Electron-phonon interaction The electron-phonon interaction plays an essential role in solid state physics. This interaction explains among other things the electrical resistivity of the metals. Nevertheless, at low temperature it will have a very different effect since it is an essential ingredient for the understanding of superconductivity by creating an effective attraction between electrons.

In this problem we consider electrons that move in a periodic potential. This potential, created by the ions, is not static, but undergoes small fluctuations, called phonons. The wave function that describes an electron moving in a periodic potential is the following (Bloch's theorem):

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}),$$

where $u_{\mathbf{k}}(\mathbf{r})$ is a function that has the periodicity of the lattice.

The position of the ions that make up the lattice can be described thanks to the creation and annihilation operators of phonons. First, a change of coordinates is made to switch to the normal coordinates that can be quantified, and then we express the latter with creation and annihilation operators:

$$s_{n,\alpha,i}(t) = \frac{1}{\sqrt{NM_\alpha}} \sum_{j,\vec{q}} Q_j(\vec{q},t) e^{(j)}_{\alpha,i}(\vec{q}) e^{i\vec{q}\cdot\vec{R}_n}$$

where n denotes the unit cells of the lattice, α the position of the ion in the unit cell, and i the spatial direction. N is the number of unit cells in the lattice, and M_α the mass of the ion α; $s_{n,\alpha,i}(t)$ is the displacement relative to the equilibrium position $\vec{R}_{n,\alpha}$. The quantities $e^{(j)}_{\alpha,i}$ are called polarization vectors. The quantities $Q_j(\vec{q},t)$ are called normal coordinates. They can be considered as the new variables of the problem (see course notes on pages 82-85 for more details on the calculation leading to this result). In second quantization, they can be rewritten using phonon creation and annihilation operators such as:

$$Q_j(\vec{q}) = \sqrt{\frac{\hbar}{2\omega_j(\vec{q})}} (a^\dagger_j(-\vec{q}) + a_j(\vec{q}))$$

The electron-phonon interaction is described via a Coulomb repulsion potential of the form

$$\sum_{l,n,\alpha} V(\vec{r}_l - \vec{R}_{n,\alpha}(t)).$$

The position of the ions can be described as a vector of the lattice plus a small displacement: $\vec{R}_{n,\alpha}(t) = \vec{R}_{n,\alpha} + \vec{s}_{n,\alpha}(t)$.

1. Assuming that the $\vec{s}_{n,\alpha}(t)$ displacements are small, show that the electron-phonon interaction can be written as:

$$H_{\text{el-ph}} = -\sum_{\alpha,n,l} \frac{1}{\sqrt{NM_\alpha}} \sum_{j,\vec{q}} Q_j(\vec{q}) \vec{e}^{(j)}_\alpha(\vec{q}) \cdot \vec{\nabla} V_\alpha(\vec{r}_l - \vec{R}_{n,\alpha}) e^{i\vec{q}\cdot\vec{R}_n}$$

   N.B.: The static potential $\sum_{l,n,\alpha} V(\vec{r}_l - \vec{R}_{n,\alpha})$ is already taken into account by the Bloch theorem.

   We now want to express this interaction in second quantisation. We already know the transformation for the coordinates $Q_j(\vec{q})$, but not for the positions of the electrons.

2. By expanding the potential in Fourier series $V_\alpha(\vec{r}) = \sum_{\vec{K}} e^{i\vec{K}\cdot\vec{r}} V_{\alpha,\vec{K}}$, show that the matrix elements of the gradient can be written as:

$$\left\langle \vec{k}', \sigma' \middle| \vec{\nabla} V_\alpha \middle| \vec{k}, \sigma \right\rangle = \sum_{\vec{K}} e^{-i\vec{K}\vec{R}_{n,\alpha}} V_{\alpha,\vec{K}} i\vec{K} \int d\vec{r} u^*_{\vec{k}'}(\vec{r}) u_{\vec{k}}(\vec{r}) e^{i(-\vec{k}'+\vec{K}+\vec{k})\vec{r}} \delta_{\sigma,\sigma'}$$

3. What condition must k, k', and K satisfy so that the integral does not cancel?

4. Returning to the initial expression of the interaction, prove that in the sum, only terms satisfying $\vec{K} = \vec{q} + \vec{G}$ contribute.

   In the end, the condition is written as: $\vec{q} = \vec{k}' - \vec{k} + \vec{G}$

$$\begin{cases} \vec{G} = \vec{0} & \text{for normal processes} \\ \vec{G} \neq \vec{0} & \text{for Umklapp processes} \end{cases}$$

5. Gather all the terms and show that the electrons-phonons interaction expressed in second quantisation reads:

$$\begin{aligned} H &= -\sum_{\alpha,\sigma,\vec{k},\vec{q},j} \sqrt{\frac{N\hbar}{2M_\alpha \omega_j(\vec{q})}} \\ &\times \sum_{\vec{G}'} \left[\vec{e}^{(j)}_{\alpha,\vec{q}} \cdot i(\vec{q}+\vec{G}') \right] \int V_\alpha(\vec{r}') e^{-i(\vec{q}+\vec{G}')\cdot(\vec{r}'+\vec{R}_\alpha)} d\vec{r}' \\ &\times \int u^*_{\vec{k}+\vec{q}+\vec{G}}(\vec{r}) u_{\vec{k}}(\vec{r}) e^{-i(G-\vec{G}')\vec{r}} d\vec{r} \\ &\times \left[a^\dagger_{-\vec{q}}(j) + a_{\vec{q}}(j) \right] c^\dagger_{\vec{k}+\vec{q}+\vec{G},\sigma} c_{\vec{k},\sigma} \end{aligned}$$

   where for each $\vec{k}$ and $\vec{q}$, the value of $\vec{G}$ is given by the constraint that $\vec{k} + \vec{q} + \vec{G}$ must be in the first Brillouin zone.

In a generic way, this interaction can be written in the form

$$H = -\sum_{\vec{k},\vec{k}',\vec{q},j,\sigma} M(\vec{k},\vec{k}',\vec{q},j) \left[a^\dagger_{-\vec{q}}(j) + a_{\vec{q}}(j) \right] c^\dagger_{\vec{k}',\sigma} c_{\vec{k},\sigma}$$

This formula is the one used in the course to explain electrical resistivity as well as the pairing of electrons in Cooper pairs.

Reminder concerning second quantization: In order to write a one-body operator in second quantization, it is necessary to calculate the matrix elements of this operator with respect to one-particle states:

$$\hat{F}^{(1)} = \sum_{i,j} \langle i | \hat{f}^{(1)} | j \rangle \, c^\dagger_i c_j$$

where $\hat{f}$ acts in the one-particle Hilbert space, and the states i and j are states of that same space.