LECTURE # 31

Note Title 4/6/2009

CHAPT 21 - 22 - 23

(1) CONDUCTIVITY

BLOCH ELECTRON HAS $\tau = \infty$

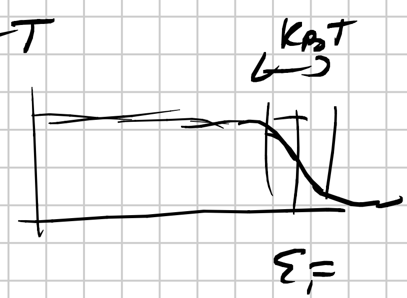
τ IN FINITE BECAUSE LATTICE IS NOT STATIC

ELECTRON - PHONON INTERACTION

(2) SPECIFIC HEAT OF SOLIDS

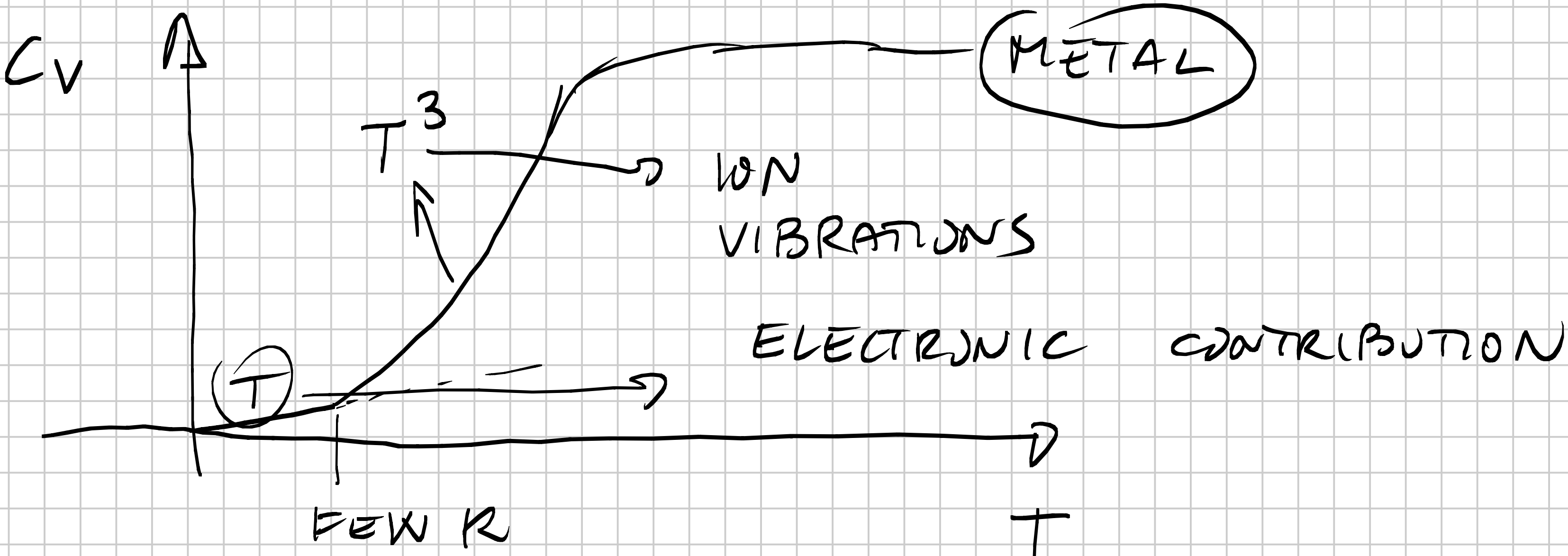
ELECTRONIC SPECIFIC HEAT

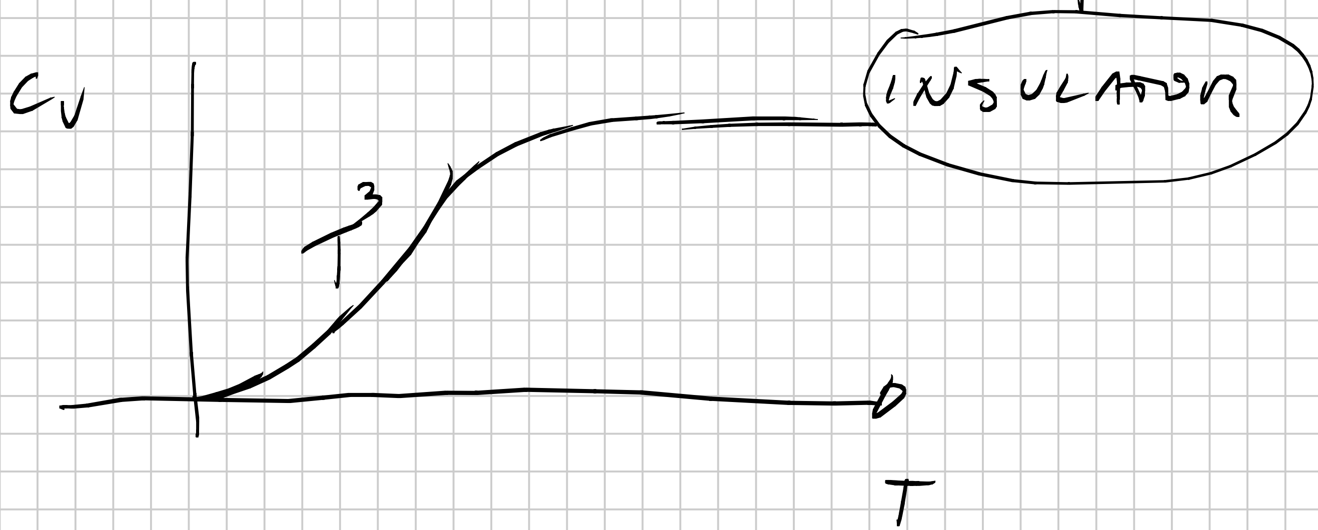
IN SOMMERFELD

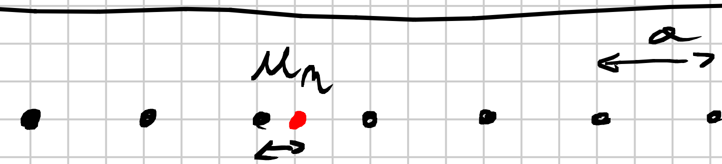


$$U \sim K_B T \left(\frac{K_B T}{\varepsilon_F} \right)$$

$$C_V \sim \frac{dU}{dT} \sim T$$







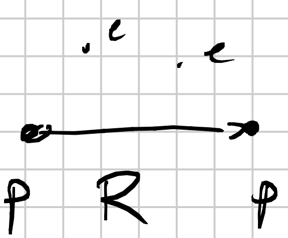
FOR EACH ION WE DEFINE u_n DEVIATION FROM EQUILIBRIUM

TOTAL ENERGY $U(\{u_m\})$

U INCLUDES BOTH ELECTRONS + IONS

HOW IS U FOR 2 IONS H_2 MOLECULE

2 P + 2 e



MOLECULAR SYSTEMS

BORN- OPPENHEIMER APPROX:

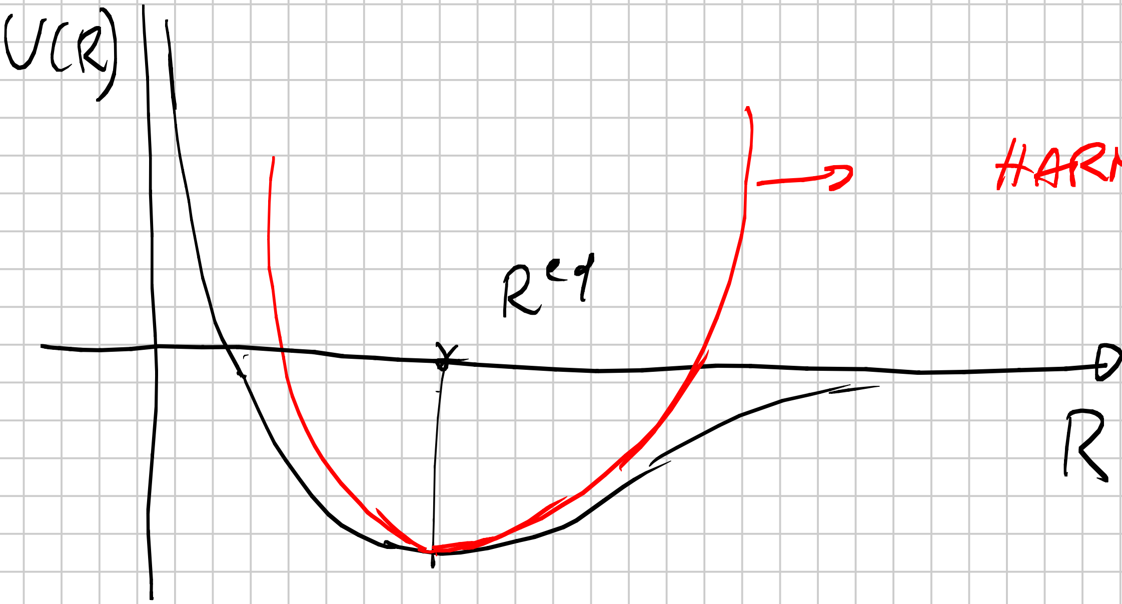
① FIX POSITION OF PROTONS AT R

② SOLVE PROBLEM FOR 2 ELECTRONS AS A FUNCTION OF R

$$U(R) = U_{eL}(R) + \frac{e^2}{R}$$

$\frac{e^2}{R}$ → P-P REPULSION

⊕ ⊖ ⊕ → COVALENT BONDING



HARMONIC APPROXIMATION FOR $U(R)$

$$U^H \sim \frac{\partial^2 U(R)}{\partial R^2}(R-R_{eq})^2$$

1D LATTICE

$$U = U_0 + \frac{1}{2}\sum_{nm} \left.\frac{\partial^2 U}{\partial u_n \partial u_m}\right|_{\{u_n\}=0} u_n u_m + O(u_n^3)$$

(1) HARMONIC POTENTIAL BETWEEN IONS

$$U = \sum_n \Phi(u_n - u_{n-1} + a)$$

↗ Φ IS ALWAYS THE SAME (2)

KEEP ONLY FIRST NEIGHBORS INTERACTION

$$\left.\frac{\partial^2 \Phi}{\partial u_n \, \partial u_{n-1}}\right|_{eq} = -\Phi''(a)$$

$$\left.\frac{\partial^2 \Phi}{\partial u_n^2}\right|_{equil} = 2\Phi''(a)$$

$$\Phi''(a) = K$$

$$U = U_0 + \frac{K}{2}\sum_n \left(2u_n^2 - u_n u_{n-1} - u_n u_{n+1}\right)$$

PERIODIC BC : $u_N = u_0$

EQ OF MOTIONS FOR IONS

$$M\ddot{u}_n = -\frac{\partial U}{\partial u_n} = -K\left(2u_n - u_{n+1} - u_{n-1}\right)$$

N EQUATIONS (# DEGREES OF FREEDOM)

$\Rightarrow$ N SOLUTIONS

LOOK FOR SOLUTION

$u_n = e^{i(qna - \omega t)}$ WAVE FORM

$u_n(q)$ $\quad q \to q + \frac{2\pi}{a}$

$e^{i\left(q + \frac{2\pi}{a}\right)na}$ $\quad u_n(q) = u_n\left(q + \frac{2\pi}{a}\right)$

$\Rightarrow \quad u_n(q) = u_n(q + G)$ $\quad G \in$ RECIPROCAL LATTICE

⇒ WE CAN TAKE

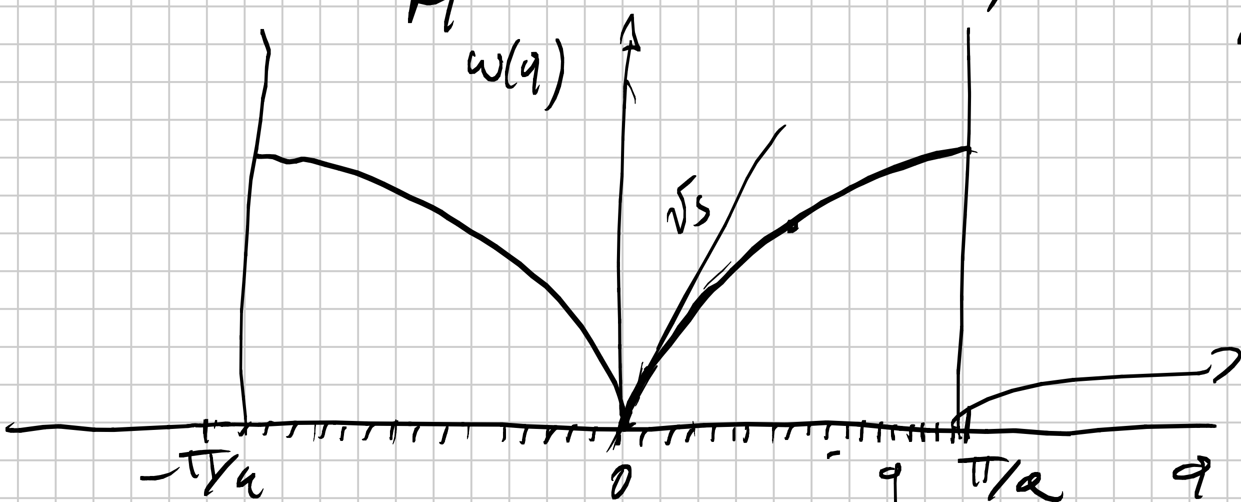
q IN THE FIRST BRILLOUIN ZONE

$\omega(q)$ $\qquad u_n(q) = e^{i(qna - \omega t)}$

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

$$-M\omega^2 u_n = -K(2u_n - u_{n+1} - u_{n-1}) = -K(2 - e^{iqa} - e^{-iqa}) u_n$$

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



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

$$\Delta q = \frac{2\pi}{Na}$$

ELASTIC WAVES IN THE CHAIN

ACOUSTIC MODE

$$V_G = \frac{d\,\omega(q)}{dq}$$

LIMIT OF SMALL q

$$V_G = \frac{d}{dq}\sqrt{\frac{4K}{M}}\,\frac{qa}{2} \to \sqrt{\frac{K}{M}}\,a = V_S$$

SPEED OF SOUND IN THE CHAIN