

ELECTRON - PHONON INTERACTIONS

- The first goal is to derive a form of e-ph interaction Hamiltonian in second quantization, \mathcal{H} .
- We start by considering electrons moving in the ionic potential:

$$\mathcal{H}_1 = \sum_{k, k', e} \langle \vec{k} | U_0 (\vec{r} - \vec{R}_e - \vec{u}_e) | \vec{k}' \rangle c_{k'}^+ c_k' \quad (1)$$

↑
 single-ion
 potential ↑ displacement
 on equilibrium position

$$|\vec{k}\rangle = \frac{1}{\sqrt{N}} e^{i\vec{k}\cdot\vec{r}}$$

$$\mathcal{H}_1 = \sum_{k, k', e} e^{i(\vec{k}' - \vec{k}) \cdot (\vec{R}_e + \vec{u}_e)} V_{k-k'} c_{k'}^+ c_k' \quad (2)$$

Here V_k is the Fourier transform of $U_0(\vec{r})$.

- We now assume that displacement \vec{u}_e is small and expand

$$\begin{aligned}
 e^{i(\vec{k}' - \vec{k}) \cdot \vec{u}_e} &\approx 1 + i(\vec{k}' - \vec{k}) \cdot \vec{u}_e \\
 &= 1 + i \frac{1}{\sqrt{N}} (\vec{k}' - \vec{k}) \sum_q e^{i\vec{q} \cdot \vec{R}_e} u_q
 \end{aligned} \quad (3)$$

The leading term gives the usual Bloch Hamiltonian

$$\begin{aligned}
 \mathcal{H}_{\text{Bloch}} &= \sum_{k, k'} \left(\sum_e e^{i(\vec{k}' - \vec{k}) \cdot \vec{R}_e} \right) V_{k-k'} c_{k'}^+ c_k' \\
 &= N \sum_{k, G} V_G c_{k+G}^+ c_k
 \end{aligned} \quad (4)$$

e-ph interaction follows from the second term,

$$\mathcal{H}_{e-p} = \frac{i}{\sqrt{N}} \sum_{k, k'} (\vec{k}' - \vec{k}) \cdot \vec{u}_{k-k'} V_{k-k'} c_{k'}^+ c_k' \quad (5)$$

- We finally express \vec{H}_e in terms of phonon operators

$$\mathcal{H}_{e-p} = i \sum_{\epsilon, \epsilon', s} \left(\frac{N_k}{2M\omega_{k+\epsilon, s}} \right)^{1/2} (\vec{\epsilon} - \vec{k}) \cdot \vec{V}_{k+\epsilon} (a_{k+\epsilon, s}^+ + a_{k+\epsilon, s}) c_s^+ c_\epsilon$$

- in the following we assume (i) isotropic phonon spectrum (so that phonons are either longitudinally or transversely polarized) and (ii) we neglect the effect of H_{Bloch} (consider free electrons). This leads to FÖLICHT Hamiltonian:

$$\mathcal{H} = \sum_k \epsilon_k c_k^+ c_k + \sum_q \hbar \omega_q a_q^+ a_q + \sum_{k, q} H_q (a_{-q}^+ + a_q) c_{k+q}^+ c_k \quad (6)$$

$$H_q = i \sqrt{\frac{N_k}{2M\omega_q}} q V_q$$

- This is the simplest model for e-ph coupling in solids.

The Kohn anomaly: effect of electrons on the phonon frequencies

- How does e-ph coupling change the phonon spectrum?
- we consider a single phonon, propagating in the presence of the Fermi sea of electrons.
- assume WEAK e-ph interaction, treat \mathcal{H}_{e-p} as a perturbation

Unperturbed states: $|\phi_i\rangle : \mathcal{H}_0 |\phi_i\rangle = \epsilon_i |\phi_i\rangle$

Consider $|\phi_i\rangle = \underbrace{|\text{FS}\rangle}_{e} \underbrace{a_p^+ |0\rangle}_{\text{1 phonon with momentum } \vec{p}}$ (7)

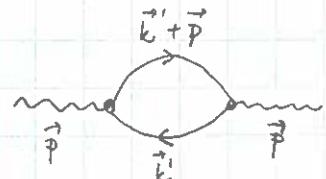
- second-order perturbation theory:

$$E_i \simeq E_i^{(0)} + \langle \phi_i | \mathcal{H}' | \phi_i \rangle + \langle \phi_i | \mathcal{H}' (E_i^{(0)} - \mathcal{H}_0)^{-1} \mathcal{H}' | \phi_i \rangle \quad (8)$$

Evaluate the second-order correction:

$$E_1^{(2)} = \langle \phi_1 | \sum_{kq} H_q (a_{-q}^+ + a_q) c_{k+q}^+ c_k (\epsilon_1 - \epsilon_0)^{-1} \times \sum_{k'q'} H_{q'} (a_{-q'}^+ + a_{q'}) c_{k'+q'}^+ c_{k'} | \phi_1 \rangle \quad (9)$$

Two possibilities: ① $-\vec{q} = \vec{q}' = \vec{p}$



$$\textcircled{2} \quad q = -q'$$

$$\textcircled{1} \quad \langle \phi_1 | \sum_{k'k} H_p H_{-p} a_p^+ c_{k-p}^+ c_k (\epsilon_1 - \epsilon_0)^{-1} c_{k+p}^+ c_{k'} a_p | \phi_1 \rangle \Rightarrow \rightarrow \vec{k} - \vec{p} = \vec{k}' \quad (10)$$

$$(\epsilon_1 - \epsilon_0) \rightarrow -(\epsilon_{k+p} - \epsilon_{k'} - \hbar\omega_p) \quad (11)$$

$$\textcircled{1} = - \sum_k |H_p|^2 \frac{\langle \phi_1 | a_p^+ c_{k-p}^+ c_k c_k^+ c_{k-p} a_p | \phi_1 \rangle}{\epsilon_k - \epsilon_{k-p} - \hbar\omega_p} \quad (12)$$

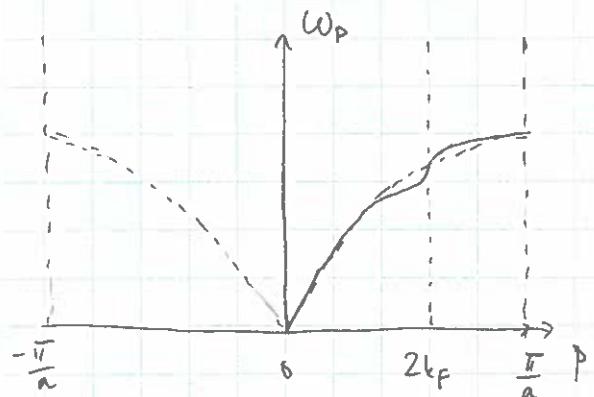
$$= - \sum_k |H_p|^2 \frac{\langle \phi_1 | c_{k-p}^+ c_{k-p} (1 - c_k^+ c_k) a_p^+ a_p | \phi_1 \rangle}{\epsilon_k - \epsilon_{k-p} - \hbar\omega_p}$$

$$\Rightarrow \boxed{\hbar\delta\omega_p = -|H_p|^2 \sum_k \frac{u_k (1 - u_{k+p})}{\epsilon_{k+p} - \epsilon_k - \hbar\omega_p}} \quad (13)$$

3 dimensions:

$\delta\omega_p$ is finite but exhibits an INFINITE SLOPE ($\delta\omega_p/dp \rightarrow \infty$) as $p \rightarrow 2k_F$

This is known as the "KOHN ANOMALY" and is often observed in phonon spectra in metals.

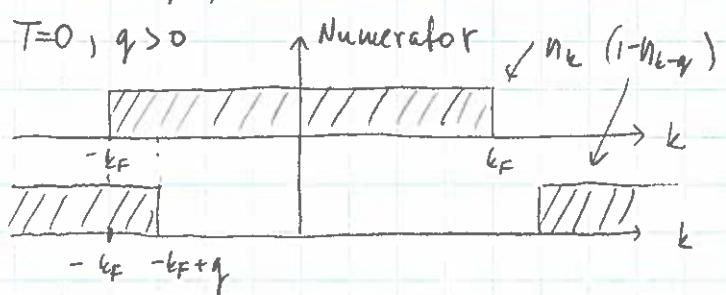


- Intuitively, Kohn anomaly can be interpreted as phonon spending some fraction of time as electron-hole pair  Because $v_F \gg v_{ph}$ the phonon speed of propagation effectively goes up.

- 1 dimension: "PEIERLS INSTABILITY"

- assume ω_q small compared to E_q , evaluate (13)

$$-\int_{-\infty}^{\infty} dk \frac{n_k (1 - n_{k-q})}{E_{k-q} - E_k}$$



$$\rightarrow - \int_{-k_F}^{-k_F+q} dk \frac{1}{(k-q)^2 - k^2}$$

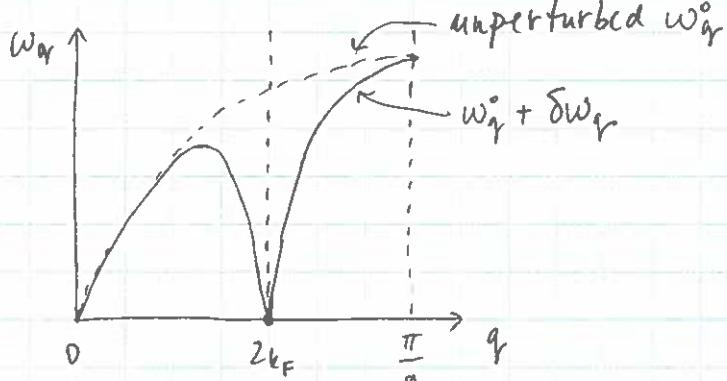
$$= - \int_{-k_F}^{q-k_F} \frac{dk}{q(q-2k)} = \frac{1}{2q} \ln |q-2k| \Big|_{-k_F}^{q-k_F} \quad (14)$$

We find

$$\delta\omega_q \sim \frac{1}{2q} (\ln |q-2k_F| - \ln |q+2k_F|) \quad (15)$$

- valid for all q .

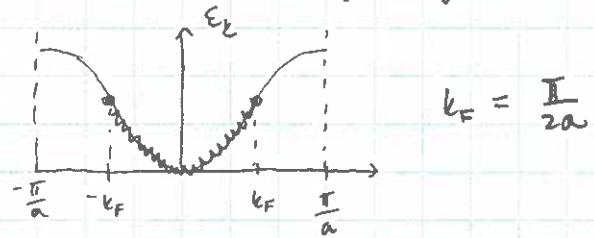
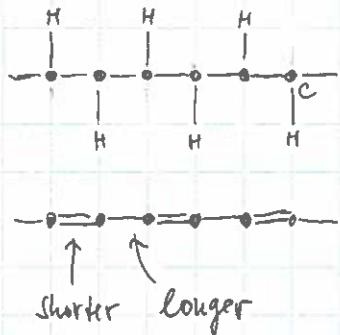
The correction is DIVERGENT as $q \rightarrow \pm 2k_F$.



A more careful treatment shows that $\omega_q \rightarrow 0$ as $q \rightarrow \pm 2k_F$ (not $\rightarrow -\infty$).

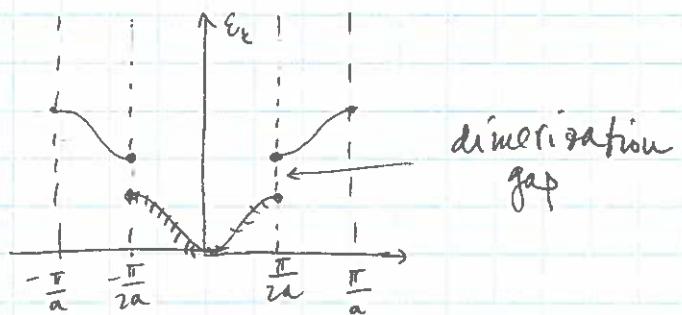
- This leads to "Bose-condensation" of $q = \pm 2k_F$ phonons. The result is a STATIC DISTORTION of the ion lattice, known as the Peierls instability.

- A classic example of Peierls physics occurs in polyacetylene



Peierls instability occurs at
 $q = \pm 2k_F = \pm \frac{\pi}{a}$

This leads to "dimerization" of the carbon chain

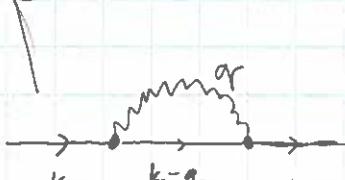


POLARONS AND THE MASS ENHANCEMENT

- What is the effect of e-ph interaction on the electron spectra? This can be understood from contraction ② in Eq. (9)

$$\rightarrow - \sum_{kq} |M_{kq}|^2 \frac{\langle \phi_0 | a_q c_k^+ c_{k-q} a_q^\dagger c_{k-q}^\dagger c_k | \phi_0 \rangle}{\epsilon_k - \epsilon_{k-q} - \hbar\omega_q} \quad (16)$$

- this expression can be regarded as "electron self-energy"



- electron emits a phonon and then absorbs it back
- evaluating as before we obtain

$$E_0^{(2)} = \sum_{k,q} |H_q|^2 \frac{n_k(1-n_{k+q})}{\epsilon_k - \epsilon_{k+q} - \hbar\omega_q} \quad (17)$$

- Because the effective single-electron Hamiltonian reads

$$\begin{aligned} H_e &= \sum_k (\epsilon_k + \delta\epsilon_k) c_k^\dagger c_k \\ &= \sum_k (\epsilon_k + \delta\epsilon_k) n_k \end{aligned} \quad (18)$$

we seek the e-ph correction to the energy by taking

$$\begin{aligned} \delta\epsilon_k &= \frac{\partial E_0^{(2)}}{\partial n_k} = \sum_q |H_q|^2 \left[\frac{1-n_{k+q}}{\epsilon_k - \epsilon_{k+q} - \hbar\omega_q} - \frac{n_{k+q}}{\epsilon_{k+q} - \epsilon_k - \hbar\omega_q} \right] \\ &= \sum_q |H_q|^2 \left[\frac{1}{\epsilon_k - \epsilon_{k+q} - \hbar\omega_q} - \frac{2\hbar\omega_q n_{k+q}}{(\epsilon_k - \epsilon_{k+q})^2 - (\hbar\omega_q)^2} \right] \end{aligned} \quad (19)$$

- The first term represents correction indep. of n_k and would be present even in an insulating crystal
 - it changes the effective mass of electron near the bottom of the band \rightarrow electron is "dressed" with a cloud of phonons and becomes "polaron"
- The second term leads to velocity change near the Fermi level:

$$\begin{aligned} \hbar v_e &= \frac{\partial (\epsilon_k + \delta\epsilon_k)}{\partial k} \\ &= \frac{\partial \epsilon_k}{\partial k} \left[1 - \frac{1}{\partial \epsilon_k / \partial k} \sum_q |H_q|^2 \frac{2\hbar\omega_q n_{k+q}}{(\epsilon_k - \epsilon_{k+q})^2 - (\hbar\omega_q)^2} \right] \\ &\approx \hbar v_e^0 (1-\alpha) \quad (\text{near } k_F) \end{aligned} \quad (20)$$

- velocity becomes REDUCED near FS which can be attributed to electron being slowed down by the phonon cloud.