Electron - Phonon Coupling

When discussing phonons, the Born-Oppenheimer approximation ensures that the electronic degrees of freedom and the lattice dynamics are decoupled. Corrections to this decoupling exist and are of order $\sqrt{\frac{m}{M}}$ where m is the electron and M is the ion mass.

Let's consider the electronic part of the total lattice Hamiltonian:

$$\mathcal{H} = \sum_{i=1}^{N_e} \frac{p_i^2}{2m} + \underbrace{\sum_{i=1}^{N_e} V(r_i)}_{\text{lattice potential} \rightarrow \text{periodic}} + \sum_{i<j} u(r_i - r_j)$$

$$V(\vec{r}+\vec{R}) = V(\vec{r})$$

strictly speaking, the lattice potential can be periodic only at $T=0$. At finite temperature, the ions move around their equilibrium positions.

The lattice potential can be written as a linear combination of contributions from each unit cell:

$$V(\vec{r}) = \sum_{n=1}^{N} v(\vec{r}-\vec{R}_n)$$

where the $\vec{R}_n$ are not necessarily lattice vectors of the Bravais lattice as the ions may vibrate around these positions.

$$\rightarrow \vec{R}_n = \vec{R}_{n0} + \vec{u}_n$$

$\uparrow$ lattice vector $\quad \nwarrow$ small deviation

We assume here that there is only one atom in the unit cell.

For small $\vec{u}_n$, we can write

$$v(\vec{r}-\vec{R}_n) = v(\vec{r}-\vec{R}_{n0}-\vec{u}_n)$$

$$= v(\vec{r}-\vec{R}_{n0}) - \vec{\nabla} v(\vec{r}-\vec{R}_{n0}) \cdot \vec{u}_n$$

and so the one-particle part of the Hamiltonian, H_0, can be written

$$\mathcal{H}_0 = \sum_{i=1}^{N_e} h(\vec{r}_i)$$

with $h(\vec{r}_i) = \frac{\vec{p}_i}{2m} + \underbrace{\sum_{n=1}^{N} v(\vec{r}_i-\vec{R}_{n0})}_{V_{periodic}} - \underbrace{\sum_{n=1}^{N} \vec{\nabla} v(\vec{r}_i-\vec{R}_{n0}) \cdot \vec{u}_n}_{V_{el-ph}(\vec{r}_i)}$

In 2^{nd} quantization, the first two terms of the right-hand side are diagonal in a representation based on Bloch wavefunctions. The first two terms are (lattice) translational invariant.

The term $V_{el-ph}(\vec{r})$ will have non-diagonal elements, as this term in general lacks translational invariance.

$$H_0 = \sum_{k\sigma} \mathcal{E}(\underline{k})\, c^+_{\underline{k}\sigma} c_{\underline{k}\sigma} - \sum_{\underline{k},\sigma} \langle \underline{k} | V_{el-ph}(\underline{r}) | \underline{k}' \rangle\, c^+_{\underline{k}'\sigma} c_{\underline{k}\sigma}$$

- $V_{el\text{-}ph}(\vec{r})$ is spin-diagonal

- $\langle \underline{k} | V_{el-ph} | \underline{k}' \rangle = \int d^3r\, \psi^*_{\underline{k}}(\underline{r}) \sum_{l=1}^{N} \nabla v(\vec{r} - \vec{R}_{l0}) \cdot \vec{u}_l\, \psi_{\underline{k}'}(\underline{r})$

The potential $v(\vec{r})$ of a single ion can be written in a Fourier series as

$$v(\vec{r}) = \sum_{\vec{k}} v_k\, e^{i\vec{k}\cdot\vec{r}} \quad \text{where} \quad v_k = \frac{1}{V}\int d^3r\, e^{-i\vec{k}\cdot\vec{r}}\, v(\vec{r})$$

$$\rightarrow \nabla v(\vec{r}) = \sum_{k} i\vec{k}\, v_k\, e^{i\vec{k}\cdot\vec{r}}$$

and therefore

$$\langle \underline{k} | V_{el-ph} | \underline{k}' \rangle = \sum_{\underline{k}} i\vec{k}\, v_{\underline{k}} \int d^3r\, \psi^*_{\underline{k}}(\underline{r}) \sum_{l=1}^{N} e^{i\vec{k}\cdot(\vec{r} - \vec{R}_{l0})}\, \vec{u}_l\, \psi_{\underline{k}'}(\vec{r})$$

The deviation from the equilibrium position, $\vec{u}_e$, can be written in terms of phonon creation and annihilation operators. This is very similar to expressing the displacement $\hat{x}$ of the harmonic oscillator in terms of the ladder operators:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\,(\hat{a}+\hat{a}^+)$$

$$\left(\text{and } \hat{p} = -i\sqrt{\frac{m\hbar\omega}{2}}\,(\hat{a}-\hat{a}^+)\right)$$

$$\rightsquigarrow \vec{u}_e = \frac{1}{\sqrt{N}} \underbrace{\sum_{q,j}}_{\text{different modes}} \sqrt{\frac{\hbar}{2M\omega_j(\vec{q})}}\,\left(b_{\vec{q}j} + b^+_{-\vec{q}j}\right) \underbrace{\vec{e}_j(\vec{q})}_{\text{displacement direction}}\, e^{i\vec{q}\cdot\vec{R}_{e0}}$$

and so

$$\langle \underline{k} | V_{el\text{-}ph} | \underline{k}' \rangle = \frac{1}{\sqrt{N}} \sum_{q\tilde{k}j} i\tilde{k}\cdot\vec{e}_j(\vec{q})\, v_{\tilde{k}} \overbrace{\sum_{i=1}^{N} e^{i(\underline{q}-\underline{\tilde{k}})\cdot\vec{R}_{e0}}}^{N\sum_G \delta_{\tilde{k}\,q+G}}$$

$$\times \underbrace{\frac{1}{V}\int d^3r\, e^{i(\underline{k}'-\underline{k})\cdot\underline{r}}\, u^*_{\underline{k}}(\underline{r})\, e^{i\underline{\tilde{k}}\cdot\underline{r}}\, u_{\underline{k}'}(\underline{r})}_{\frac{1}{N}\sum_R e^{i(\underline{k}'+\underline{k}-\tilde{k})\vec{R}}\, \frac{1}{V_{EZ}}\int_{EZ} d^3r\, e^{i(k'+\tilde{k}-k)\vec{r}}\, u^*_k(r)\, u_{k'}(r)} \sqrt{\frac{\hbar}{2M\omega_j(\vec{q})}}\,\left(b_{qj} + b^+_{-qj}\right)$$

$$\rightsquigarrow \langle \underline{k} | V_{el-ph} | \underline{k}' \rangle = \sqrt{N} \sum_{\vec{G}\vec{q}j} i(\vec{q}+\vec{G})\cdot\vec{e}_j(\vec{q})\, v_{q+G} \sqrt{\frac{\hbar}{2M\omega_j(\vec{q})}} \left(b_{qj} + b^+_{-qj}\right)$$

$$\times \frac{1}{V_{EZ}} \int d^3r\, u_k^*(\vec{r})\, u_{k-q-G}(\vec{r})\, \delta_{k'k-q-G}$$

We therefore have in 2^{nd} quantization

$$\mathcal{H}_0 = \sum_{k\sigma} \varepsilon(\underline{k})\, c^+_{k\sigma} c_{k\sigma} + \sum_{kqGj\sigma} M^j_{k,q+G} \left(b_{qj} + b^+_{-qj}\right) c^+_{k\sigma}\, c_{k-q-G\sigma}$$

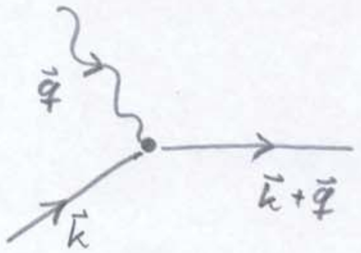
$$= \sum_{k\sigma} \varepsilon(\underline{k})\, c^+_{k\sigma} c_{k\sigma} + \sum_{\substack{kq\\Gj\sigma}} M^j_{k,q+G} \left(b_{qj} + b^+_{-qj}\right) c^+_{k+q+G\sigma}\, c_{k\sigma}$$

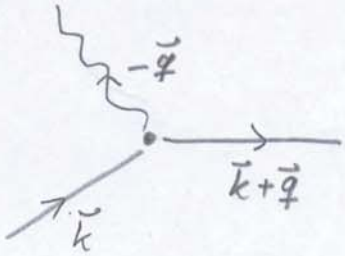
where the matrix element of the electron-phonon coupling

$$M^j_{k,q+G} = -\sqrt{\frac{\hbar N}{2M\omega_j(\vec{q})}}\; i(\vec{q}+\vec{G})\cdot\vec{e}_j(\vec{q})\, v_{\vec{q}+\vec{G}}\, \frac{1}{V_{EZ}} \int_{EZ} d^3r\, u^*_{\vec{k}+\vec{q}+\vec{G}}(\vec{r})\, u_{\vec{k}}(\vec{r})$$

This hamiltonian is called the <u>Fröhlich model</u> for the electron-phonon interaction.

The electrons scatter at the displacements: an electron with wavevector $\underline{k}$ is being scattered into state $k' = k + q$ by absorbing (distroying) a phonon of wavevector q or by emitting (creating) a phonon with wave vector $-q$.





At the interaction vertex momentum conservation holds

$\vec{k}$ can be confined to the 1^{st} Brillouin zone

if $\vec{k}+\vec{q}$ lies outside of the 1^{st} Brillouin zone, a reciprocal lattice vector $\vec{G}$ can be added, so that $\vec{k}+\vec{q}+\vec{G}$ again lies in the 1^{st} Brillouin zone.

Such processes are called <u>Umklapp processes</u>.

If several atoms in the unit cell exist, optical phonons will also exist.

Our solid state Hamiltonian then assumes the following form:

$$\mathcal{H} = \sum_{\substack{k\nu \\ \sigma}} \varepsilon_\nu(\underline{k})\, c^+_{\underline{k}\nu\sigma} c_{\underline{k}\nu\sigma} + \sum_{\substack{\underline{k}\nu\underline{q} \\ \underline{G} j\sigma}} M^{j}_{\underline{k},\underline{q}+\underline{G}} \left(b_{\underline{q}j} + b^+_{-\underline{q}j}\right) c^+_{\underline{k}+\underline{q}+\underline{G}\,\nu\sigma} c_{\underline{k}\nu\sigma}$$

$$+\frac{1}{2}\sum_{\substack{k_1 k_2 \\ q}} \sum_{\substack{\sigma\sigma' \\ \nu\nu'}} U_{k_1+q\,\nu\, k_2-q\,\nu',\, \underline{k}_2\nu' k_1\nu}\, c^+_{k_1+q\,\nu\sigma}\, c^+_{\underline{k}_2-\underline{q}\,\nu'\sigma'}\, c_{\underline{k}_2\nu'\sigma'}\, c_{\underline{k}_1\nu\sigma}$$

$$+\sum_{qj} \hbar\omega_j(\underline{q})\left(b^+_{qj} b_{qj} + \frac{1}{2}\right)$$

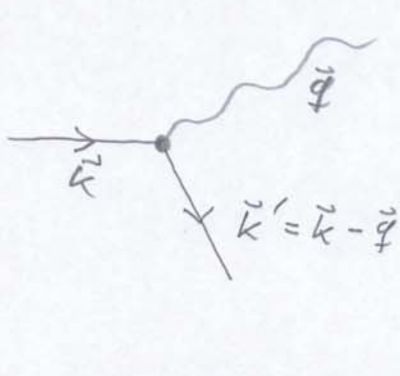
where ν is a band index and interband scattering has been neglected.

• consequences of the electron-phonon coupling:

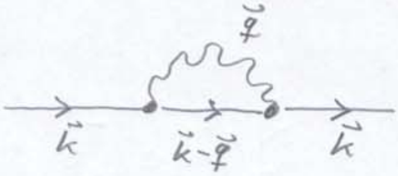
The wave vector $\underline{k}$ is no longer a good quantum number as electrons are scattered from $\underline{k}$ to $\underline{k}'$.

→ electrons have a finite life-time in the bloch state $\underline{k}$

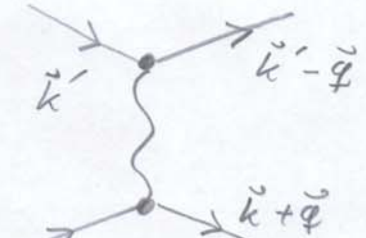
This results in a contribution to the electric resistivity.



- The electronic eigenstates and eigenvalues will be modified. In particular, a lattice polarization can accompany the propagation of the electron. This can lead to a new quasiparticle, the <u>polaron</u>, consisting of an electron and the polarization cloud

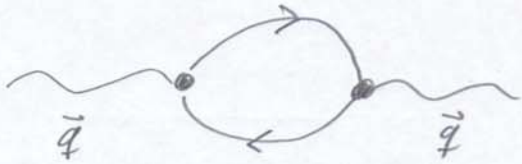


- The phonon emitted by an electron can be absorbed by another electron
This leads to an effective electron-electron interaction.
This interaction <u>may</u> be attractive which is the root for (conventional) superconductivity



- The phonon properties will also be renormalized by the electron phonon coupling.

These exist in particular processes where a propagating phonon generates an electron-hole pair which subsequently decays and emits a phonon:



These processes (and their theoretical treatment) resemble processes between electrons and photons in QED (quantum electrodynamics).

86

Effect of screening on phonon dispersion and electron-phonon interaction

The electron-phonon interaction is generated by the attractive potential that the electrons experience due to the positively charged ions.

→ The Coulomb interaction is at the root of the electron-phonon coupling

The Coulomb potential is screened.
What are the effects of screening of the ion potentials on phonons and electron-phonon interaction?

When discussing accustic phonons, you learned that in the long-wavelength limit ($q \to 0$) a uniform displacement of all ions. The ions are charged.
If the electrons would remain in their equilibrium position, a collective plasma oscillation of the ions should ensue, where the ionic plasma frequency would be $\Omega_p^2 = 4\pi \frac{Z^2 e^2 n_i}{M}$

where n_i is the ion density and M is the ion mass.
Ze is the positive charge of an ion.

$$M \frac{d^2x}{dt^2} = -Ze\underbrace{|\vec{E}|}_{4\pi \frac{Q}{A_{\text{area}}} = 4\pi \frac{Zen_iV}{A} = 4\pi Zen_i x} = -4\pi Z^2 e^2 n_i x \leadsto \frac{d^2x}{dt^2} + \omega^2 x = 0$$

87

This expectation of ionic plasma oscillations contradict the results for accustic phonons: $\omega_{AP} \to 0$ for $q \to 0$. The reason is that the assumption of electrons remaining in their equilibrium position is incorrect. Electrons will tend to screen the lattice polarization.

Using Thomas-Fermi approximation:

$$\varepsilon(q) = 1 + \frac{k_{TF}^2}{q^2} \quad \text{with} \quad k_{TF}^2 = 4\pi e^2 \frac{\partial n_0}{\partial \mu}$$

The field driving back the ions is therefore reduced by a factor $\frac{1}{\varepsilon(q)}$

$$\rightsquigarrow \quad \omega^2 = \frac{\Omega_P^2}{\varepsilon(q)} = \frac{4\pi Z^2 e^2 n_i}{M(q^2 + k_{TF}^2)} q^2$$

and so $\omega(q) = \sqrt{\frac{4\pi Z^2 e^2 n_i}{M k_{TF}^2}}\, q$

as expected for accustic phonons.

The sound velocity is therefore $c = \sqrt{\frac{4\pi Z^2 e^2 n_i}{M k_{TF}^2}}$

charge neutrality implies $n_i = n_e / Z$ for the electron density

$n_e = \frac{k_F^3}{3\pi^2}$, $k_{TF}^2 = 4me^2 k_F / \pi\hbar^2$

$$\rightsquigarrow \quad c^2 = \frac{4\pi Z^2 e^2 n_i}{M k_{TF}^2} = \frac{1}{3} Z \frac{m}{M} v_F^2 \qquad \left(m v_F^2 = \frac{\hbar^2 k_F^2}{m} \right)$$

The relation between sound and Fermi velocity: $\frac{c}{v_F} \sim \sqrt{\frac{m}{M}}$
"Bohm-Staver relation"

The ions themselves also screen electrostatic potentials. As their dynamics is much slower than that of the electrons, one has to consider dynamic screening and work with a frequency-dependent dielectric constant while we can use the static one to describe the electronic screening:

$$\varepsilon^{(0)}_{ion} = 1 - \frac{\Omega_p^2}{\omega^2}$$

the ions themselves are screened : $\Omega_p = \omega(q)\,\varepsilon_{el}(q)$

$$\rightsquigarrow \quad \varepsilon_{ion} = 1 - \frac{\omega^2(q)}{\omega^2}$$

the total dielectric constant (electronic + ionic) is

$$\frac{1}{\varepsilon} = \frac{1}{\varepsilon_{el}(q)}\,\frac{1}{\varepsilon_{ion}} = \frac{1}{1+\frac{k_{TF}^2}{q^2}}\;\frac{1}{1-\frac{\omega^2(q)}{\omega^2}}$$

The bare Coulomb potential therefore becomes

$$\frac{4\pi e^2}{q^2}\,\frac{1}{\varepsilon} = \frac{4\pi e^2}{q^2+k_{TF}^2}\left(1+\frac{\omega^2(q)}{\omega^2-\omega^2(q)}\right)$$

(89)

Two electrons with momenta k, k' experience in a metal a screened interaction

$$V_{\underline{k},\underline{k}'} = \frac{1}{V} \frac{4\pi e^2}{(\underline{k}-\underline{k}')^2 + k_{TF}^2} \left(1 + \frac{\omega^2(\underline{k}-\underline{k}')}{\omega^2 - \omega^2(k-k')}\right)$$

where $\hbar\omega = \varepsilon_k - \varepsilon_{k'}$

If $\hbar\omega$ is much larger than the phonon energies (of order of the Debye frequency) we recover the Thomas-Fermi approximation.

If $\hbar\omega$ is smaller than the Debye frequency, the 2nd term is negativ and the total interaction may become negativ, that is, attractive.

This is the microscopic origin of (conventional) superconductivity.