

(EPI)

Electrons can participate in the dynamics.

# Electron-Phonon Interaction in Metals

Two main effects:

$$\textcircled{1} [\text{He} + \text{He-ion}] \psi_n(\{\vec{r}_i\}, \{\vec{R}_i\}) = E_n(\{\vec{R}_i\}) \psi_n$$

We'll no longer assume that the ions are fixed at their equilibrium positions (on the lattice sites).

Then, He-ion will involve the instantaneous positions of the ions. At any finite  $T$  (even at  $T=0$ , there is zero-pt. motion), there will be phonons present.

This will modify the energy spectrum of the electrons. (The effect is appreciable only near the Fermi surface)  $\Rightarrow$  mass renormalization (Effective mass,  $\text{d} \omega$  at the Fermi surface changes). \*\*

$$\textcircled{2} [\text{H-ion} + E_n(\{\vec{R}_i\})] \phi_{mn}(\{\vec{R}_i\}) = E_m \phi_{mn}(\{\vec{R}_i\})$$

We'll now consider the  $\{\vec{R}_i\}$  dependence of this term. This will modify the <sup>bare</sup> phonon frequencies.

In metals, the main effect is the screening of the bare Coulomb interaction between the ions.

## Bohm-Staver Relation

\*\* Effective el-el. interaction  $\Leftarrow$  Superconductivity.

(EP2) Plasma dispersion relation

"Bare" plasma

$$H = \sum_i \frac{p_i^2}{2M} + \frac{1}{2} \sum_{i \neq j} V_{ion}(\vec{R}_i - \vec{R}_j)$$

"Bare"  
Potential is the long-range Coulomb potential.  
↑↑  
Ions: Charged particles with charge Ze.

Ionic system => a system of charged particles interacting via the bare Coulomb potential.

Collective motion => Plasma oscillation.

$$\omega_p^2 = \frac{4\pi n_e e^2}{m} \text{ for electron gas. at } k=0.$$

Here, ~~number density~~ number density =  $n_e/z$   
charge =  $ze$ .  
mass =  $M$ .

$$\Rightarrow \Omega_p^2 = \frac{4\pi \frac{n_e}{z} (ze)^2}{M} = \frac{4\pi n_e e^2 z}{M}$$
$$= \left(\frac{Zm}{M}\right) \omega_p^2.$$

This is much smaller than  $\omega_p$ , but it does not go to zero as  $k \rightarrow 0$ . (This is a consequence of the long-range nature of the Coulomb interaction.)

(EP3)

Experimentally, however we know that there are acoustic phonons in metals (Newton's eq.,  $T^3$  law etc). So, this result has to be modified. The modification comes from the response of electrons to the ionic motion, namely screening. Consider the phonon in the long wavelength limit ( $k \rightarrow 0$ ). A phonon of wavevector  $\vec{k}$  corresponds to a displacement of the ions with a periodicity given by  $e^{i\vec{k}\cdot\vec{r}}$ . The effect of the screening by the electrons is to reduce the electric field associated with this disturbance by an amount  $1/\epsilon(\vec{k})$ . Since the restoring force seen by an ion is  $\propto$  to the electric field, and the phonon frequency  $\propto \sqrt{\text{restoring force}}$ , the square of the phonon frequency is reduced by the same factor,  $1/\epsilon(\vec{k})$ .

$$\Rightarrow \omega^2(\vec{k}) = \frac{\Omega_p^2}{\epsilon(\vec{k})}$$

In the long wavelength limit, we can use the Thomas-Fermi form for  $\epsilon(\vec{k})$ :  $\epsilon(\vec{k}) = 1 + \frac{k_{FT}^2}{k^2}$

As  $k \rightarrow 0$ ,  $\epsilon(\vec{k}) \Rightarrow \frac{k_{FT}^2}{k^2}$

$$\omega^2(\vec{k}) = \frac{\Omega_p^2}{k_{FT}^2} k^2 \quad \omega(\vec{k}) = C k$$

(EPA) where  $C^2 = \frac{\Omega_p^2}{k_{FT}^2} = \frac{1}{3} Z \frac{m}{M} v_F^2$

$$\frac{4\pi e^2}{k_{FT}^2} = \frac{\hbar^2 \pi^2}{mk_F}$$

Free electron value

$$\frac{Zm}{M} \sim 10^{-4} \Rightarrow C \sim 10^{-2} v_F$$

(reasonable)

### Bohm-Staver Relation

At large <sup>values of k</sup> ~~wave lengths~~, the Thomas-Fermi result is not adequate, and one must consider the more accurate Lindhard (RPA) form. In this approximation,  $\epsilon(k)$  has a weak singularity

when  $k = 2k_f$ .  $\left( \frac{\partial \epsilon}{\partial k} \rightarrow \infty \text{ at this point} \right)$

$\Rightarrow \frac{\partial \omega}{\partial k} \rightarrow \infty$  at  $k = 2k_f$  ← Extremal radius of the Fermi surface

(Kink in the  $\omega$  vs  $k$  curve)

### Kohn anomaly

### Effective el.-el. interaction

Total dielectric ~~constant~~ function of a metal

⇓  
Conduction electrons + ions.

Total polarizability = Electronic pol. + ionic pol.

EPS

$$\alpha = \alpha_{el} + \alpha_{ion}^{base}$$

$$\left. \begin{aligned} \epsilon &= 1 + 4\pi\alpha \\ \epsilon_{el} &= 1 + 4\pi\alpha_{el} \\ \epsilon_{ion}^{base} &= 1 + 4\pi\alpha_{ion} \end{aligned} \right\} \begin{aligned} \alpha_{el} &= \frac{\epsilon_{el} - 1}{4\pi} \\ \alpha_{ion} &= \frac{\epsilon_{ion}^{base} - 1}{4\pi} \end{aligned}$$

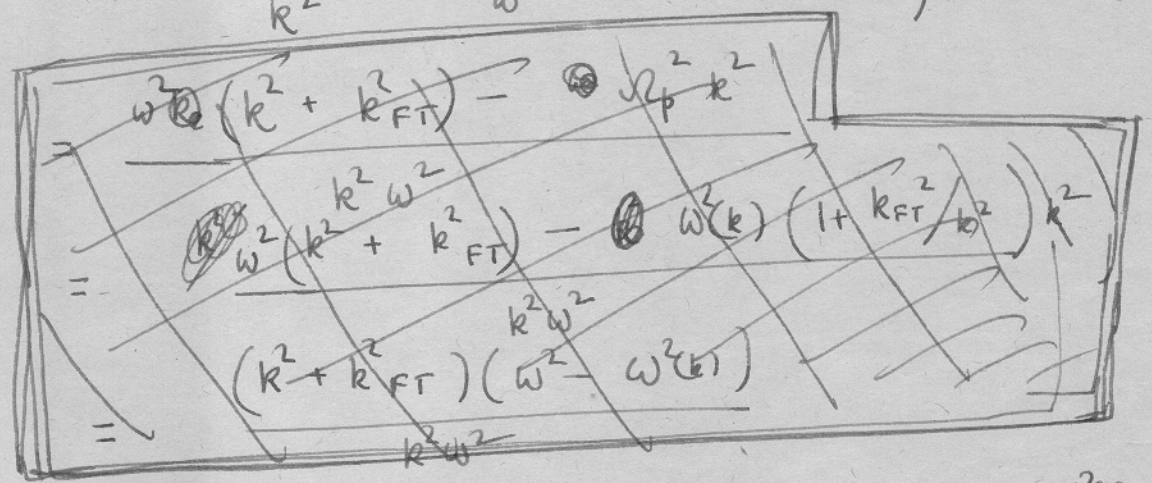
$$\Rightarrow \epsilon = 1 + 4\pi \left( \frac{\epsilon_{el} - 1}{4\pi} + \frac{\epsilon_{ion}^{base} - 1}{4\pi} \right)$$

$$= \epsilon_{el} + \epsilon_{ion}^{base} - 1$$

Use  $\epsilon_{el} = 1 + \frac{k_{FT}^2}{k^2}$  (low freq.  $\omega \sim \Omega_p$ , so that  $\omega \rightarrow 0$  formula ok for the electronic part)

$$\epsilon_{ion}^{base} = 1 - \frac{\Omega_p^2}{\omega^2}$$

$$\Rightarrow \epsilon = 1 + \frac{k_{FT}^2}{k^2} - \frac{\Omega_p^2}{\omega^2} = \left(1 + \frac{k_{FT}^2}{k^2}\right) - \left(1 + \frac{k_{FT}^2}{k^2}\right) \frac{\omega^2(k)}{\omega^2}$$



$$\frac{1}{\epsilon(\vec{k}, \omega)} = \frac{\omega^2}{\omega^2 - \omega^2(k)} \frac{1}{1 + k_{FT}^2/k^2} = \frac{1}{1 + \frac{k_{FT}^2}{k^2}} \left[ 1 + \frac{\omega^2(k)}{\omega^2 - \omega^2(k)} \right]$$

(E16)

Now consider the effective interaction between two electrons. In  $\vec{k}$ -space, the Fourier component of the bare Coulomb interaction with wave number  $k$  is

$$\frac{4\pi e^2}{k^2}$$

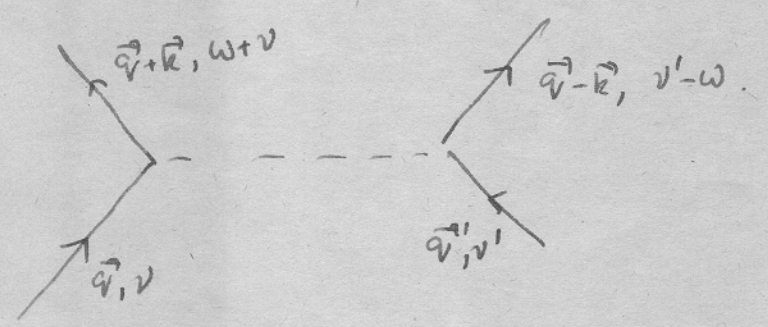
This is modified by the total dielectric function of the solid.

$$\Rightarrow \text{Eff. int.} = \frac{4\pi e^2}{k^2} \cdot \frac{1}{\epsilon(\vec{k}, \omega)}$$

$$= \frac{4\pi e^2}{k^2 + k_{FT}^2} \left[ 1 + \frac{\omega^2(k)}{\omega^2 - \omega^2(k)} \right]$$

Screened Coulomb interaction. (no effect from the lattice)  
Effect of the lattice.

We have to understand what  $\vec{k}$  and  $\omega$  refers to.  
It can be shown that  $\vec{k}$ : momentum transfer  
 $\hbar\omega$ : energy transfer in the scattering of two electrons.



(EFT)

In most situations,  $\omega \sim \epsilon_f / \hbar \gg \omega(k)$   
 and the second term can be neglected. However,  
 when  $\omega \approx \omega(k)$ , this term becomes very large  
 and if  $\omega \leq \omega(k)$ , this term may dominate and  
 make the overall effective interaction negative.

Only happens when  $q$  is close to  $k_f$ .

~~$q < k_f$~~   ~~$q > k_f$~~   $\hbar v < \epsilon_f / \hbar$   
 $\hbar(\omega + v) > \epsilon_f / \hbar$

$$\hbar\omega \leq \hbar\omega_D \quad \left[ \epsilon_f \geq \hbar v \geq \epsilon_f - \hbar\omega_D \right]$$

Only those electrons in a thin shell about the  
 Fermi surface may have an attractive eff. int.

$\Rightarrow$  Superconductivity.

One el. produces a local distortion of the ions

$\Rightarrow$  field which may attract another electron.

e) Linear response theory. Dynamical susceptibility.

Books: Same as before.  
 Homework + Term paper.  
 Solutions to homeworks?  
 Student opinion forms?

## Electron-phonon Interaction

Adiabatic (Born-Oppenheimer approximation)

$$\begin{aligned}
 H = & \sum_i p_i^2 / 2m + \frac{1}{2} \sum_{i \neq j} e^2 / |\vec{r}_i - \vec{r}_j| \quad \leftarrow \text{el.} \\
 & + \sum_i P_i^2 / 2M + \frac{1}{2} \sum_{i \neq j} V_{\text{ion}}(\vec{R}_i - \vec{R}_j) \quad \leftarrow \text{ion} \\
 & + \sum_{ij} V_{\text{el-ion}}(\vec{r}_i - \vec{R}_j) \quad \leftarrow \text{el-ion.}
 \end{aligned}$$

~~Born-Oppenheimer~~

$$\rightarrow [H_{\text{ion}} + E_n(\{\vec{R}_i\})] \phi_{mn}(\{\vec{R}_i\}) = E_m \phi_{mn}(\{\vec{R}_i\}) \quad (2)$$

$$[H_{\text{el}} + H_{\text{el-ion}}] \psi_n(\{\vec{r}_i\}, \{\vec{R}_i\}) = E_n(\{\vec{R}_i\}) \psi_n \quad (1)$$

The second equation solves the motion of the electrons in a potential given by the instantaneous positions of the ions. This gives an energy which is a function of the ionic positions, and this energy acts as an effective potential in the first



equation, which solves the motion of the ions.

In obtaining these two equations, we had to neglect terms of order  $\lambda = (m/M)^{1/4}$  and higher. The physical picture is the following. Since the mass of the electron is  $\ll$  ionic mass, the ions vibrate much more slowly than the electrons.

Electronic motion:  $\omega_p \sim 10^{16} \text{ sec}^{-1}$

Ionic motion:  $\omega_{\text{phonon}} \leq 10^{13} \text{ sec}^{-1}$

Thus, the potential an electron sees is essentially determined by the instantaneous positions of the ions. The ions, on the other hand, see the average effect of the electronic motion. One can treat the neglected term in perturbation theory, but we'll not consider that here.

Instead, we'll try to solve these two equations more carefully. Previously, we put  $\vec{R}_i = \vec{L}_i$  in the second equation. i.e., we assumed that, when dealing with the dynamics of the electrons, we can take the ions to be at rest at their equilibrium positions. This led to band structure calculations of study of e-e interaction. This gave an  $E_n$  which is a constant, and then the first equation was used to study phonons. In this approximation, electrons of phonons were completely decoupled. Now, we'll go beyond this approximation of consider the dependence of Hel-ion on

$$H_{\text{el-phin}} = \int d\vec{r} \rho(\vec{r}) \sum_e \vec{u}_e \cdot \vec{\nabla}_{\vec{r}} V(\vec{r} - \vec{R}_e) \Big|_{\vec{R}_e = \vec{L}}$$

$$- \sum_e \int d\vec{r}' \rho(\vec{r}' + \vec{R}_e) \vec{u}_e \cdot \vec{\nabla}_{\vec{r}'} V(\vec{r}')$$

The first term represents the interaction of the electron density with the external electric field. The second term represents the interaction of the electron density with the internal electric field. The first term is evaluated at the position of the external field, and the second term is evaluated at the position of the internal field. The external field is assumed to be uniform, and the internal field is assumed to be zero. The external field is represented by the vector  $\vec{u}_e$ , and the internal field is represented by the vector  $\vec{u}_i$ . The external field is represented by the vector  $\vec{u}_e$ , and the internal field is represented by the vector  $\vec{u}_i$ . The external field is represented by the vector  $\vec{u}_e$ , and the internal field is represented by the vector  $\vec{u}_i$ .

the instantaneous positions of the ions. This will lead to an interaction between the electron and the phonons.

The interaction Hamiltonian

$$H_{el} = \sum_i \frac{p_i^2}{2m} + H_{el-el}$$

not considered for the time being,  
can be put in later on.

$$H_{el-ion} = \sum_{i \in \text{cell}} V(\vec{r}_i - \vec{R}_e)$$

one atom/unit cell.

$$\vec{R}_e(t) = \vec{L} + \vec{U}_e(t)$$

$$V(\vec{r}_i - \vec{R}_e) = V(\vec{r}_i - \vec{L}) + \vec{U}_e \cdot \vec{\nabla}_R V(\vec{r}_i - \vec{R}_e) \Big|_{\vec{R}_e = \vec{L}}$$

"static" lattice term. ↑ el-phon. int.

Perturbing potential seen by the  $i$ th electron =  $V_p(\vec{r}_i) =$

$$+ \sum_e \vec{U}_e \cdot \vec{\nabla}_R V(\vec{r}_i - \vec{R}_e) \Big|_{\vec{R}_e = \vec{L}}$$

$$\Rightarrow H_{el-phon} = + \int d\vec{r} \psi^\dagger(\vec{r}) \sum_e \vec{U}_e \cdot \vec{\nabla}_R V(\vec{r} - \vec{R}_e) \Big|_{\vec{R}_e = \vec{L}} \psi(\vec{r})$$

$$\vec{U}_e = \frac{1}{\sqrt{NM}} \sum_{\vec{k}, \sigma} \left[ \frac{\hbar}{2\omega(\vec{k}, \sigma)} \right]^{1/2} \vec{E}_\sigma(\vec{k}) e^{i\vec{k} \cdot \vec{L}} \times [a_\sigma(\vec{k}) + a_\sigma^\dagger(-\vec{k})]$$

These phonons are the ~~not~~ "bare" phonons, where el-phon effects are neglected.

$$\psi(\vec{r}) = \sum_{n, \vec{k}} \phi_n(\vec{k}, \vec{r}) C_n(\vec{k})$$

$n$ : band index  
 $\vec{k}$ : crystal momentum

The  $\phi$ 's are Bloch states, so that

$$\phi_n(\vec{k}, \vec{r} - \vec{L}) = e^{-i\vec{k}' \cdot \vec{L}} \phi_n(\vec{k}, \vec{r})$$

$$\Rightarrow H_{\text{el-phonn}} = \sum_{\vec{k}, n} \int d\vec{r} \sum_{\vec{k}', n'} C_n^+(\vec{k}) \phi_n^*(\vec{k}, \vec{r})$$

$$\times \sum_{\vec{q}, \sigma} \frac{1}{\sqrt{NM}} \left[ \frac{\hbar}{2W(\vec{q}, \sigma)} \right]^{1/2} \vec{\epsilon}_\sigma(\vec{q}) e^{i\vec{q} \cdot \vec{L}} [a_\sigma(\vec{q}) + a_\sigma^+(\vec{q})] \cdot [\vec{\nabla} V(\vec{r} - \vec{L})]$$

$$\times \sum_{\vec{k}', n'} C_{n'}(\vec{k}') \phi_{n'}(\vec{k}', \vec{r})$$

$$\phi_{n'}(\vec{k}', \vec{r}) = e^{i\vec{k}' \cdot \vec{L}} \phi_{n'}(\vec{k}, \vec{r} - \vec{L})$$

$$\phi_n^*(\vec{k}, \vec{r}) = e^{-i\vec{k} \cdot \vec{L}} \phi_n^*(\vec{k}, \vec{r} - \vec{L}) \quad \left[ \begin{array}{l} \text{change variables} \\ \vec{r} \rightarrow \vec{r} - \vec{L} \end{array} \right]$$

$$\Rightarrow \vec{r} \text{ integration: } \int d\vec{r} \phi_n^*(\vec{k}, \vec{r}) \vec{\nabla} V(\vec{r}) \phi_{n'}(\vec{k}', \vec{r}) = C_{nn'}(\vec{k}, \vec{k}')$$

$$e\text{-dependent term: } \sum_{\vec{q}} e^{i\vec{q} \cdot \vec{L}} e^{i\vec{k}' \cdot \vec{L}} e^{-i\vec{k} \cdot \vec{L}} = N \delta_{\vec{q} + \vec{k}' - \vec{k}, \vec{K}}$$

$$\vec{q} = \vec{k} - \vec{k}' + \vec{K} \quad \vec{q} \text{ in 1st BZ}$$

$\Rightarrow$  If  $\vec{k} - \vec{k}'$  in 1st BZ,  $\vec{K} = 0$ , if  $\vec{k} - \vec{k}'$  outside 1st BZ, we must have  $\vec{K} \neq 0$  in order to bring  $\vec{q}$  back to 1st BZ (Umklapp).

$$\Rightarrow H_{\text{el-phonn}} = + \sum_{\vec{k}, \vec{k}'} \sum_{n, n', \sigma} C_n^+(\vec{k}) C_{n'}(\vec{k}')$$

$$\times [a_\sigma(\vec{k} - \vec{k}') + a_\sigma^+(\vec{k}' - \vec{k})] D_{nn', \sigma}(\vec{k}, \vec{k}')$$

[ It is understood that if  $\vec{k} - \vec{k}'$  is outside the 1st BZ, we must add or subtract a rec. lat. vect. ]

Longitudinal acoustic phonons, conduction electrons

$$D(\vec{k}-\vec{k}') = -\sqrt{\frac{N}{M}} \sqrt{\frac{\hbar}{2\omega(\vec{k}-\vec{k}')}} \frac{1}{V} i |\vec{k}-\vec{k}'|$$

$$\frac{4\pi z e^2}{|\vec{k}-\vec{k}'|^2 + k_0^2} \leftarrow \text{Screened Coulomb}$$

$$|D|^2 = \frac{N}{M} \frac{1}{V^2} \frac{\hbar}{2\omega(\vec{k}-\vec{k}')} |\vec{k}-\vec{k}'|^2 \frac{(ze^2)^2 16\pi^2}{(|\vec{k}-\vec{k}'|^2 + k_0^2)^2}$$



$$\omega^2(\vec{k}-\vec{k}') = \frac{4\pi N/V (ze^2)^2 |\vec{k}-\vec{k}'|^2}{M (|\vec{k}-\vec{k}'|^2 + k_0^2)}$$

$$\frac{|D|^2}{\omega(\vec{k}-\vec{k}')} = \frac{\cancel{N}}{\cancel{M}} \frac{1}{\cancel{V^2}} \frac{\hbar}{2} \frac{\cancel{V} M (|\vec{k}-\vec{k}'|^2 + k_0^2)}{4\pi \cancel{N} z^2 e^2 |\vec{k}-\vec{k}'|^2} \frac{16\pi^2}{(|\vec{k}-\vec{k}'|^2 + k_0^2)^2}$$

$$\nabla_{\vec{k}} E(\vec{k}) = \hbar v(\vec{k})$$

$$= \frac{\hbar}{2V} \frac{4\pi e^2}{|\vec{k}-\vec{k}'|^2 + k_0^2}$$

$$\frac{2V}{(2\pi)^3} \int d^3k' \frac{ds_{k'}}{\hbar v(\vec{k}')} \frac{1}{2V} \frac{4\pi e^2}{|\vec{k}-\vec{k}'|^2 + k_0^2}$$

$$= \int \frac{ds_{k'}}{8\pi^3} \frac{1}{v(\vec{k}')} \frac{4\pi e^2}{|\vec{k}-\vec{k}'|^2 + k_0^2} \leftarrow \text{Ashcroft & Mermin}$$

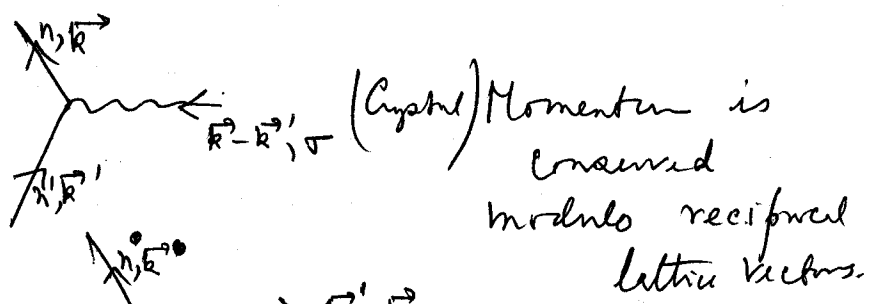
$$\vec{C}_{nn'}(\vec{k}, \vec{k}') \equiv \int d\vec{r} \phi_n^*(\vec{k}, \vec{r}) \vec{\nabla} V(\vec{r}) \phi_{n'}(\vec{k}', \vec{r}) \quad (4b)$$

$V(\vec{r})$ : P.T. seen by electron at  $\vec{r}$  due to ion at the origin.

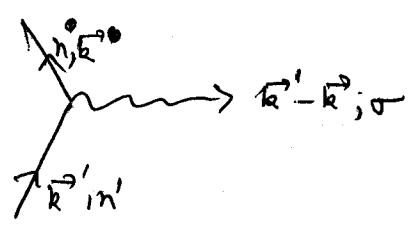
Jones & Loud  
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$$D_{nn', \sigma}(\vec{k}, \vec{k}') \equiv - \frac{1}{\sqrt{NM}} N \left[ \frac{\hbar}{2W(\vec{k}-\vec{k}', \sigma)} \right]^{1/2} \times \vec{E}_{\sigma}(\vec{k}-\vec{k}') \cdot \vec{C}_{nn'}(\vec{k}, \vec{k}')$$

1st term:



2nd term:



is only one band of the  
If we assume that these Bloch functions can be approximated by plane waves, then we have

$$\vec{C}_{nn'}(\vec{k}, \vec{k}') = \frac{1}{V} \int d\vec{r} e^{-i(\vec{k}-\vec{k}') \cdot \vec{r}} \vec{\nabla} V(\vec{r})$$

$$= \frac{1}{V} i (\vec{k}-\vec{k}') V(\vec{k}-\vec{k}') \quad \left[ \text{Integrate by parts, } V(\vec{r}) \rightarrow 0 \text{ as } r \rightarrow \infty \right]$$

This is true for normal processes. If  $\vec{k}-\vec{k}' = \vec{k}+\vec{q}$ , the  $(\vec{k}-\vec{k}') \cdot \vec{E}_{\sigma}(\vec{q})$  can be non zero for transverse mode.

$D_{nn', \sigma}(\vec{k}, \vec{k}') \sim \vec{E}_{\sigma}(\vec{k}-\vec{k}') \cdot (\vec{k}-\vec{k}')$   
which means that only longitudinal polarizations contribute. In general, the Bloch functions are not simple plane waves, and the phonons are not simply transverse or longitudinal. So all the branches have to be considered.

The electron-phonon interaction vertex  $D_{nn', \sigma}(\vec{k}, \vec{k}')$  is usually rather difficult to calculate from first principle. One complication

Comes from the effects of screening. When the ion moves, it changes the distribution of the electrons around it, so the potential seen by the another electron is modified. This effect will be taken into account (in an approximate way) later on. However, it is often convenient to take these coefficients  $D_{nn',0}$  as phenomenological parameters. In this approach, the concept of a deformation potential has been quite useful, especially in dealing with polaron effects in semiconductors.

### Deformation Potential

A state with phonons present can be thought of as a deformed state of a perfect lattice. If the phonons are of long wavelength, then the deformation changes slowly, i.e. on a length scale much larger than the lattice spacing. In this limit, the lattice can be thought of as an elastic continuum, and the concepts of continuum elasticity theory can be usefully employed. In particular, we can describe the deformation of the lattice in terms of a ~~stress~~ <sup>strain</sup> tensor  $\chi_{\alpha\beta}$ ,  $\alpha\beta \Rightarrow x, y, z$ . First, let us consider the case where  $\chi_{\alpha\beta}$  is constant in space. The energy of an electron in a Bloch state  $(n, \vec{k})$  will change as a result of this ~~stress~~ <sup>strain</sup>. ~~For~~ For small strain, we can write

$$\delta E_n(\vec{k}) = \sum_{\alpha\beta} \epsilon_{\alpha\beta}(n, \vec{k}) \gamma_{\alpha\beta}$$

The coefficients  $\epsilon_{\alpha\beta}$  can be obtained from straightforward perturbation theory. In general,  $\gamma_{\alpha\beta}$  will change the crystal structure. However, if  $\gamma_{\alpha\beta}$  is diagonal & a multiple of the unit matrix, then the strain is a simple contraction or ~~dilation~~ dilatation, and the symmetry of the crystal remain unchanged. We consider only such strains here. In that case, we can write

$$\begin{aligned} \delta E_n(\vec{k}) &= \sum_{\alpha} \epsilon_{\alpha\alpha}(n, \vec{k}) \Delta & \gamma_{\alpha\beta} &= \Delta \delta_{\alpha\beta} \\ &= C_n(\vec{k}) \Delta \end{aligned}$$

Furthermore, we neglect the  $\vec{k}$  dependence of  $C_n$ . The rationale is that we'll be interested in electrons with  $\vec{k}$  vectors in a small region in the BZ (as in the few conduction electrons in a semiconductor)

$$\Rightarrow \delta E_n \text{ [crossed out]} = C_n \Delta$$

Thus, the electron sees an extra potential (constant). Now, we let  $\Delta$  to vary slowly in space, and treat  $C_n \Delta(\vec{r})$  as an effective potential seen by the electrons.

$$\text{Deformation potential } V_p(\vec{r}) = C_n \Delta(\vec{r})$$

where  $\Delta(\vec{r})$  is the local dilatation. This simply means that the effective potential seen by an electron is determined by the ~~strain~~ distortion of the lattice in the region in which it is located.



We can now use this deformation potential to obtain a form for the electron-phonon interaction. This is done by writing the local deformation  $\Delta(\vec{r})$  in terms of the displacements of the ions from their equilibrium positions:

$$\Delta(\vec{r}) \sim \vec{\nabla} \cdot U(\vec{r}) \quad [U(\vec{r}) \leftrightarrow U_0(\vec{r})]$$

and we are treating the lattice as a continuum]

[Uniform stretching:  $\vec{R}_e = (1+\epsilon)\vec{l}$

$$\vec{U}_e = \epsilon\vec{l} \Rightarrow \vec{U}(\vec{r}) = \epsilon\vec{r}$$

$$\vec{\nabla} \cdot \vec{U}(\vec{r}) = 3\epsilon]$$

We can then write  $U$  in terms of phonon operators, & get an electron-phonon interaction which is essentially of the same form as before, but which depends only on the parameter  $C_n$ . This is thus a simplification, but this is valid only at long wavelengths.

We now proceed to examine how the electron-phonon interaction changes the properties of the electrons & the phonons.

General strategy:

$$[H_{el} + H_{el-ion}] \psi_n(\{\vec{r}_i\}, \{\vec{R}_i\}) = E_n(\{\vec{R}_i\}) \psi_n. \quad (1)$$

$$[H_{ion} + E_n(\{\vec{R}_i\})] \phi_{mn}(\{\vec{R}_i\}) = E_m \phi_{mn}. \quad (2)$$

$$\Rightarrow H_{el} + H_{el-ion}^{(static)} + H_{el-phonon} = H_{el} + H_{el-phonon}$$

We'll first try to solve the first equation, assuming that the ions are at rest at their instantaneous positions. (This we can do, because the timescale of electronic motion is much faster than that for the ionic motion). We'll thus treat  $H_{el-phonon}$  as a static potential, acting on the electrons. Also, in evaluating this potential, we'll assume that the phonons are the bare phonons, i.e., we'll assume that the potential between ions is the one ~~where~~ <sup>for which</sup> the effects of the electrons are neglected. We'll then calculate  $E_n$  in perturbation theory in  $H_{el-phonon}$ .  $E_n$  will depend upon the phonon-coordinates (displacements of the ions) because  $H_{el-phonon}$  does. We'll go only to second-order in  $H_{el-phonon}$ . This will give a  $E_n$  which contains terms bilinear in the ionic displacements. We'll then substitute this  $E_n$  in the second equation. The term in  $E_n$  quadratic in the ionic displacements will modify the phonon-frequencies. Thus, we'll get the so-called renormalized phonon. We'll study how the phonon dispersion is altered. Finally, we'll use the renormalized phonons ~~to~~ in defining  $H_{el-phonon}$ , and go back to the first equation to determine how the properties of the electrons are changed.

- a) Use Eq (1) to calculate  $E_n$  to second-order in  $H_{el-phonon}$  assuming treating  $H_{el-phonon}$  as a static potential, and assuming bare ~~to~~ ionic interaction
- b) Use the calculated  $E_n$  in Eq (2) to obtain

(48)

the renormalized phonon dispersion

- c) Use renormalized phonons in Hel-phonon to determine changes in the electronic properties from eq (1).

Justification  $\Rightarrow$  Migdal AB. Sov. Phys. JETP

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7, 996 (1958)

## Electron-phonon interaction

a) Solve for electronic energies from

$$[H_{el} + H_{el-ion}] \Psi(\{\vec{r}_i\}, \{R_i\}) = E(\{R_i\}) \Psi$$

$$H_{el-ion} = \sum_{i,e} V(\vec{r}_i - \vec{L}) + H_{el-phonon}$$

$$H_{el-phonon} = \sum_{\substack{\vec{k}_1, \vec{k}_2 \\ n_1, n_2}} V_{ep}(\vec{k}_1, \vec{k}_2) \cancel{C_{n_1}(\vec{k}_1)} \cancel{C_{n_2}(\vec{k}_2)} C_{n_1}^\dagger(\vec{k}_1) C_{n_2}(\vec{k}_2)$$

\* Treat  $H_{el-phonon}$  as static potential. Work to second order.

$V_{ep}$  can be written in terms of phonon operators, but it will be more convenient to write it directly in terms of the ionic displacements.

$$H_{el-phonon} = - \int d\vec{r} \Psi^\dagger(\vec{r}) \sum_e \vec{u}_e \cdot \vec{\nabla} V(\vec{r} - \vec{L}) \Psi(\vec{r})$$

Write  $\Psi(\vec{r})$  in terms of  $C_n(\vec{k})$

$$\Rightarrow H_{el-phonon} = - \int d\vec{r} \sum_{n_1, \vec{k}_1} \phi_{n_1}^\dagger(\vec{k}_1, \vec{r}) C_{n_1}^\dagger(\vec{k}_1) \sum_e \vec{u}_e \cdot \vec{\nabla} V(\vec{r} - \vec{L}) \sum_{n_2, \vec{k}_2} \phi_{n_2}(\vec{k}_2, \vec{r}) C_{n_2}(\vec{k}_2)$$

$$= \int d\vec{r} - \sum_{n_1, n_2} \left[ \int d\vec{r} \phi_{n_1}^\dagger(\vec{k}_1, \vec{r}) \vec{\nabla} V(\vec{r}) \phi_{n_2}(\vec{k}_2, \vec{r}) \right]$$

$$\cdot \sum_e e^{i(\vec{k}_2 - \vec{k}_1) \cdot \vec{L}} \vec{u}_e C_{n_1}^\dagger(\vec{k}_1) C_{n_2}(\vec{k}_2)$$

$$= - \sum_{\substack{n_1, n_2 \\ \vec{k}_1, \vec{k}_2}} \vec{M}(n_1, \vec{k}_1; n_2, \vec{k}_2) \cdot \sum_e e^{i(\vec{k}_2 - \vec{k}_1) \cdot \vec{L}} \vec{u}_e C_{n_1}^\dagger(\vec{k}_1) C_{n_2}(\vec{k}_2)$$

$$\vec{M}(n_1, \vec{k}_1; n_2, \vec{k}_2) \equiv \int d\vec{r} \phi_{n_1}^\dagger(\vec{k}_1, \vec{r}) \vec{\nabla} V(\vec{r}) \phi_{n_2}(\vec{k}_2, \vec{r})$$

$$\vec{M}(n_1 \vec{k}_1; n_2 \vec{k}_2) \equiv \vec{C}_{n_1 n_2}(\vec{k}_1, \vec{k}_2) \quad (6)$$

$$\Rightarrow V_{ep}(n_1 \vec{k}_1; n_2 \vec{k}_2) = - \sum \vec{Q}(n_1 \vec{k}_1, n_2 \vec{k}_2) \cdot \vec{u}_e \\ \cdot x e^{i(\vec{k}_2 - \vec{k}_1) \cdot \vec{r}}$$

$$(*) H_{el} = \sum_i \frac{p_i^2}{2m} + H_{el-el}$$

We neglect  $H_{el-el}$  for the time being. We'll put it in later.

$$\Rightarrow H_{el} + H_{el-ion} = H_{band} + H_{el-phonon}$$

$$H_{band} = \sum_i \frac{p_i^2}{2m} + \sum_{i,e} V(\vec{r}_i - \vec{r})$$

Eigenstates of  $H_{band}$ :  $\phi_n(\vec{k}, \vec{r}) \rightarrow E_n(\vec{k})$  (energy)  
Operator  $\rightarrow C_n(\vec{k})$

$$\Rightarrow H_{band} = \sum_{n, \vec{k}} E_n(\vec{k}) C_n^\dagger(\vec{k}) C_n(\vec{k})$$

Here, we make a simplification. We'll assume that only the electrons in the highest occupied band are important in the electron-phonon interaction. This means conduction electrons in metals, and valence electrons in semiconductors or insulators. The assumption we are making here is that the electrons in the inner core levels do not take part in the electron-phonon interactions. These electrons are tightly bound to the nucleus, and the rigid-

~~lattice~~ approximation is a reasonable one for them. Thus, we drop the band index  $n$ .

$$\langle \psi | \psi \rangle = \int |\psi|^2 d\tau$$

$$\langle \psi | \psi \rangle = \int |\psi|^2 d\tau = \int |\psi|^2 d\tau$$

a

$$\sum_{\vec{k}_1, \vec{k}_2} \frac{|V_{ep}(\vec{k}_1, \vec{k}_2)|^2 [1-f(\vec{k}_1)] f(\vec{k}_2)}{E(\vec{k}_1) - E(\vec{k}_2)}$$

b

$$= \sum_{\vec{k}_1, \vec{k}_2} \frac{|V_{ep}(\vec{k}_1, \vec{k}_2)|^2 [1-f(\vec{k}_2)] f(\vec{k}_1)}{E(\vec{k}_1) - E(\vec{k}_2)}$$

$$= \frac{a+b}{2} = \frac{1}{2} \sum_{\vec{k}_1, \vec{k}_2} \frac{|V_{ep}(\vec{k}_1, \vec{k}_2)|^2 [f(\vec{k}_1) - f(\vec{k}_2)]}{E(\vec{k}_1) - E(\vec{k}_2)}$$

$\uparrow$   $\times 2$  (spin)

$$\langle \psi | \psi \rangle = \int |\psi|^2 d\tau$$

Handwritten notes at the bottom of the page, including the phrase "x 2 (spin)" and other illegible text.

$$H = H_0 + H_I$$

$$H_0 = H_{\text{band}}, \quad H_I = \sum_{\vec{k}_1, \vec{k}_2} V_{ep}(\vec{k}_1, \vec{k}_2) c^\dagger(\vec{k}_1) c(\vec{k}_2)$$

$$V_{ep}(\vec{k}_1, \vec{k}_2) = - \sum_e \vec{A}(\vec{k}_1, \vec{k}_2) \cdot \vec{u}_e e^{i(\vec{k}_2 - \vec{k}_1) \cdot \vec{r}}$$

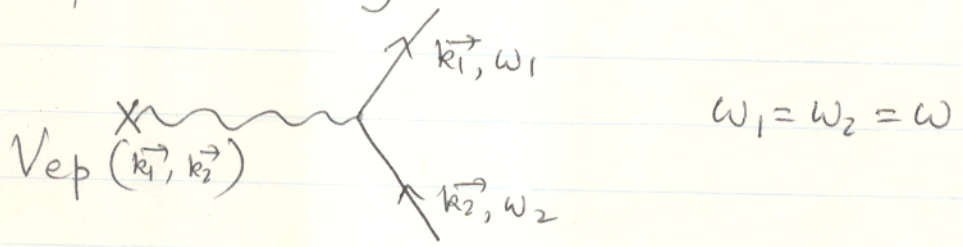
We'll now try to calculate the change in the ground-state energy of the electronic system due to the presence of  $H_I$ . We'll work to second order in  $H_I$ . This will give

$$E(\{\vec{R}_i\}) = \Delta E^{(2)} + E_0 \quad \text{where } E_0 \text{ is the ground-state energy in the absence of el-phonon int.}$$

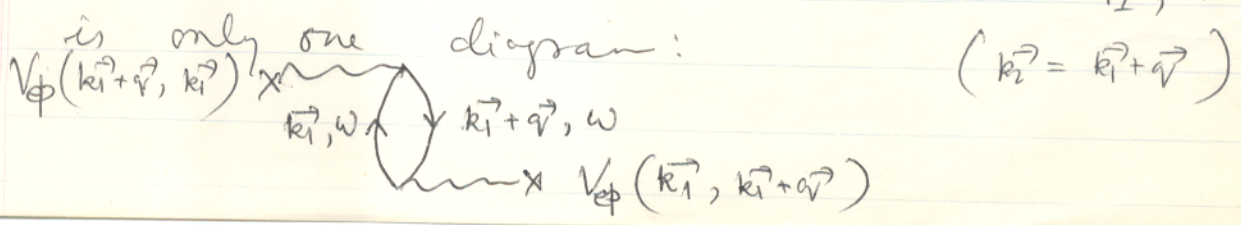
$\Delta E^{(2)} \sim \sum (\dots) U_e^\alpha U_e^\beta$ , which, when used in the S-equation for the ionic co-ordinates, will give modified (renormalized) phonon dispersion.

Calculation of  $\Delta E^{(2)}$

We are treating Hel-phonon as a static potential. Thus, the interaction vertex can be represented by



The ground-state energy diagrams contain no external lines. To second order in  $H_I$ , there



$[\vec{q}$  doesn't have to be in 1st BZ]

(8)

Contribution from this diagram:

Spins  $\rightarrow \frac{2}{2!} \sum_{\vec{k}, \vec{q}} V_{ep}(\vec{k}, \vec{k}+\vec{q}) V_{ep}(\vec{k}+\vec{q}, \vec{k})$   
 $\times \int \frac{d\omega}{2\pi i} G_0(\vec{k}, \omega) G_0(\vec{k}+\vec{q}, \omega)$

$$G_0(\vec{k}, \omega) = \frac{1}{E(\vec{k}) - \omega - i\eta(\vec{k})}$$

$\eta(\vec{k}) = \pm 0^{\pm}$   
 depending on whether  $\vec{k}$  is inside or outside Fermi surface.

Doing the integral is quite straightforward. It is the same as calculating the polarization bubble. Contribution is zero if both  $\vec{k}, \vec{k}+\vec{q}$  are inside or outside the Fermi surface. The result is

$$\Delta E^{(2)} = \sum_{\vec{k}, \vec{q}} |V_{ep}(\vec{k}, \vec{k}+\vec{q})|^2 \frac{f(\vec{k}) - f(\vec{k}+\vec{q})}{E(\vec{k}) - E(\vec{k}+\vec{q})}$$

$f=1 \Rightarrow$  occ.  
 $f=0 \Rightarrow$  unocc.

The same result could be obtained by second-order perturbation theory.

$$H_I = \sum_{\vec{k}_1, \vec{k}_2} V_{ep}(\vec{k}_1, \vec{k}_2) c_0^{\dagger}(\vec{k}_1) c(\vec{k}_2)$$

$$\Delta E^{(2)} = \sum_n \frac{|\langle n | H_I | 0 \rangle|^2}{E_0 - E_n}$$

(1)  ~~$(\vec{k}_1)$~~  unocc,  $\vec{k}_2$  occ.  $E_n = E_0 + E(\vec{k}_1) - E(\vec{k}_2)$

$$\Rightarrow \frac{|V_{ep}|^2 (1-f_{\vec{k}_1}) f_{\vec{k}_2}}{E(\vec{k}_2) - E(\vec{k}_1)} \Rightarrow \frac{1}{2} \sum_{\vec{k}_1, \vec{k}_2} |V_{ep}(\vec{k}_1, \vec{k}_2)|^2 \frac{f(\vec{k}_1) - f(\vec{k}_2)}{E(\vec{k}_1) - E(\vec{k}_2)}$$

Spin indices

(2)  $(\vec{k}+\vec{q})$  occ,  $\vec{k}$  unocc  $E_n = E_0 + E(\vec{k}) - E(\vec{k}+\vec{q})$



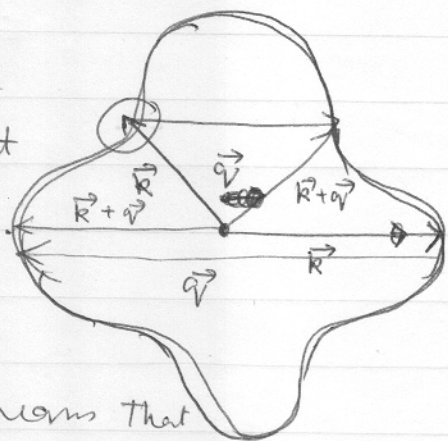
④ For insulators/semiconductors, there is a gap at the Fermi surface, and the energy denominator never vanishes. ④

We are using diagrams because it'll be easier to generalize the treatment to include the effects of el-el interaction.

Before going into that, we note that <sup>for metals,</sup> the energy denominators  $E(\vec{k}+\vec{q}) - E(\vec{k})$  can be arbitrarily small. \* For a given  $\vec{q}$ , the maximum contribution will come from the region within the Fermi surface for which  $E(\vec{k}+\vec{q}) \approx E(\vec{k})$ .

But ~~one~~ of these two wavevectors  $\vec{k}, \vec{k}+\vec{q}$  must lie on opposite sides of the Fermi surface. Thus, ~~for small  $\vec{q}$ , the values of  $\vec{k}$  which contribute, the must will come from~~ <sup>would restrict</sup> ~~very close to the Fermi surface.~~ and for which

Both  $\vec{k}$  &  $\vec{k}+\vec{q}$  must be close to the Fermi surface.



[ This means that electrons close to the Fermi surface determine the effects of el-phonon interaction ]

~~the~~ the energy denominator is close to zero. Such regions for the  $\vec{k}$  vector can be found only if  $q$  is less than ~~the~~ ~~the~~ the width of the Fermi surface. If  $q$  is greater than the width, the  $E(\vec{k}+\vec{q})$  can not be equal to  $E(\vec{k})$ , and ~~the~~ the energy denominator can not

be close to zero. This ~~will~~ effect will show up in the phonon dispersion. To see how that would happen, we look at  $|V_{ep}(\vec{k}, \vec{k}+\vec{q})|^2$

$$V_{ep}(\vec{k}, \vec{k}+\vec{q}) = - \sum_e \vec{M}(\vec{k}, \vec{k}+\vec{q}) \cdot \vec{u}_e i \vec{q} \cdot \vec{r}$$

(10)

This  $q$  is in the 1st BZ

(Can be different from the  $q$  appearing in  $M$  by  $\vec{k}$ )

$$\Rightarrow \Delta E^{(2)} \sim \sum_{\vec{k}, \vec{q}} M^\alpha(\vec{k}, \vec{k} + \vec{q}) M^\beta(\vec{k} + \vec{q}, \vec{k}) U^\alpha(\vec{q}) U^\beta(-\vec{q}) \times \frac{f(\vec{k}) - f(\vec{k} + \vec{q})}{E(\vec{k}) - E(\vec{k} + \vec{q})}$$

Thus, the extra term <sup>that changes</sup> in the harmonic phonon frequency Hamiltonian for wave-vector  $q$

$$\sim \sum_{\vec{k}} M^\alpha(\vec{k}, \vec{k} + \vec{q}) M^\beta(\vec{k} + \vec{q}, \vec{k}) \frac{f(\vec{k}) - f(\vec{k} + \vec{q})}{E(\vec{k}) - E(\vec{k} + \vec{q})}$$

For  $q < q_m$ , the width of Fermi surface, the energy denominator can be zero, whereas for  $q > q_m$ , it can not. Thus, there is a non-analytic behavior in this term ~~at  $q = q_m$  goes through the width~~, and this non-analyticity would be reflected in the phonon frequency as a kink in  $\omega(q)$  at  $q = q_m$ . The form of this singularity depends upon the shape of the Fermi surface in the direction of  $\vec{q}$ . In general, the Fermi surface is not spherical, so the magnitude of  $q_m$  also depends upon the direction of  $\vec{q}$ . These singularities are known as Kohn anomalies. They are closely related to the non-analytic behavior of the dielectric function  $\epsilon(q, 0)$  at  $q = 2k_f$  (which, we found, gives rise to the Friedel oscillations). The form of the Kohn anomaly is modified when we take into account  $e-e$  interaction.

the expression for the change in energy  
 Note that the term  $(*)$  can be thought  
 of a interaction potential between the ions  
 at  $O$  and  $R$ , mediated by the electrons. We  
 can do the  $q^2$  integrations, and obtain how  
 this potential depends upon the separation  $R$ .  
 Because of the non-analytic behavior of  $\epsilon(q)$   
 at  $q = 2k_f$  ( $q = q_m$  is general), this potential  
 will have long-range oscillations of the  
 Friedel type. Thus, in a metal, even if the  
 bare ion-ion interaction is short-range, ~~there~~  
 the interaction with the electrons induce effective  
 long-range interactions, and this makes the  
 problem of calculating phonon frequencies difficult.  
 However, calculations have been done, ~~and~~ with  
 realistic band structures (instead of assuming  
 plane waves) and the results do agree with ~~expt~~  
 (neutron scattering).

### Electron mass renormalization

We have now reached the third stage  
 of the calculation that we have to do. This  
 stage is to calculate the change in the electron-  
 energies (quasiparticle energies) due to the el-  
 phonon interaction. The change in the quasiparticle  
 energies at the Fermi surface can be expressed  
 as a change in the effective mass of these  
 quasiparticles, hence the name mass renormalization\*.  
 We'll do this by calculating the self-energy

(2)

of an electron due to the el-phonon interaction. Again, the self-energy will have both real & imaginary parts, real part  $\rightarrow$  quasiparticle energy (mass renormalization) and imaginary part  $\rightarrow$  quasiparticle lifetime (comes into transport theory).

$$\text{Hamiltonian } H = \sum_{\vec{k}} E(\vec{k}) c_{\vec{k}}^{\dagger} c_{\vec{k}} + \sum_{\sigma, \vec{k}, \vec{k}'} D_{\sigma}(\vec{k}, \vec{k}') c_{\vec{k}}^{\dagger} c_{\vec{k}'} \left[ a_{\sigma}(\vec{k}-\vec{k}') + a_{\sigma}^{\dagger}(\vec{k}'-\vec{k}) \right] + \sum_{\vec{q}, \sigma} \hbar \omega_{\sigma}(\vec{q}) a_{\sigma}^{\dagger}(\vec{q}) a_{\sigma}(\vec{q})$$

(only one band)

$D_{\sigma}, a, a^{\dagger} \Rightarrow$  Renormalized phonons.

Also, assume  $D_{\sigma}(\vec{k}, \vec{k}') = D_{\sigma}(\vec{k}-\vec{k}')$

$$\Rightarrow \sum_{\sigma, \vec{k}, \vec{q}} D_{\sigma}(\vec{q}) c_{\vec{k}+\vec{q}}^{\dagger} c_{\vec{k}} \left[ a_{\sigma}(\vec{q}) + a_{\sigma}^{\dagger}(-\vec{q}) \right]$$

Electron-electron interactions are not present. They have been taken into account in defining the renormalized phonons. Also, we should look at  $E(\vec{k})$  as the quasiparticle energy, not the single-electron band energy.

(\*) The actual values of the quasiparticle energies do not change by much. This is because the energy scale of the phonons is set by the Debye energy which is  $\sim 20-30$  meV, whereas the electronic energy  $\sim$  Fermi energy  $\sim$  several eV. However, the actual self energy is small, but its derivative w.r.t.  $\vec{k}$  is large  $\Rightarrow$  large correction to the effective mass.

(12)

## Mass renormalization (of electrons)

$$\begin{aligned}
 H = & \sum_{\vec{k}} E(\vec{k}) C^\dagger(\vec{k}) C(\vec{k}) \\
 & + \sum_{\sigma, \vec{k}, \vec{k}'} D_\sigma(\vec{k}, \vec{k}') C^\dagger(\vec{k}) C(\vec{k}') \left[ a_\sigma(\vec{k}-\vec{k}') + a_\sigma^\dagger(\vec{k}'-\vec{k}) \right] \\
 & + \sum_{\vec{p}} \hbar \omega_\sigma(\vec{p}) a_\sigma^\dagger(\vec{p}) a_\sigma(\vec{p})
 \end{aligned}$$

We'll calculate the self-energy of an electron due to the electron-phonon interaction term. The phonons in the above expression are the renormalized ones, and the single-electron energies  $E(\vec{k})$  are the quasiparticle energies. The real part of the self-energy  $\Rightarrow$  mass renormalization. Im. part  $\Rightarrow$  lifetime.

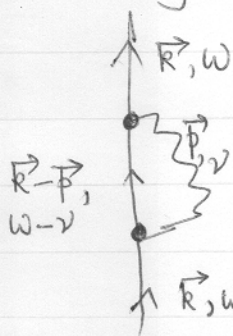
Simplification:  $D_\sigma(\vec{k}+\vec{p}, \vec{k}) = D_\sigma(\vec{p})$

$$\Rightarrow \sum_{\sigma, \vec{p}} D_\sigma(\vec{p}) C^\dagger(\vec{k}+\vec{p}) C(\vec{k}) \left[ a_\sigma(\vec{p}) + a_\sigma^\dagger(-\vec{p}) \right]$$

$\Uparrow$  electron-phonon vertex.

To calculate the self-energy, we have to look at the irreducible diagrams for the 1-electron Green's function. We'll consider terms upto second order in the el-phonon interaction. The contributions from higher order terms are small.

$\Rightarrow$  The only diagram that we have to consider is



The wavy line corresponds to either

- ① Emission of phonon of wave number  $\vec{p}$  and subsequent absorption.
- ② Absorption of phonon of wave no.

$(-\vec{p})$  and subsequent emission.

Vertex (1):  $c_{(\vec{k}-\vec{p})}^+ c_{(\vec{k})} \otimes v_{\sigma}(-\vec{p})$

$= c_{(\vec{k}-\vec{p})}^+ c_{(\vec{k})} [a_{\sigma}(-\vec{p}) + a_{\sigma}^+(\vec{p})]$

Vertex (2):  $c_{(\vec{k}+\vec{p})} c_{(\vec{k})}^+ [a_{\sigma}(\vec{p}) + a_{\sigma}^+(-\vec{p})]$

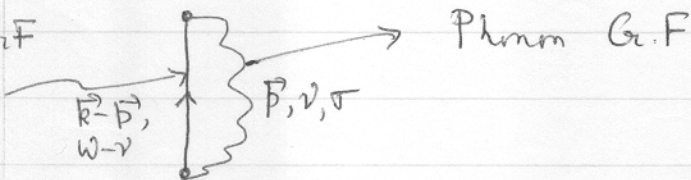
Second term. First term.

$v_{\sigma}^+(\vec{p})$

Self-energy  $\Sigma(\vec{k}, \omega)$

For simplicity, we'll work here at zero temperature.

El. G.F



Finite temperature  $\Rightarrow$  Matsubara frequencies  $\Rightarrow$  discrete sum.

Zero temperature  $\Rightarrow$  integral.

Harmonic 1-phonon Green's function

$$G_p(\vec{k}, \sigma, i\omega_n) = \frac{1}{\beta} \frac{2\omega_{\sigma}(\vec{k})}{\omega_n^2 + \omega_{\sigma}^2(\vec{k})} \quad \omega_n = \frac{2\pi n}{\beta}$$

(Diagonal in the polarization  $\sigma$ )

$T=0 \Rightarrow \beta \rightarrow \infty, \omega_n \rightarrow \omega$ , a continuous variable.

$$\sum_n \Rightarrow \frac{\beta}{2\pi} \int d\omega. \quad [i\omega_n \rightarrow z_n \rightarrow z]$$

$$\Rightarrow G_p(\vec{k}, \sigma, z) = \frac{1}{\beta} \frac{2\omega_{\sigma}(\vec{k})}{-z^2 + \omega_{\sigma}^2(\vec{k})} \otimes \frac{\beta}{2\pi}$$

$$= \frac{1}{2\pi} \left[ \frac{1}{\omega_{\sigma}(\vec{k}) - z - i\eta} + \frac{1}{\omega_{\sigma}(\vec{k}) + z - i\eta} \right]$$

$\eta \rightarrow 0^+$  to assure correct analytic properties.

(B)

Electron green's function  $G_e(\vec{k}, \omega) = \frac{1}{E(\vec{k}) - \omega - i\eta(\vec{k})}$

$\eta(\vec{k}) = 0^+$   $\vec{k}$  outside Fermi surface

$0^-$   $\vec{k}$  inside "  $|D_\sigma(\vec{p})|^2$

$$\Sigma(\vec{k}, \omega) = \sum_{\sigma} \sum_{\vec{p}} \int \frac{d\nu}{2\pi} G_e(\vec{k}-\vec{p}, \omega-\nu) G_p(\vec{p}, \sigma, \nu)$$

The integral over  $\nu$  gives rise to two terms.

(1)

$$\frac{1}{E(\vec{k}-\vec{p}) - \omega + \nu - i\eta(\vec{k}-\vec{p})} \cdot \frac{1}{\omega_\sigma(\vec{p}) - \nu - i\eta}$$

This term contributes only if  $\eta(\vec{k}-\vec{p}) = 0^+$   
 then the pole of the first term is above the real axis,  
 the pole of the second term is below.

Contribution: 
$$\frac{1 - f(\vec{k}-\vec{p})}{E(\vec{k}-\vec{p}) - \omega + \omega_\sigma(\vec{p})}$$

(2)

$$\frac{1}{E(\vec{k}-\vec{p}) - \omega + \nu - i\eta(\vec{k}-\vec{p})} \cdot \frac{1}{\omega_\sigma(\vec{p}) + \nu - i\eta}$$

$\eta(\vec{k}-\vec{p}) = 0^- \Rightarrow (\vec{k}-\vec{p})$  inside Fermi surface.

Contribution: 
$$\frac{f(\vec{k}-\vec{p})}{E(\vec{k}-\vec{p}) - \omega - \omega_\sigma(\vec{p})}$$

Putting these two terms together, we get

$$\Sigma_1(\vec{k}, \omega) = \sum_{\vec{p}, \sigma} |D_\sigma(\vec{p})|^2 \times \left[ \frac{1 - f(\vec{k}-\vec{p})}{E(\vec{k}-\vec{p}) - \omega + \omega_\sigma(\vec{p})} \right]$$

(16)

$$+ \frac{f(k^2 - p^2)}{E(k^2 - p^2) - \omega - \omega_0(p^2)} \Big]$$

$$G_e^R(k^2, \omega) = \frac{1}{E(k^2) - \omega - \Sigma^R(k^2, \omega)}$$

Quasiparticle energy: Real part of the pole.

For  $D_0$  small, this energy can be approximately obtained [by

$$E^R(k^2) = E(k^2) - \Sigma^R(k^2, E(k^2) + i\eta)$$

$$= E(k^2) + \sum_{\vec{p}, \sigma} \left| D_0(p^2) \right|^2 \left[ \frac{1 - f(k^2 - p^2)}{E(k^2) - E(k^2 - p^2) - \omega_0(p^2) + i\eta} + \frac{f(k^2 - p^2)}{E(k^2) - E(k^2 - p^2) + \omega_0(p^2) + i\eta} \right]$$

$$\Rightarrow E(k^2) + \sum_{\vec{p}, \sigma} \int \frac{d^3 p}{(2\pi)^3} \left| D_0(p^2) \right|^2 \left[ \frac{1 - f(k^2 - p^2)}{E(k^2) - E(k^2 - p^2) - \omega_0(p^2)} + \frac{f(k^2 - p^2)}{E(k^2) - E(k^2 - p^2) + \omega_0(p^2)} \right]$$

There are different other ways of getting this result. We could get this by looking at  $\Delta E^{(2)}$  and determining how it changes as we add another electron to the system. The extra energy is the electron-photon contribution to the quasi-particle energy. Now,

$$\Delta E^{(2)} \sim \sum_{\vec{p}, \sigma, \vec{k}} \left| D_0(p^2) \right|^2 \frac{f(k^2) [1 - f(k^2 - p^2)]}{E(k^2) - E(k^2 - p^2)}$$



$$E(\vec{k}) - E(\vec{k}-\vec{p}) - \hbar\omega(\vec{p}) = \frac{E(\vec{k}-\vec{p}) - \hbar\omega(\vec{p})}{E(\vec{k}) - \hbar\omega(\vec{p})} + \frac{\hbar\omega(\vec{p})}{E(\vec{k}) - \hbar\omega(\vec{p})}$$

For  $\vec{p}$  small, the energy can be approximated by

$$E(\vec{k}) - [2E(\vec{k}) - E(\vec{k}-\vec{p}) + \hbar\omega(\vec{p})] = E(\vec{k}-\vec{p}) - E(\vec{k}) - \hbar\omega(\vec{p})$$

$$\text{Initial (-) sign} \rightarrow E(\vec{k}) - E(\vec{k}-\vec{p}) + \hbar\omega(\vec{p})$$

Intermediate state

$$E_{int} = E_0 - E(\vec{k}-\vec{p}) + \hbar\omega(\vec{p})$$

Initial state:  $E(\vec{k}) + \text{Filled Fermi sea}$

Intermediate state:  $E(\vec{k}) + \text{Filled Fermi sea} - E(\vec{k}-\vec{p}) + E(\vec{k}) + \hbar\omega(\vec{p})$

$$\text{Initial} - \text{Intermediate} = E(\vec{k}-\vec{p}) - E(\vec{k}) - \hbar\omega(\vec{p})$$

there are different ways of getting the result. We could get the result by looking at  $\Delta E$  and determining how it changes as we add another electron to the system. The extra energy is the electron-phonon contribution to the ground state energy.

$$\Delta E_0 = \sum_{\vec{k}, \vec{p}} \frac{E(\vec{k}) - E(\vec{k}-\vec{p})}{E(\vec{k}) - \hbar\omega(\vec{p})} \hbar\omega(\vec{p})$$

(17)

Now, we add an electron in the state  $\vec{k}_0$ , and try to calculate the change in  $\Delta E^{(2)}$ . This has two terms. First one:  $\vec{k} = \vec{k}_0$   $f = 0$  prev. = 1 now.

$$\Rightarrow \sum_{\sigma, \vec{p}} |D_{\sigma}(\vec{p})|^2 \frac{1 - f(\vec{k}_0 - \vec{p})}{E(\vec{k}_0) - E(\vec{k}_0 - \vec{p})}$$

Second term:  $\vec{k} - \vec{p} = \vec{k}_0$   $\vec{k} = \vec{k}_0 + \vec{p}$

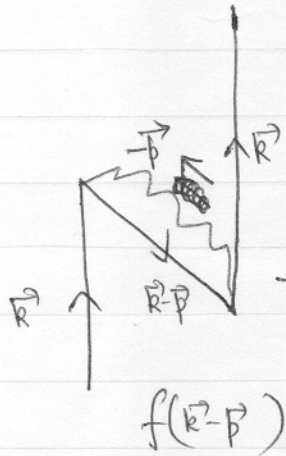
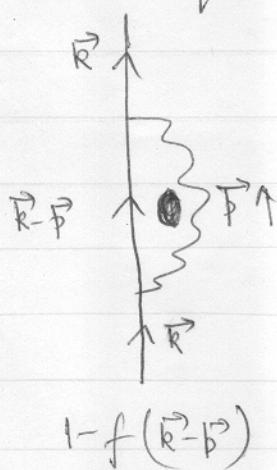
$1 - f = 1$  prev.,  $0$  now.

$$\Rightarrow \text{Contribution: } - \sum_{\sigma, \vec{p}} |D_{\sigma}(\vec{p})|^2 \frac{f(\vec{k}_0 + \vec{p})}{E(\vec{k}_0 + \vec{p}) - E(\vec{k}_0)}$$

$$(\vec{p} \rightarrow -\vec{p}) = \sum_{\sigma, \vec{p}} |D_{\sigma}(\vec{p})|^2 \frac{f(\vec{k}_0 - \vec{p})}{E(\vec{k}_0) - E(\vec{k}_0 - \vec{p})}$$

These two terms are identical to the ones obtained above, with the exception of  $\omega_{\sigma}(\vec{p})$ . But this is to be expected, because in calculating  $\Delta E^{(2)}$ , we assumed static potentials, i.e. we put  $\omega_{\sigma}(\vec{p}) = 0$ .

A third way to look at this result is to consider diagrams in real time instead of in frequency. Then we have two diagrams!



time.

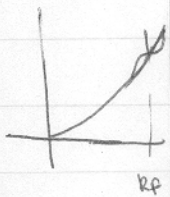
emits  $E$  in  $(\vec{k}-\vec{p})$  absorbs  $\text{phon}(\vec{p})$ , emits electron  $\vec{k}$  (hole is created in  $(\vec{k}-\vec{p})$ ) This hole then annihilates with the initial electron, ~~releasing~~ <sup>absorbing</sup>  $\text{phon}(-\vec{p})$

(18)



From the expression for  $E(\vec{k}^{\sigma})$ , we can obtain the mass-renormalization factor. To do this, we rewrite the expression for  $E^R(\vec{k}^{\sigma})$ :

$$E^R(\vec{k}^{\sigma}) = E(\vec{k}^{\sigma}) + \sum_{\vec{p}, \sigma'} |D_{\sigma}(\vec{p})|^2 \left[ \frac{1}{E(\vec{k}^{\sigma}) - E(\vec{k}^{\sigma} - \vec{p}^{\sigma}) - \omega(\vec{p}^{\sigma})} - \frac{2 f(\vec{k}^{\sigma} - \vec{p}^{\sigma}) \omega_{\sigma}(\vec{p}^{\sigma})}{[E(\vec{k}^{\sigma}) - E(\vec{k}^{\sigma} - \vec{p}^{\sigma})]^2 - \omega_{\sigma}^2(\vec{p}^{\sigma})} \right]$$



The first term is a slowly varying function of  $\vec{k}^{\sigma}$ . There is a tendency we are interested in  $E^R(\vec{k}^{\sigma})$  for  $k \approx k_f$  because only in this region, the quasiparticles are well-defined. Also, all the low-energy excitations ~~for~~ involve  $k \approx k_f$ . ~~At~~ ~~in~~ the first term, contributions from regions above of below the Fermi surface tend to cancel each other, and the total contribution  $\approx \omega_D$ . (Come back to this when discussing polarons). The second term is also  $\approx \omega_D$  because of the presence of  $\omega_{\sigma}(\vec{p}^{\sigma})$ , but it involves a sharp cutoff in the factor  $f(\vec{k}^{\sigma} - \vec{p}^{\sigma})$ . Thus, its derivative w.r.t  $\vec{k}^{\sigma}$  can be quite large. This is the term that leads to a renormalization of the effective mass near the Fermi surface. To calculate it, we note that

$$\frac{\partial f(E)}{\partial E} = -\delta(E - E_f) \quad \text{at zero temperature. Considering only the second term,}$$

$$\Rightarrow \nabla_{\vec{k}} E^R(\vec{k}^{\sigma}) = \nabla_{\vec{k}} E(\vec{k}^{\sigma}) + \sum_{\vec{p}, \sigma'} |D_{\sigma}(\vec{p}^{\sigma})|^2 \times \left[ + \frac{2 \omega_{\sigma}(\vec{p}^{\sigma}) \nabla_{\vec{k}} E(\vec{k}^{\sigma} - \vec{p}^{\sigma}) \delta[E(\vec{k}^{\sigma} - \vec{p}^{\sigma}) - E_f]}{[E(\vec{k}^{\sigma}) - E(\vec{k}^{\sigma} - \vec{p}^{\sigma})]^2 - \omega_{\sigma}^2(\vec{p}^{\sigma})} \right]$$

(19)

Change of variables;  $\vec{k} - \vec{p} = \vec{k}'$

Both  $\vec{k}$ ,  $\vec{k}'$  are close to Fermi surface.

$$\Rightarrow \vec{\nabla}_{\vec{k}} E(\vec{k} - \vec{p}) \approx \vec{\nabla}_{\vec{k}} E(\vec{k}), \quad E(\vec{k} - \vec{p}) \approx E(\vec{k})$$

$$\text{Also } \sum_{\vec{p}} \Rightarrow \frac{V}{(2\pi)^3} \int d\vec{k}'$$

$$\Rightarrow \vec{\nabla}_{\vec{k}} E^R(\vec{k}) = \vec{\nabla}_{\vec{k}} E(\vec{k}) \left[ 1 + \frac{V}{(2\pi)^3} \sum_{\sigma} \int d\vec{k}' \frac{2 \omega_{\sigma}(\vec{k} - \vec{k}')}{\omega_{\sigma}^2(\vec{k} - \vec{k}')} \delta(E(\vec{k}') - E_f) |D_{\sigma}(\vec{k} - \vec{k}')|^2 \right]$$

$$= \vec{\nabla}_{\vec{k}} E(\vec{k}) [1 - \alpha(\vec{k})]$$

$$\alpha(\vec{k}) = \frac{2V}{(2\pi)^3} \sum_{\sigma} \int |D_{\sigma}(\vec{k} - \vec{k}')|^2 \frac{1}{\omega_{\sigma}(\vec{k} - \vec{k}')} \frac{dS_{k'}}{|\vec{\nabla}_{\vec{k}'} E(\vec{k}')|}$$

Now, we replace  $\alpha(\vec{k})$  by its average value  $\bar{\alpha}$  for  $\vec{k}$  on the Fermi surface, and write

$$\vec{\nabla}_{\vec{k}} E^R(\vec{k}) = \vec{\nabla}_{\vec{k}} E(\vec{k}) (1 - \bar{\alpha})$$

The effective mass, for isotropic Fermi surface, is given by

$$\frac{1}{m^*} = \frac{1}{3k^2} \nabla_{\vec{k}}^2 E(\vec{k}) \Big|_{k=k_f}$$

Thus, we have

$$\frac{1}{m_R^*} = (1 - \bar{\alpha}) \frac{1}{m^*}$$

$$\Rightarrow m_R^* = (1 + \bar{\alpha}) m^* \quad \text{to first order in } \bar{\alpha}.$$

$\bar{\alpha}$  is also called the el-phonon mass enhancement factor.

(20)

A rough estimate of  $\bar{\alpha}$  can be obtained by assuming that  $D_0$  is independent of  $(\vec{k}-\vec{k}')$ , and replacing  $\omega_0(\vec{k}-\vec{k}')$  by an average phonon frequency  $\bar{\omega}$  which is of the order of the Debye frequency  $\omega_D$ . We then have

$$\bar{\alpha} \approx D^2 \frac{1}{\bar{\omega}} G_0(E_f) \quad \text{where } G_0: \text{density}$$

of states at the Fermi surface. This gives, for simple metals like sodium,  $\bar{\alpha} \approx 0.5$ .

Actually,  $\bar{\alpha} \approx 0.1 - 0.4$  and this implies a substantial change in the effective mass at the Fermi surface. This parameter  $\bar{\alpha}$  is a direct measure of the strength of electron-phonon coupling, and plays an important role in the theory of superconductivity. Low  $\bar{\alpha}$  means weak coupling, less tendency towards superconductivity, whereas large  $\bar{\alpha}$  means strong coupling. Actually, the classification of superconductors into strong & weak coupling classes is often done according to the value of  $\bar{\alpha}$  (often called  $\lambda$ ). The value of  $\bar{\alpha}$  can be measured directly in electron tunneling experiment.

## ORIGIN OF SUPERCONDUCTIVITY

Superconductivity results from an effective attractive interaction between electrons, produced by phonon exchange. Here, we'll try to understand