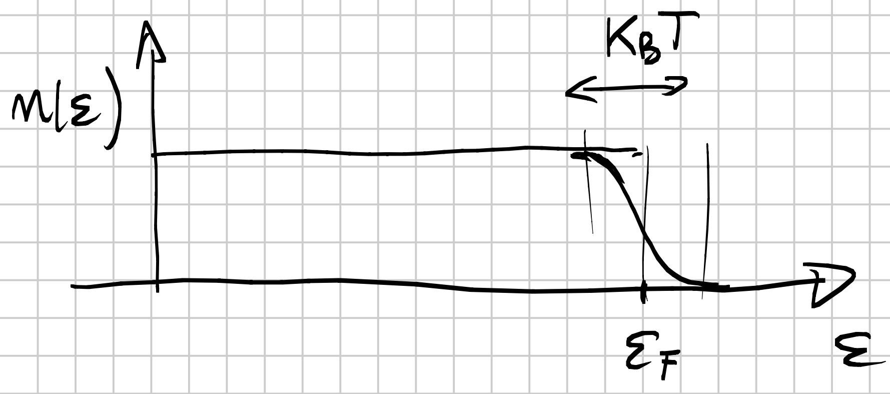
CANNOT EXPLAIN RESISTIVITY OF METALS

SPECIFIC HEAT

$$C_V = \frac{\partial U}{\partial T}$$

METAL CASE

FREE ELECTRONS IN A BOX



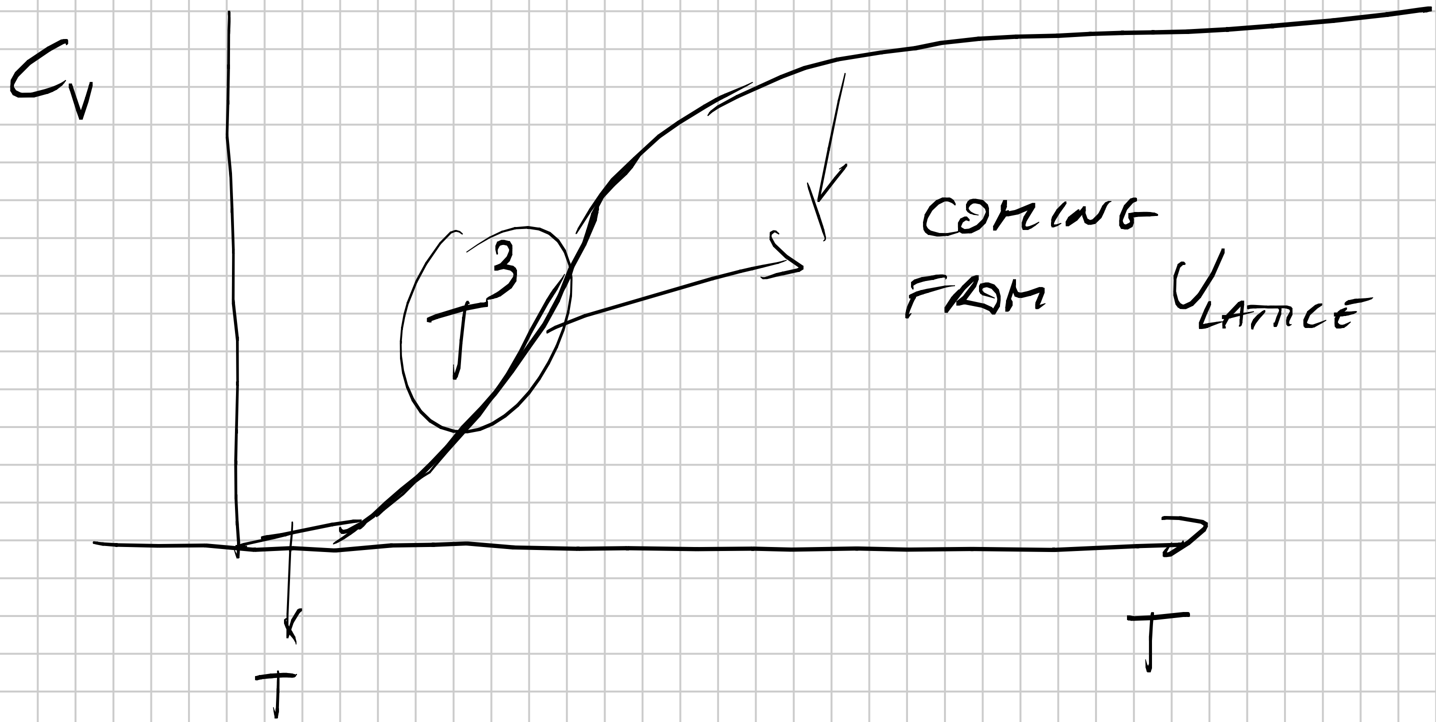
$$U \sim K_B T \left(\frac{K_B T}{E_F} \right)$$

% OF ELECTRONS ON FERMI SURFACE COMPARED TO TOTAL # ELECTRONS

$$U \sim T^2 \Rightarrow C_V \sim T$$

METALS!

$$U_{TOT}(T) = \underbrace{U(T)}_{ELECTRONS} + \underbrace{U(T)}_{LATTICE}$$



INSULATOR $U_{TOT}(T) \sim U_{LATTICE}(T)$

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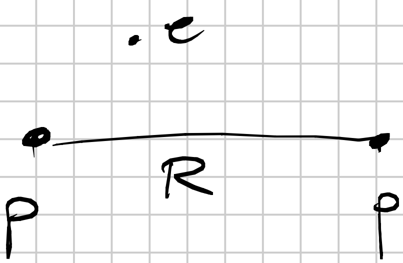
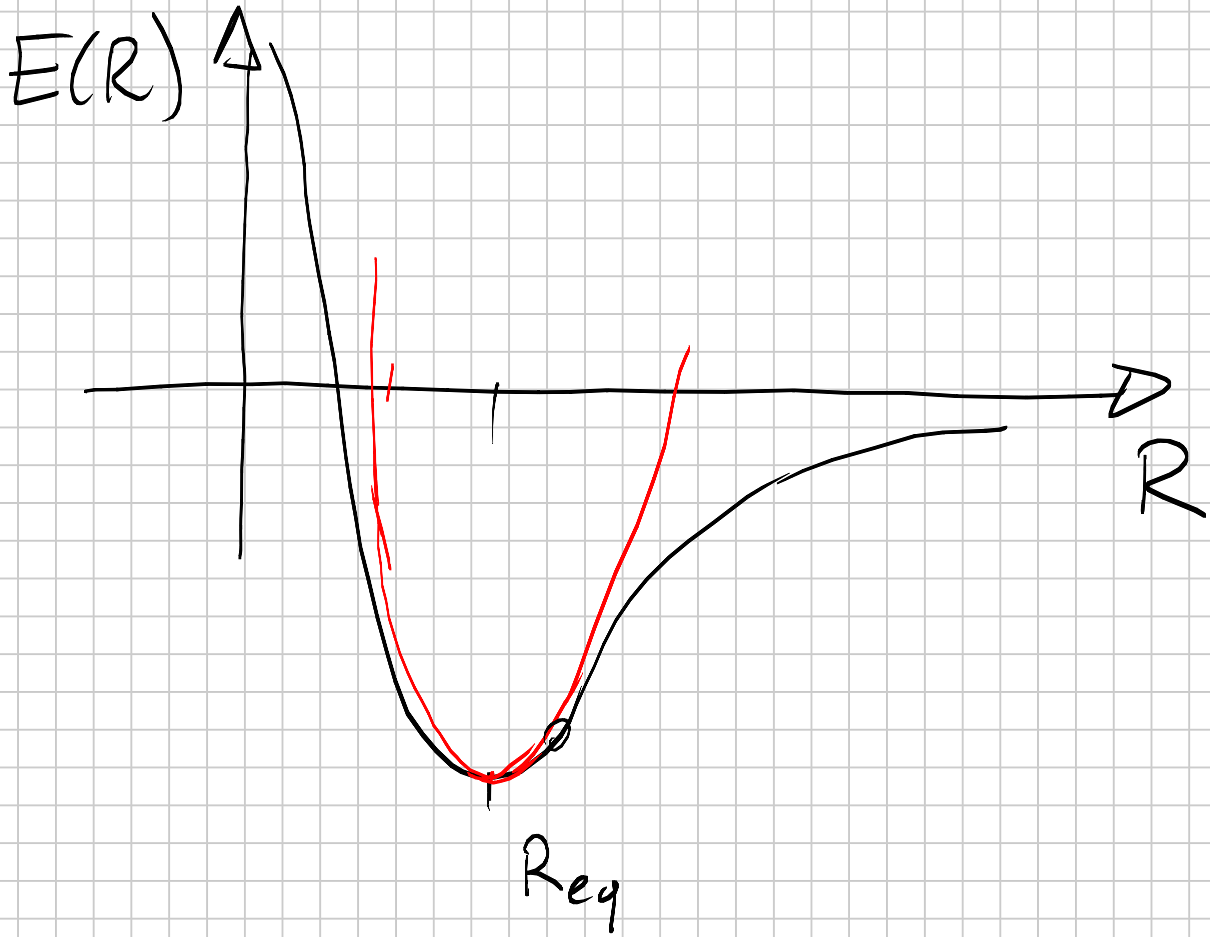
(3) → TRANSMISSION OF SOUND

→ MELTING

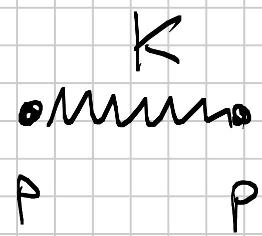
GO BACK TO H_2^+ MOLECULE



BORN-OPPENHEIMER APPROXIMATION

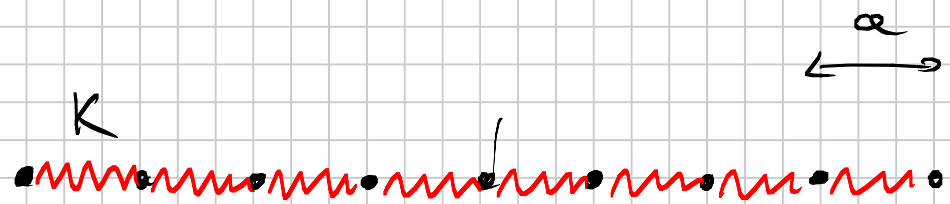


① HARMONIC APPROXIMATION



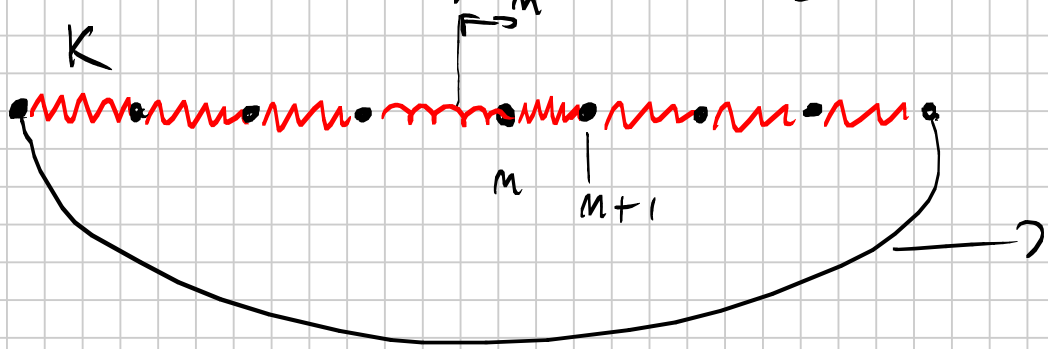
$$K = \left.\frac{d^2E(R)}{dR^2}\right|_{R=R_{eq}}.$$

LATTICE IN 1D



② ONLY FIRST NEIGHBOR INTERACTION

u_m → DEVIATION FROM EQUILIBRIUM POSITION



③ BORN - VON KARMAN BOUNDARY CONDITION

$$u_N = u_0$$

CLASSICAL EQUATION OF MOTION

$$M \ddot{u}_m = \underbrace{-K\left(u_m - u_{m+1}\right)}_{\text{RIGHT SPRING}} \underbrace{- K\left(u_m - u_{m-1}\right)}_{\text{LEFT SPRING}}$$

LOOK FOR SOLUTIONS OF THE FORM

$$u_m = e^{i(qma - \omega t)} \qquad q = \frac{2\pi}{\lambda} \qquad \lambda \text{ WAVE LENGTH}$$

$\frac{\omega(q)}{2\pi}$ = FREQUENCY OF OSCILLATION FOR THE OSCILLATION MODE q

$$u_{m+1}(q) = e^{i(q(m+1)a - \omega t)} = e^{iqa} u_m(q)$$

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

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

$$\frac{1-\cos x}{2} = \sin^2\frac{x}{2}$$

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

$$K = \frac{2\pi}{a}$$

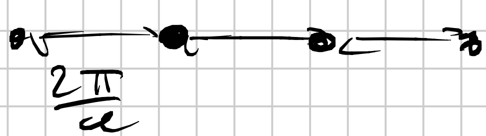
$$\omega(q + K)$$

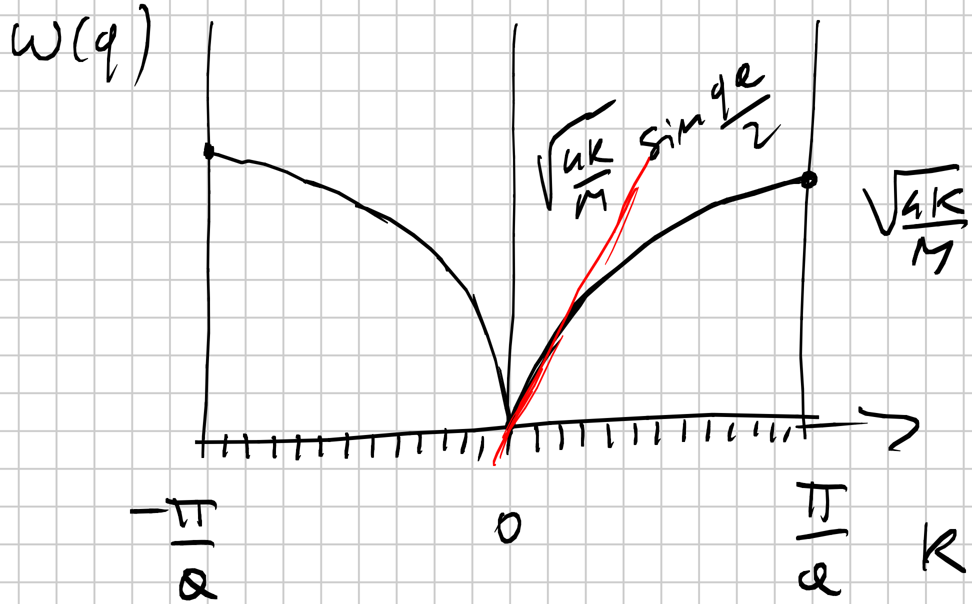
$$u_n \sim e^{iqna} \qquad e^{i(q+K)na}$$

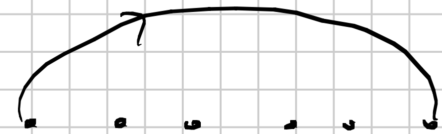
$$u_n(q) = u_n(q+K) \Rightarrow \omega(q) = \omega(q+K)$$

$\forall$ K VECTOR OF RECIPROCAL LATTICE

REAL SPACE







N ATOMS

$$e^{iqNa} = 1 \Rightarrow q = \frac{2\pi}{a}\frac{n}{N}$$

K (OR q) CRYSTAL MOMENTUM

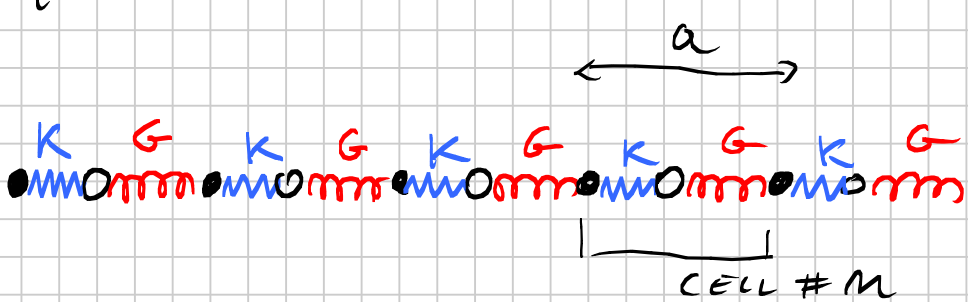
FOR SMALL q $\Rightarrow$ LARGE λ $(\lambda \gg a)$

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

GROUP VELOCITY FOR OSCILLATIONS (v_g)

$$v_g = \frac{d\,\omega(q)}{dq} \sim \sqrt{\frac{K}{M}}\,a$$ = SPEED OF SOUND IN SOLID

CRYSTAL WITH BASIS



$\bullet$, $\circ$ $\Big\}$ SAME MASS

I HAVE TO FIND

BOTH $u_{1,m}$ FOR $\bullet$

$u_{2,m}$ FOR $\circ$

$$\left.\begin{aligned} M\ddot{u}_{1m} &= -K\left(u_{1m}-u_{2m}\right)-G\left(u_{1m}-u_{2,m-1}\right) \\ M\ddot{u}_{2m} &= -G\left(u_{2m}-u_{1,m+1}\right)-K\left(u_{2m}-u_{1m}\right) \end{aligned}\right\}$$

LOOK FOR WAVE SOLUTIONS

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

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

$$\left(K + G e^{iqa}\right)\varepsilon_1 + \left[M\omega^2 - (K+G)\right]\varepsilon_2 = 0 \qquad (1)$$

$$\vec{\varepsilon} = \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \end{pmatrix}$$

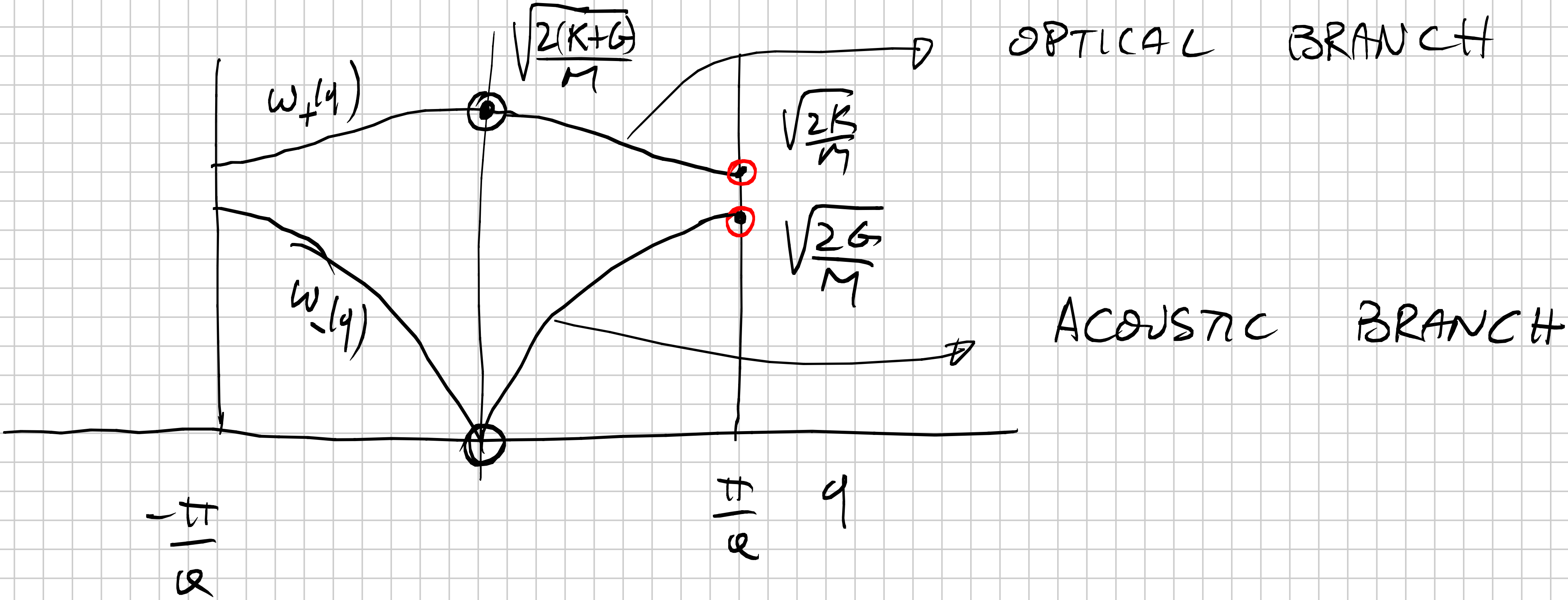
$$(1) = \left[A(\omega^2)\right] \cdot \vec{\varepsilon} = 0$$

2×2 MATRIX

SOLUTION WITH $\vec{\varepsilon} \neq 0$ ONLY IF

$$\text{DET } A = 0$$

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

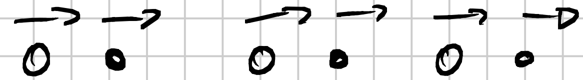


$$\omega_{\pm}(q) \Rightarrow \frac{\varepsilon_1(q)}{\varepsilon_2(q)} = \mp \frac{K+Ge^{iqa}}{|K+Ge^{iqa}|}$$

FOR $q \to 0$

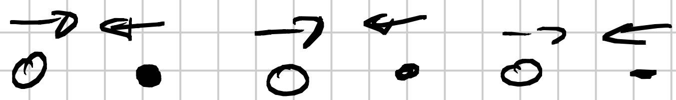
ACOUSTIC ω_- $\varepsilon_1 = \varepsilon_2$

MOVE TOGETHER SAME DIRECTION



OPTICAL ω_+ $\varepsilon_1 = -\varepsilon_2$

MOVE IN OPPOSITE DIRECTION



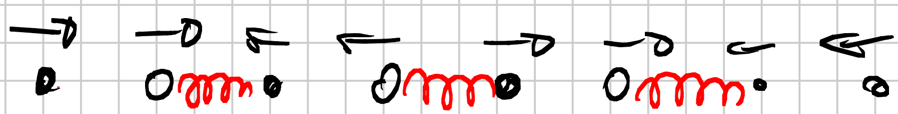
FOR $q = \frac{\pi}{a}$ $u_{n+1}\left(\frac{\pi}{a}\right) = -u_n\left(\frac{\pi}{a}\right)$

$\sqrt{\frac{2G}{M}}$

ACOUSTIC BRANCH $\varepsilon_1 = \varepsilon_2$

ONLY G

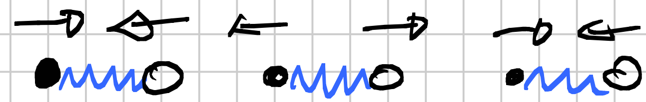
SPRING ENLARGED/COMPRESSED



OPTICAL BRANCH $\quad \varepsilon_1 = -\varepsilon_2$

$$\omega\left(\frac{\pi}{a}\right) \sim \sqrt{\frac{2K}{m}}$$

ONLY K SPRING IS ENLARGED/COMPRESSED



OPTICAL MODES

OSCILLATING DIPOLE

COUPLED TO LIGHT