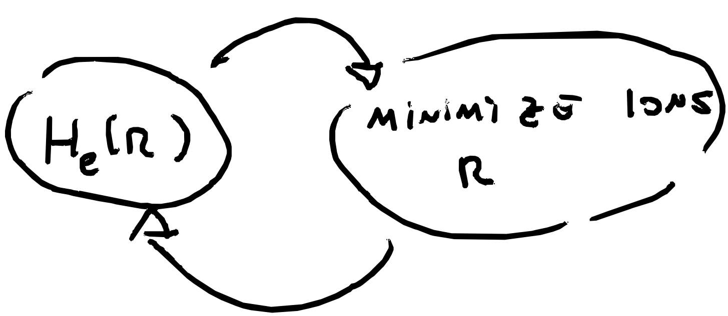
ELECTRON - PHONON

PHONON - PHONON and other scattering

BO DYNAMICS

$$\begin{cases} \left[T_e + V(r;R)\right]\psi(r;R) = E_0(R)\,\psi(r;R) \\ \\ \left[-\frac{h^2}{2M}\frac{\partial^2}{\partial R^2} + E(R_0) + \frac{1}{2}C\,(R-R_0)^2\right]\chi = \\ \\ \omega_m \chi_m \end{cases}$$

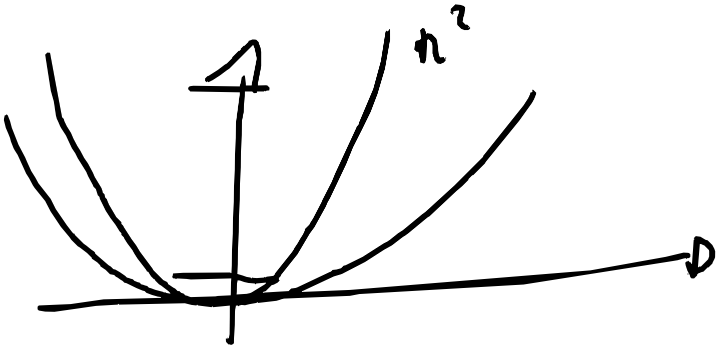


WHAT IS MISSING ?

A) HIGHER TERMS IN THE PHONON HAMILTONIAN

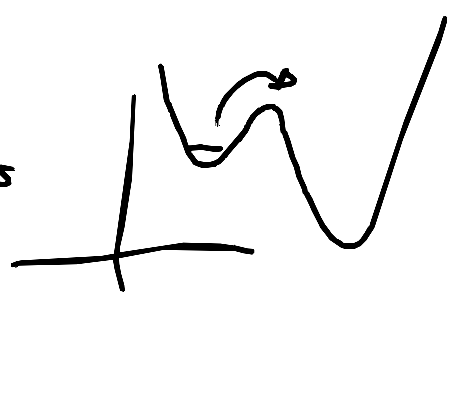
$$E(r_0) + \frac{1}{2} c \, (r-r_0)^2 + \frac{1}{6} D \, (r-r_0)^3$$

$$+ \frac{1}{4!} (r-r_0)^4 + \ldots\ldots$$

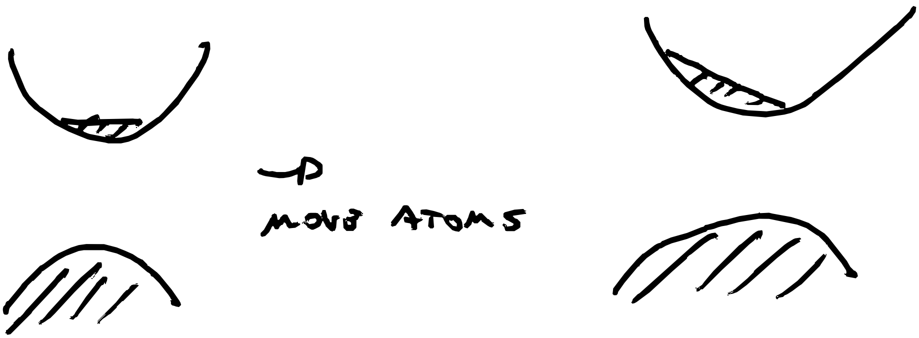


- AT LOW T THEY ARE LESS IMPORTANT

- PHASE TRANSITIONS



B) NON-ADIABATIC CORRECTION IN PHONON HAMILTONIAN

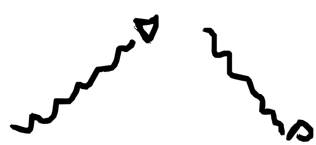


IMPORTANT FOR METAL/SEMIMETALS

C) OTHER SCATTERING FOR PHONONS

DEFECTS

BOUNDARY



D) ELECTRON - PHONON COUPLING

$$H_e \Psi = E(R_0)\Psi_0$$

MINIMIZE $E(R_0)$

$\downarrow$ BUT ATOMIC VIBRATION AFFECT ELECTRONS

$$H_e = T_e + V(r; R_0) + \nabla V \cdot \Delta r + \dots$$

Electron Phonon Coupling

$$H_{e\text{-}ion} = V(r - R)$$

$$H_{e\text{-}ion} \simeq V(r - R^\circ) + \underbrace{\nabla_R V(r - R)\big|_{R^\circ} \Delta u_I}_{V_{e\text{-}ph}}$$

$$\Delta u_I = \varphi(q,\omega)\left[e^{i(qR - \omega_0 t)} + e^{-i(qR + \omega t)}\right]$$

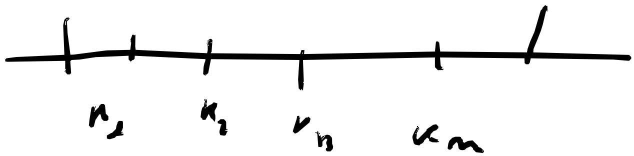
WE SUPPOSE WE ALREAD SOLVED THE PROBLEM AT EQUILIBRIUM

$$H_{el}(r; R^\circ)\,\phi_i(R^\circ) = E_i(R^\circ)\,\phi_i(R^\circ)$$

- WE WANT TO CALCULATE

$\langle \phi_i | V_{e\text{-}ph} | \phi_j \rangle$ MATRIX ELEMENTS

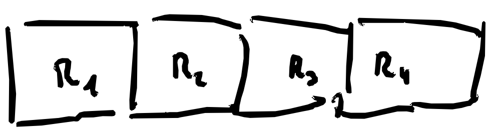
WE CONSIDER A SOLID



$$H_k \phi_{ik} = E_{ik} \phi_{ik}$$

$$\phi_{ik} = e^{ikr} u_{ki}(r)$$ BLOCH FUNCTIONS

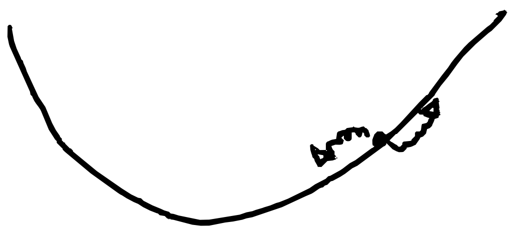
$$\langle \phi_{ik} | V_{e-ph} | \phi_{jk'} \rangle = \sum_L \int_{cell} \phi^*_{ik} | V_{e-p} | \phi_{jk'} \cdot dv(r)$$



$$= \underbrace{\sum_R e^{iR(k-k'+q)}}_{\to\ \delta(k-k'+q)} \cdot \int_{cell} \phi^*_{ik} V^{(q)}_{e-ph} \phi_{jk'}$$

$$\langle \phi_{ik} | V(q) | \phi_{k+q} \rangle = g^{ij}_{k,k+q}$$

WHAT IT MEANS?



$q = k' - k$

IF WE CALCULATE THE PROBABILITY TO JUMP WE GOT ALSO ENERGY CONSERVATION $E_i(k+q) - E_j(k) = \omega_q$!

IN ANOTHER WAY:

$$H = \begin{pmatrix} H_{k_1} & V_{en} & V_{en} \\ & H_{k_2} & \\ & & H_{k_3} \end{pmatrix}$$

e-ph COUPLES ELECTRONS AT DIFFERENT MOMENTUM !

EFFECT OF PHONONS ON ELECTRONS

$$\tilde{E}^i = E^i + \langle \phi_i | V_{e-ph} | \phi_i \rangle \langle u(r) \rangle$$

$$+ \sum_{i \neq j} \frac{|\langle \phi_i | V_{e-ph} | \phi_j \rangle|^2}{E^i - E^j} \langle u^2 \rangle$$

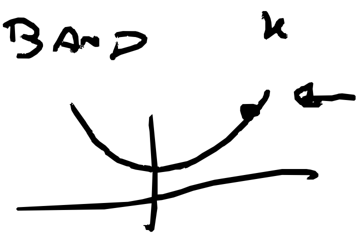
AVERAGE ON PHONONS TOO

$\langle u(r) \rangle = 0$! BECAUSE

$\chi_0 = e^{-(r-r_0)^2/\sigma^2}$ r IS ODD !

CONSIDER NOW THE ENTIRE BZ

CONSIDER NOW AN ELECTRON IN A BAND

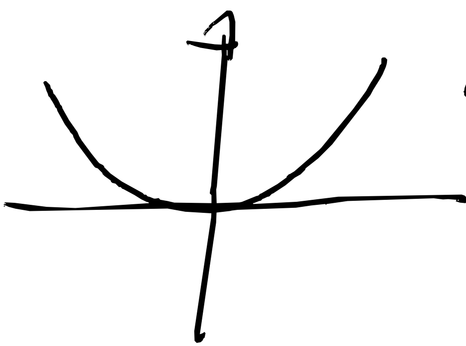


ITS INTERACTION WITH PHONONS

$$\tilde{E}(k) = E(k) - \frac{1}{N}\sum_q \frac{|g_{k,k+q}|^2}{E(k+q) + \hbar\omega_q - E(k)}$$

$$g_{k,k+q} \simeq g(q)$$

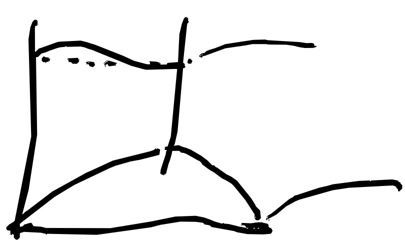
WE SUPPOSE TO HAVE PARABOLIC BANDS



$$E(k) = \frac{\hbar^2 k^2}{2m}$$

SUPPOSE optical PHONON AND

$\omega_q \sim \omega_0$



$$\tilde{E}(k) = E(k) - \frac{1}{N}\sum_q \frac{|g(q)|^2}{\frac{h^2(k+q)^2}{2m} + h\omega_0 - \frac{h^2k^2}{2m}}$$

$$= E(k) - \frac{1}{N}\sum_q \frac{|g(q)|^2}{h\omega_0 + \frac{h^2q^2}{2m} + \frac{h^2 k\cdot q}{2m}}$$

$$= E(k) - \frac{1}{N}\sum_q \frac{|g(q)|^2}{h\omega_0 + \varepsilon(q)}\left[1 - \frac{\frac{h^2\vec{k}\cdot\vec{q}}{m}}{h\omega_0+\varepsilon(q)}\right.$$

$$\left. + \left(\frac{h^2\vec{k}\cdot\vec{q}}{h\omega_0+\varepsilon(q)}\right)^2 + \dots\right]$$

FOR SMALL k THIS TERM CANCEL WITH INTERAL IN p

$$\Downarrow$$

$$E(k) - G_p - \frac{h^2k^2}{2m} \quad ;)$$

$$E_p = +\frac{1}{N}\sum_q \frac{|g(q)|^2}{\hbar\omega_0 + E(q)} > 0$$

$$\lambda = \frac{|g(q)|^2 q^2 \hbar^2}{[\hbar\omega_0 + E(q)]^2} \ll 1$$

USING $1 - \lambda \simeq \frac{1}{1+\lambda}$ FOR SMALL λ

$$E(k) = -E_p + \frac{\hbar^2 k^2}{2m(1+\lambda)} = -E_p + \frac{\hbar^2 k^2}{2m^*}$$

$m^* > m$!

- COUPLING WITH PHONONS LOWER ENERGY
- INCREASE MASS HEAVIER PARTICLES

POLARONS

AN ELECTRON SURROUNDED BY PHONONS

- WE CAN WRITE DOWN ITS WF.

$$|\psi(k)\rangle = |\psi_0\rangle + \frac{1}{\sqrt{N}} \sum_q \frac{g(q)}{E(k+q) + \hbar\omega_q - E(k)} \cdot |\psi_{k+q}\rangle |\chi_q\rangle$$

ELECTRON AND PHONONS TOGETHER !!

NOT SEPARATED ANYMORE

- E_p ENERGY OF LOCALLY DISTORTED LATTICE, POLARON ENERGY

- DISTORTIONS MOVES WITH ELECTRONS

$m^* > m$

IF WE HAVE QUANTUM PHONONS

$$\tilde{E}(k) = E(k) - \frac{1}{N}\sum_q \frac{(1 - \langle n_q \rangle)\, |g(q)|^2}{\hbar\omega_0 + \tilde{E}(k+q) - \tilde{E}(k)}$$

$$\langle n_q \rangle = \frac{1}{e^{\hbar\omega_0/kT} - 1}$$ BOSE DISTRIBUTION

- DIVERGENCES DUE TO LOW PERTURBATION ORDER
- THEORY VALID FOR DOPED SYSTEMS
- WITH MANY ELECTRONS ONLY CLOSE TO THE FERMI