SOLID STATE PHYSICS III **Solution session 9** November 27th 2025

Electron-phonon interaction: The goal of this exercise is to express the electron-phonon interaction with the formalism of second quantization.

1. Under the assumption that the displacements $s_{n,\alpha}(t)$ are small, we expand the interaction:

$$\sum_{l,n,\alpha} V_\alpha\big(\vec{r}_l - \big(\vec{R}_{n,\alpha} + \vec{s}_{n,\alpha}(t)\big)\big) \approx \sum_{l,n,\alpha} V_\alpha(\vec{r}_l - \vec{R}_{n,\alpha}) - \vec{s}_{n,\alpha}(t) \cdot \vec{\nabla} V_\alpha(\vec{r}_l - \vec{R}_{n,\alpha}) \tag{1}$$

In this exercise, the static term of the potential is neglected, and we only consider the part related to the vibrations of the lattice.

$$\mathcal{H}_{\text{el-ph}} \approx -\sum_{l,n,\alpha} \vec{s}_{n,\alpha}(t) \cdot \vec{\nabla} V_\alpha(\vec{r}_l - \vec{R}_{n,\alpha}) \tag{2}$$

By replacing $\vec{s}_{n,\alpha}(t)$ with their expression in terms of normal coordinates we obtain

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

then in terms of phonon creation and annihilation operators, we obtain:

$$H_{\mathrm{el-ph}} = -\sum_{\alpha,n,l,j,\vec{q}} \sqrt{\frac{\hbar}{2NM_\alpha\omega_j(\vec{q})}} \left[a^\dagger_j(-\vec{q}) + a_j(\vec{q})\right] \vec{e}^{(j)}_\alpha(\vec{q}) \cdot \vec{\nabla} V_\alpha(\vec{r}_l - \vec{R}_{n,\alpha}) e^{i\vec{q}\cdot\vec{R}_n}$$

We still need to express in second quantization the electronic part of this interaction. Since the only operators concerning the electrons are the positions $\vec{r}_l$, this amounts to expressing $\sum_l \vec{\nabla} V_\alpha(\vec{r}_l - \vec{R}_{n,\alpha})$ in second quantization. We use the result presented in the course (see the course appendix):

$$\sum_l \vec{\nabla} V_\alpha(\vec{r}_l - \vec{R}_{n,\alpha}) = \sum_{\vec{k},\vec{k}',\sigma,\sigma'} \left\langle \vec{k}',\sigma' \middle| \vec{\nabla} V_\alpha(\vec{r}_l - \vec{R}_{n,\alpha}) \middle| \vec{k},\sigma > \right\rangle c^\dagger_{k',\sigma'} c_{k,\sigma}$$

2. Calculation of $\left\langle \vec{k}',\sigma' \middle| \vec{\nabla} V_\alpha(\vec{r} - \vec{R}_{n,\alpha}) \middle| \vec{k},\sigma \right\rangle$:

$$\left\langle \vec{k}',\sigma' \middle| \vec{\nabla} V_\alpha(\vec{r} - \vec{R}_{n,\alpha}) \middle| \vec{k},\sigma \right\rangle = \sum_{\vec{K}} e^{-i\vec{K}\vec{R}_{n,\alpha}} V_{\alpha,\vec{K}} i K \left\langle \vec{k}',\sigma' \middle| e^{i\vec{K}\vec{r}} \middle| \vec{k},\sigma \right\rangle \tag{3}$$

as the operator $e^{i\vec{K}\vec{r}}$ does not involve the spin of the electrons we have:

$$\begin{aligned} \left\langle \vec{k}',\sigma' \middle| e^{i\vec{K}\vec{r}} \middle| \vec{k},\sigma \right\rangle &= \delta_{\sigma,\sigma'} \int d\vec{r} \psi^*_{\vec{k}'}(\vec{r}) \psi_{\vec{k}}(\vec{r}) e^{i\vec{K}\vec{r}} \\ &= \delta_{\sigma,\sigma'} \int d\vec{r} u^*_{\vec{k}'}(\vec{r}) u_{\vec{k}}(\vec{r}) e^{i(-\vec{k}'+\vec{K}+\vec{k})\vec{r}} \end{aligned} \tag{4}$$

in the end we get:

$$\left\langle \vec{k}', \sigma' \middle| \vec{\nabla} V_\alpha(\vec{r} - \vec{R}_{n,\alpha}) \middle| \vec{k}, \sigma \right\rangle = \sum_{\vec{K}} e^{-i\vec{K}\vec{R}_{n,\alpha}} V_{\alpha,\vec{K}} i\vec{K} \delta_{\sigma,\sigma'} \int d\vec{r} u^*_{\vec{k}'}(\vec{r}) u_{\vec{k}}(\vec{r}) e^{i(-\vec{k}'+\vec{K}+\vec{k})\vec{r}} \tag{5}$$

3. The functions $u_{\vec{k}}(\vec{r})$ et $u_{\vec{k}'}(\vec{r})^*$ have the periodicity of the lattice. The product $u_{\vec{k}}(\vec{r}) u_{\vec{k}'}(\vec{r})^*$ has the same property. The expansion of $u_{\vec{k}}(\vec{r}) u_{\vec{k}'}(\vec{r})^*$ in Fourier series will thus only contain the modes corresponding to the vectors of the reciprocal lattice.

$$u_{\vec{k}}(\vec{r}) u_{\vec{k}'}(\vec{r})^* = \sum_{\vec{G}} f(\vec{G}) e^{i\vec{G}\vec{r}} \tag{6}$$

where $\vec{G}$ are vectors of the reciprocal lattice (such that $\vec{G} \cdot \vec{R}_n = 2\pi m$, m integers). By replacing this expression in the integral of Eq. (5), we have:

$$\int d\vec{r} u^*_{\vec{k}'}(\vec{r}) u_{\vec{k}}(\vec{r}) e^{i(-\vec{k}'+\vec{K}+\vec{k})\vec{r}} = \sum_{\vec{G}} f(\vec{G}) \int d\vec{r} e^{i(-\vec{k}'+\vec{K}+\vec{k}+\vec{G})\vec{r}} \tag{7}$$

This integral is finite only if $-\vec{K} = -\vec{k}' + \vec{G} + \vec{k}$. Therefore, to make this property explicit, we can also write

$$\int d\vec{r} u^*_{\vec{k}'}(\vec{r}) u_{\vec{k}}(\vec{r}) e^{i(-\vec{k}'+\vec{K}+\vec{k})\vec{r}} = \sum_{\vec{G}} \delta_{\vec{k}',\vec{k}+\vec{G}+\vec{K}} \int d\vec{r}\, u^*_{\vec{k}'}(\vec{r}) u_{\vec{k}}(\vec{r}) e^{i(-\vec{k}'+\vec{K}+\vec{k})\vec{r}} \tag{8}$$

4. By collecting all the terms and making the sum of $\vec{k}'$ and σ' we obtain

$$\begin{aligned} H_{\text{el}-\text{ph}} \quad = \quad - \sum_{\substack{\alpha,n,j,\vec{q},\vec{K} \\ \vec{k},\vec{k}',\sigma,\sigma',\vec{G}}} & \sqrt{\frac{\hbar}{2NM_\alpha \omega_j(\vec{q})}} \left[a_j^\dagger(-\vec{q}) + a_j(\vec{q}) \right] \vec{e}_\alpha^{(j)}(\vec{q}) \cdot i\vec{K} V_{\alpha,\vec{K}} \\ & \delta_{\sigma,\sigma'} \delta_{\vec{k}',\vec{k}+\vec{G}+\vec{K}} \int u^*_{\vec{k}'}(\vec{r}) u_{\vec{k}}(\vec{r}) e^{i(-\vec{k}'+\vec{K}+\vec{k})r} d\vec{r} e^{-i\vec{K}\vec{R}_{n,\alpha}} e^{i\vec{q}\cdot\vec{R}_n} c^\dagger_{k',\sigma} c_{k,\sigma} \end{aligned} \tag{9}$$

This expression can be simplified using $\vec{R}_{n,\alpha} = \vec{R}_n + \vec{R}_\alpha$ and

$$\sum_n e^{i\vec{R}_n\vec{q}} e^{-i\vec{R}_{n,\alpha}\vec{K}} = e^{-i\vec{R}_\alpha\vec{K}} \sum_n e^{i\vec{R}_n(\vec{q}-\vec{K})} = e^{-i\vec{R}_\alpha\vec{K}} N \sum_{\vec{G}'} \delta_{\vec{K},\vec{q}+\vec{G}'} \tag{10}$$

where the $\vec{G}'$ are also vectors of the reciprocal network (note, that $\vec{K}$ is not restricted to the first Brillouin zone). By combining the conditions $\vec{K} = \vec{q} + \vec{G}'$ and $\vec{K} = \vec{k}' - \vec{G} - \vec{k}$, we get:

$$\vec{k}' = \vec{k} + \vec{q} + \vec{G}' + \vec{G}$$

Therefore, $\vec{G}' + \vec{G}$ must be the vector of the reciprocal lattice that brings $\vec{k} + \vec{q}$ back to the first Brillouin zone. Indeed, the crystal wavevectors $\vec{k}'$ et $\vec{k}$ are restricted to the first Brillouin zone.

5. After the $\vec{K}$ summation (replacing $\vec{K}$ with $\vec{q} + \vec{G}'$), the electron-phonon interaction reads

$$
\begin{aligned}
H_{\text{el}-\text{ph}} \quad = \quad - & \sum_{\substack{\alpha,n,j,\vec{q}, \\ \vec{k},\sigma,\vec{k}',\sigma',\vec{G},\vec{G}'}} \sqrt{\frac{N\hbar}{2M_\alpha \omega_j(\vec{q})}} \vec{e}_\alpha^{(j)}(\vec{q}) \cdot e^{-i(\vec{q}+\vec{G}')\vec{R}_\alpha} i(\vec{q}+\vec{G}') V_{\alpha,\vec{q}+\vec{G}'} \\
& \cdot \delta_{\sigma,\sigma'} \delta_{\vec{k}',\vec{k}+\vec{q}+\vec{G}+\vec{G}'} \int u^*_{\vec{k}'}(\vec{r}) u_{\vec{k}}(\vec{r})\, e^{i(-\vec{k}'+\vec{k}+\vec{q}+\vec{G}')\vec{r}} d\vec{r} \left[a_j^\dagger(-\vec{q}) + a_j(\vec{q})\right] c^\dagger_{k',\sigma'} c_{k,\sigma}
\end{aligned}
\tag{11}
$$

Note that because $\vec{k}'$ must be in the first Brillouin zone, for each value of $\vec{k}$, $\vec{G}'$, and $\vec{q}$, the term $\delta_{\vec{k}',\vec{k}+\vec{q}+\vec{G}+\vec{G}'}$ does not cancel out only one reciprocal lattice $\vec{G}$ that brings $\vec{k}+\vec{q}+\vec{G}$ back to the first Brillouin zone. For this reason the electron-phonon interaction is written as:

$$
\begin{aligned}
H_{\text{el}-\text{ph}} = - \sum_{\substack{\alpha,j,\vec{q},\vec{G}' \\ \vec{k},\sigma}} \Bigg[& \sqrt{\frac{N\hbar}{2M_\alpha \omega_j(\vec{q})}} \vec{e}_\alpha^{(j)}(\vec{q}) \cdot i(\vec{q}+\vec{G}') \int V_\alpha(\vec{r}') e^{-i(\vec{q}+\vec{G}')(\vec{r}'+\vec{R}_\alpha)} d\vec{r}' \\
& \cdot \int u^*_{\vec{k}+\vec{q}+\vec{G}+\vec{G}'}(\vec{r}) u_{\vec{k}}(\vec{r}) e^{-i\vec{G}\vec{r}} d\vec{r} \quad \left[a_j^\dagger(-\vec{q}) + a_j(\vec{q})\right] c^\dagger_{\vec{k}+\vec{q}+\vec{G}+\vec{G}',\sigma} c_{\vec{k},\sigma} \Bigg]_{\vec{G}\,:\,\vec{k}+\vec{q}+\vec{G}+\vec{G}' \in 1^{\text{st}} \text{ B. Z.}}
\end{aligned}
\tag{12}
$$

Finally, if we introduce the variable $\vec{G}'' = \vec{G} + \vec{G}'$, we obtain the desired form of the electron-phonon interaction

$$
\begin{aligned}
H_{\text{el}-\text{ph}} = - \sum_{\substack{\alpha,j,\vec{q},\vec{G}' \\ \vec{k},\sigma}} \Bigg[& \sqrt{\frac{N\hbar}{2M_\alpha \omega_j(\vec{q})}} \vec{e}_\alpha^{(j)}(\vec{q}) \cdot i(\vec{q}+\vec{G}') \int V_\alpha(\vec{r}') e^{-i(\vec{q}+\vec{G}')(\vec{r}'+\vec{R}_\alpha)} d\vec{r}' \\
& \cdot \int u^*_{\vec{k}+\vec{q}+\vec{G}''}(\vec{r}) u_{\vec{k}}(\vec{r}) e^{-i(\vec{G}''-\vec{G}')\vec{r}} d\vec{r} \quad \cdot \left[a_j^\dagger(-\vec{q}) + a_j(\vec{q})\right] c^\dagger_{\vec{k}+\vec{q}+\vec{G}'',\sigma} c_{k,\sigma} \Bigg]_{\vec{G}''\,:\,\vec{k}+\vec{q}+\vec{G}'' \in 1^{\text{st}} \text{ B. Z.}}
\end{aligned}
\tag{13}
$$