Lecture 14 | Electron phonon interaction

Positively charged ions produce charged background for electron's motion. When ion's motion produces change in density the electron density will follow. Relative change in density is $\delta n = -n \, \mathrm{div}\, u$. As a result Fermi level which is $\propto n^{2/3}$ will change by the amount $\sim \frac{\delta n}{n} \varepsilon_F$. Thus we can estimate the strength of the electron phonon interaction as

$$V_{e\text{-}ph} \sim \varepsilon_F \, \mathrm{div}\, \vec{u}$$

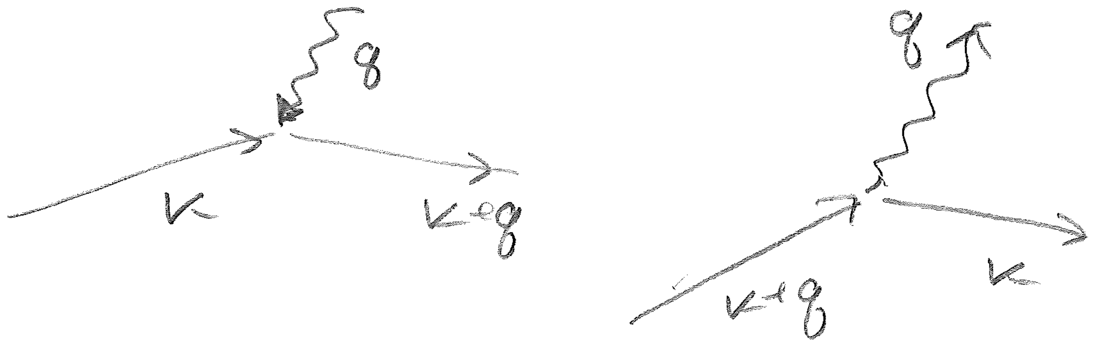
The main interaction is with longitudinal phonons. Transverse phonons produce much weaker interaction.

In second quantization we can write the electron-phonon coupling as

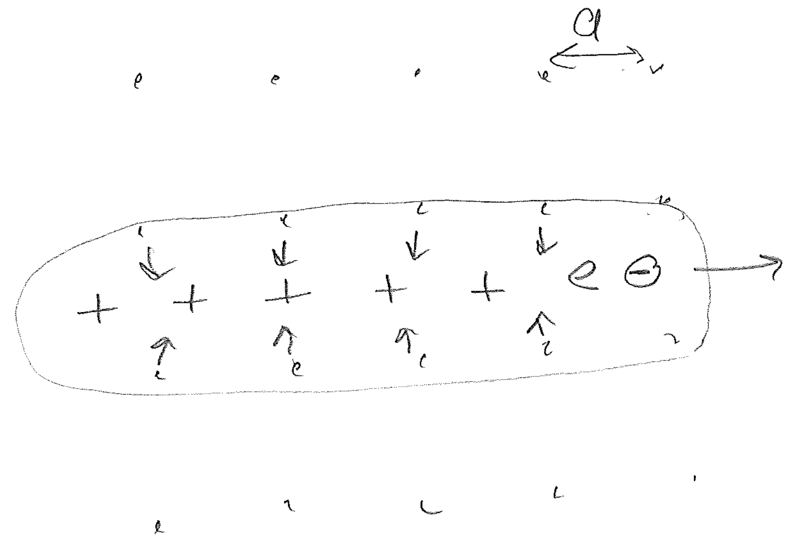
$$H_{e\text{-}ph} = \frac{i}{2} \sum q \left(V_{-q} u_q a^+_{k+q} a_k - V_q u_{-q} a^+_k a_{k+q} \right)$$

with $u_q = \left(\frac{\hbar}{2 M \omega_q} \right)^{1/2} \vec{e}_q \left(b_k + b^+_{-k} \right)$

b^+_{-k} and b_k a phonon creation and annihilation operators. This Hamiltonian corresponds to emission or absorption of phonon

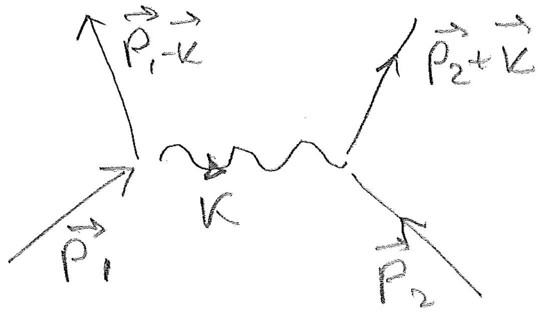


Electron-phonon interaction leads to effective attraction between the electrons which is responsible for superconductivity



An electron moving through the lattice attracts ions. Ion relaxation is relatively slow thus there will be long living ion cloud.
Typical lattice frequency $\omega_D \simeq c k_F \simeq \varepsilon_F \sqrt{\frac{m}{M}} \Rightarrow$ Ion trace is elongated along the motion for $L \sim \sqrt{\frac{M}{m}}\, a_0$. Second electron moving in the opposite direction passes through the same cloud and lowers it's energy. Attraction is most efficient for two electrons with the opposite momenta

Interaction between the electrons due to exchange of phonon can be represented by the following diagram. One electron with momentum $\vec{p}_1$

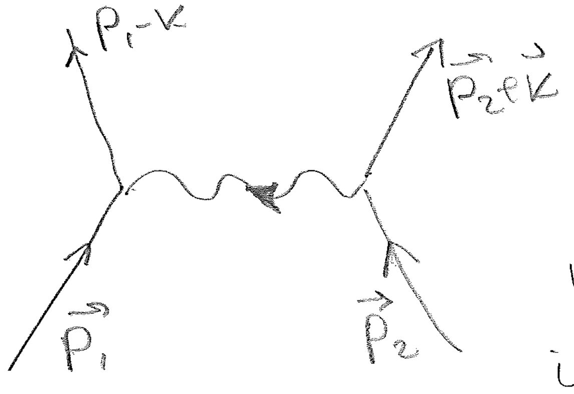


emits the phonon of momentum $\vec{k}$. The phonon is absorbed by a second electron which has had momentum $\vec{p}_2$ before the absorption. $\vec{p}_1 \to \vec{p}_1{}' = \vec{p}_1 - \vec{k}$, $\vec{p}_2 \to \vec{p}_2{}' = \vec{p}_2 + \vec{k}$. The amplitude of this process in second order of perturbation theory is given by

$$\frac{|V_k|^2}{\varepsilon(p_1) - \varepsilon(p_1') - \hbar\omega(k)},$$

where V_k is the matrix element for electron phonon interaction.

On the other hand there is another process



Here an electron $(\vec{p}_2)$ emits a phonon with momentum $(-\vec{k})$ which is then absorbed by the first electron $(\vec{p}_1)$

The amplitude of this process is

$$\frac{|V_k|^2}{\mathcal{E}(p_2) - \mathcal{E}(p_2') - \hbar\omega(k)}$$

We have to add both amplitudes

Since the energy conservation law gives

$$\mathcal{E}(p_1) + \mathcal{E}(p_2) = \mathcal{E}(p_1') + \mathcal{E}(p_2')$$

the total amplitude is

$$\frac{2|V_k|^2\,\omega(k)}{\hbar^2(\omega^2 - \omega^2(k))}, \quad \text{where } \hbar\omega = \mathcal{E}(p_1) - \mathcal{E}(p_1')$$

It appears that $|V_k|^2 \propto \omega(k)$ and as a result we obtain the total amplitude

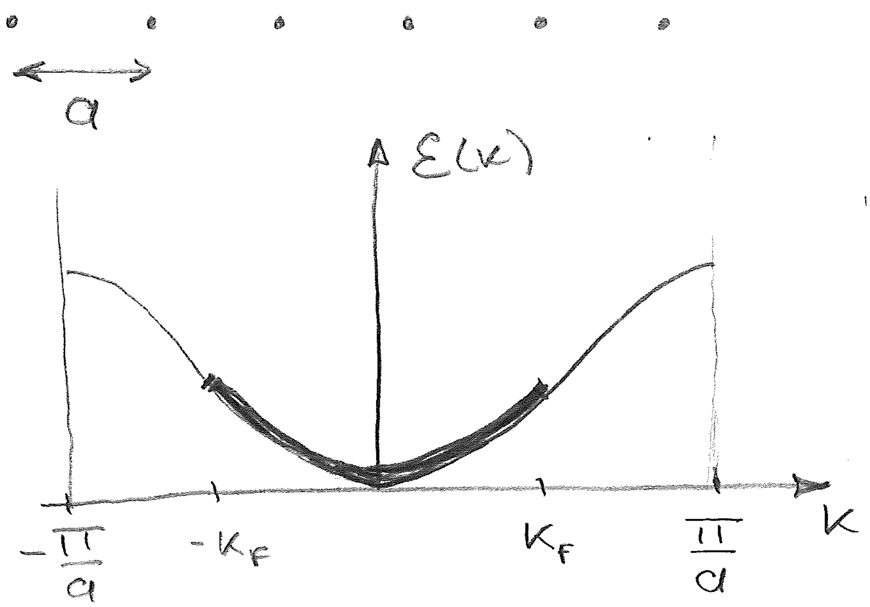
$$\sim \frac{\hbar^3}{m p_F} \frac{\omega^2(k)}{(\omega^2 - \omega^2(k))}$$

This interaction is attractive for the energy transfer $\hbar\omega = \mathcal{E}(p_1) - \mathcal{E}(p_1') < \omega(k)$

Important phonons are those with momentum of order $K_F \Rightarrow \omega(k) \simeq \omega_D$. The phonon mediated attraction occurs in a narrow layer near the Fermi surface with thickness of order $\hbar\omega_D$.

Peierls Transition

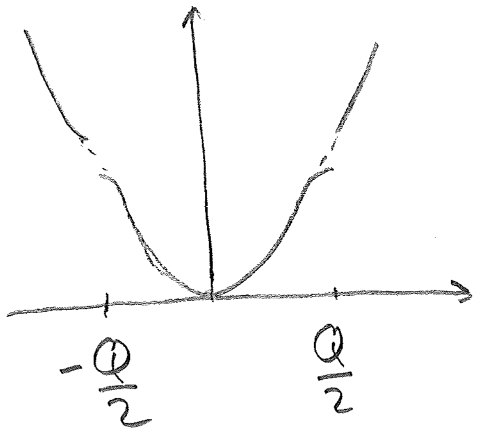
Let us consider a simple one-dimensional metal with 1 electron per unit cell (half filling)



For this filling Fermi points are at $k_F = \pm\frac{\pi}{2a}$

What happens if the lattice is deformed with some wave vector Q: $u(x) = u_0 \cos(Qx)$

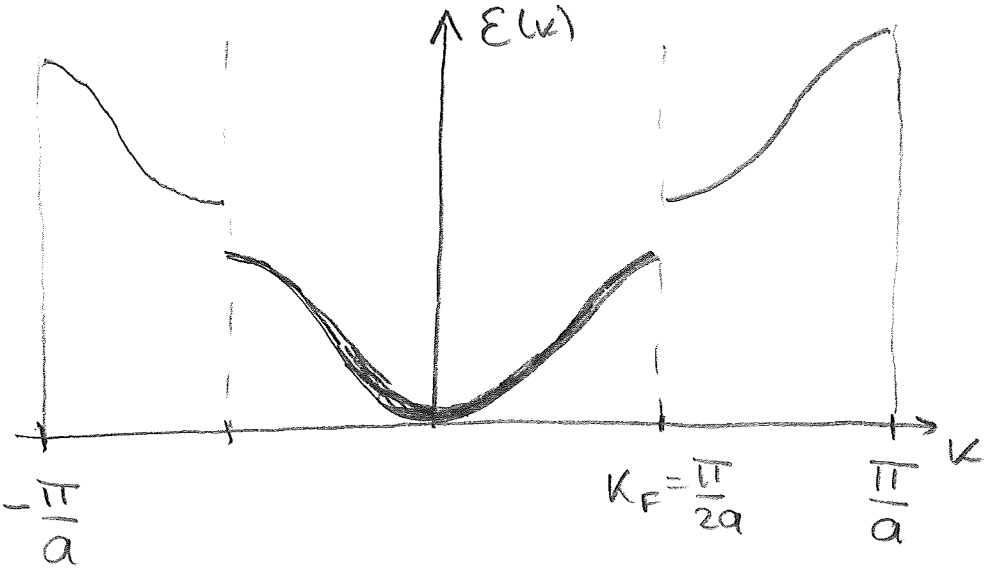
As for the case of nearly free electron in a periodic potential the gap appears at $k = \pm Q/2$.



States with k and $-k$ have the same energy. If periodic potential has matrix elements between these states it mixes them to remove degeneracy and the gap opens.

When the gap appears in the spectrum states below it go down in energy and those above it go up. If the Fermi level E_F is below the gap then we don't feel it. If E_F is above the gap then levels going up and down compensate each other and the total energy change is very small. However, if $k_F = \frac{Q}{2}$ then the Fermi energy is inside the gap and all the occupied states are going up, whereas levels that go up in energy are empty. As a result there is gain in energy

Thus 1-d metal is unstable with respect to the deformation with $Q = 2K_F$. This corresponds to the period doubling for half filling.



As a result there is Peierls transition to the Charge Density Wave state

This is rather similar to the Jahn-Teller effect.

Peierls transition in the tight binding approximation

$$H = \sum_n \left(\varepsilon_n a_n^+ a_n + t_{n,n+1}\left(a_n^+ a_{n+1} + a_{n+1}^+ a_n\right)\right)$$

If all the sites are equivalent, $t_{n,n+1} = t$ and

$$\varepsilon(k) = 2t\cos(ka)$$

If period is doubled then $u_n = (-1)^n u$

and $t_{2n,2n-1}$ t_1 $t_{2n,2n+1} = t_2$ and the spectrum

is $E_{1,2} = \pm\sqrt{t_1^2 + t_2^2 + 2t_1 t_2 \cos 2ka}$

For small $\Delta = |t_1 - t_2| << t = \frac{t_1 + t_2}{2}$, $\Delta \propto u$

we can rewrite this energy as

$$E_{1,2} = \pm\sqrt{\Delta^2 + 4t^2\cos^2 ka}$$

Icluding elastic energy we obtain

$$E = -\frac{1}{N}\sum_k \sqrt{\Delta^2 + 4t^2\cos^2 ka} + \frac{1}{2}\varkappa u^2$$

We introduce a dimensionless coupling

constant g: $\varkappa u^2 = \frac{\Delta^2}{2\pi t g^2}$

Replacing the sum by the integral we obtain

$$E(\Delta) = -\frac{1}{2\pi}\int_{-\frac{\pi}{2a}}^{\frac{\pi}{2a}} \sqrt{\Delta^2 + 4t^2\cos^2 ka}\, dka + \frac{\Delta^2}{4\pi t g^2} =$$

$$= E(\Delta=0) - \frac{\Delta^2}{4\pi}\int_0^{\frac{\pi}{a}} \frac{dk}{\sqrt{\Delta^2+4t^2\cos^2 ka}} + \frac{\Delta^2}{4\pi t g^2}$$

$$= E(\Delta=0) - \frac{\Delta^2}{4\pi t}\left(\ln\frac{8t}{\Delta} + \frac{1}{2}\right) + \frac{\Delta^2}{4\pi t g^2}$$

Minimum of this energy for small g corresponds to

$$\Delta(0) = 8t\, e^{-\frac{1}{g^2}}$$