1 Electron-Phonon Interaction

In our general many-body Hamiltonian, the interaction between each ion and the electrons is of the form

$$\begin{aligned} V_{ei} &= \sum_j V_{ei}(\mathbf{r}_j) \\ &= \sum_{i,j} V_{ei}(\mathbf{r}_j - \mathbf{R}_i). \end{aligned} \tag{1}$$

To make contact with the phonon expansion introduced in the previous section, we write the ion coordinate in terms of a deviation from the home position: $\mathbf{R}_i = \mathbf{R}_i^0 + \mathbf{Q}_i$ and Taylor series expand the electron-ion potential around $\mathbf{R}_i^0$. To first order, we have that

$$V_{ei} = \sum_{i,j} V_{ei}(\mathbf{r}_j - \mathbf{R}_i^0) - \sum_{i,j} \mathbf{Q}_i.\nabla_j V_{ei}(\mathbf{r}_j - \mathbf{R}_i^0) + O(Q^2) + \cdots \tag{2}$$

The first term defines the periodic potential seen by a conduction electron and, hence, contains no new information regarding the coupling of the electrons to the lattice distortion. Such information is contained in the second term. To simplify this term, we introduce the Fourier transform of the electron-ion potential,

$$V_{ei}(\mathbf{r}) = \frac{1}{N} \sum_{\mathbf{k}} V_{ei}(\mathbf{k}) e^{i\mathbf{k}.\mathbf{r}}. \tag{3}$$

With this definition in hand, we write the electron-ion potential as

$$V_{ei} = V_0 - \frac{i}{N} \sum_{\mathbf{k},i,j} V_{ei}(\mathbf{k}) e^{i\mathbf{k}.\mathbf{r}_j} \times \mathbf{k}. \sum_{\mathbf{q},\lambda} \left(\frac{\hbar}{2MN\omega_{\mathbf{q},\lambda}} \right)^{(} 1/2) \lambda_{\mathbf{q}} (b_{\mathbf{q},\lambda} + b^{\dagger}_{-\mathbf{q},\lambda}) e^{i(\mathbf{q}-\mathbf{k}).\mathbf{R}_i^0}, \tag{4}$$

where we have set the first term in Eq. (2) equal to V_0. We restrict the sum over $\mathbf{q}$ and $\mathbf{k}$ to the first Brillouin zone, such that

$$\frac{1}{N} \sum_i e^{i(\mathbf{q}-\mathbf{k}).\mathbf{R}_i^0} = \sum_{\mathbf{L}} \delta_{\mathbf{k},\mathbf{q}+\mathbf{L}}, \tag{5}$$

where the sum over $\mathbf{L}$ is over all reciprocal lattice vectors. We note also that the k th component of the electron density is

$$\rho_{\mathbf{k}} = \sum_j e^{i\mathbf{k}.\mathbf{r}_j}. \tag{6}$$

We introduce the electron-phonon coupling constant

$$M_{\mathbf{q},\mathbf{L},\lambda} = -i\Big(\frac{\hbar}{2MN\omega_{\mathbf{q},\lambda}}\Big)^{1/2}(\mathbf{q}+\mathbf{L}).\lambda_{\mathbf{q}}V_{ei}(\mathbf{q}+\mathbf{L}) \tag{7}$$

and recast the electron-phonon term as

$$V_{ei} = V_0 + \sum_{\mathbf{q},\mathbf{L},\lambda} M_{\mathbf{q},\mathbf{L},\lambda}(b_{\mathbf{q},\lambda} + b^{\dagger}_{-\mathbf{q},\lambda})\rho_{\mathbf{q}+\mathbf{L}} = V_0 + H_{e-ph}. \tag{8}$$

The electron-phonon coupling constant contains the product $(\mathbf{q}+\mathbf{L}).\lambda_q$. As a consequence, when λ_q is perpendicular to $\mathbf{q}+\mathbf{L}$, $M_{q+\mathbf{L},\lambda} = 0$. That is, only the longitudinal acoustic phonon modes couple to the electrons. As a result, we can drop the λ subscript, as there is only one longitudinal acoustic mode. This is an important result. However, there are certainly longitudinal optical phonons that couple to the electron motion. Such processes arise from a Coulombic rather than an elastic deformation coupling to the electron motion. In the optical phonon case, the linear q dependence of the coupling constant, M_q, is replaced by a q^{-2} dependence. The inverse $1/q^2$ term arises from the Fourier transform of the Coulomb interaction. In polar crystals, optical phonons dominate over the acoustic modes. Because we are primarily interested in superconductivity, we limit our discussion solely to the acoustic case.

Let us now compute matrix elements of H_{e-ph}. To do this, we consider the composite electron-phonon state

$$\Big|\phi_{e-ph}\Big\rangle = \Big|n_{\mathbf{k}}; N_{\mathbf{q},\lambda}\Big\rangle. \tag{9}$$

Here, the electronic state $|n_k\rangle$ represents a many-body state in which $n_{\mathbf{k}}$ electrons are in the single-particle Bloch state $\langle\mathbf{r}|\mathbf{k}\rangle \equiv e^{i\mathbf{k}.\mathbf{r}}U_{\mathbf{k}(\mathbf{r})}$, and $\Big|\langle N_{\mathbf{q},\lambda}\Big\rangle$ denotes a many-body phonon state in which $N_{\mathbf{q},\lambda}$ phonons are in the qth lattice mode of polarization $\lambda_{\mathbf{q}}$. The function $U_{\mathbf{q}}(\mathbf{r})$ has the same periodicity of the lattice as does the Fourier coefficient, $e^{i\mathbf{q}.\mathbf{r}}$, namely, $U_{\mathbf{k}}(\mathbf{r}) = U_{\mathbf{k}}(\mathbf{r}+\mathbf{R}^0_i)$. To evaluate matrix elements of the electron-phonon interaction, it is helpful to express H_{e-ph} in second-quantized form. The only electron operator in H_{e-ph} is the electron density, $\widehat{\rho_{\mathbf{k}}}$. In second-quantized form, $\widehat{\rho_{\mathbf{k}}}$ becomes

$$\widehat{\rho_{\mathbf{k}}} = \sum_{\mathbf{k}_1,\mathbf{k}_2} \langle\mathbf{k}_1|e^{i\mathbf{k}.\mathbf{r}}|\mathbf{k}_2\rangle\, a^{\dagger}_{\mathbf{k}_1}a_{\mathbf{k}_2}, \tag{10}$$

where the operator $a^{\dagger}_{\mathbf{k}}$ creates an electron in the momentum state $\mathbf{k}$. The electron-phonon interaction can now be written as

$$H_{e-ph} = \sum_{\mathbf{k},\mathbf{L},\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}} M_{\mathbf{q},\mathbf{L}} \langle \mathbf{k}_1 | e^{i(\mathbf{q}+\mathbf{L}).\mathbf{r}} | \mathbf{k}_2 \rangle \, a^{\dagger}_{\mathbf{k}_1} a_{\mathbf{k}_2} (b_{\mathbf{q}} + b^{\dagger}_{-\mathbf{q}}). \tag{11}$$

Assuming the electron wave functions are simply plane waves, we find that the matrix element of the density operator is given exactly by

$$\langle \mathbf{k}_1 | e^{i\mathbf{k}.\mathbf{r}} | \mathbf{k}_2 \rangle = \int \frac{d\mathbf{r}}{V} e^{i\mathbf{r}.(\mathbf{k}+\mathbf{k}_2-\mathbf{k}_1)} = \delta_{\mathbf{k}_1,\mathbf{k}+\mathbf{k}_2}. \tag{12}$$

In general, the electron wave functions need not be plane waves. We define

$$\alpha_{\mathbf{q}_1,\mathbf{q}_2} = \langle \mathbf{q}_1 | \mathbf{q}_2 \rangle \tag{13}$$

to be the general overlap between two electronic states. Because the $U'_{\mathbf{k}}s$ have the periodicity of the lattice, the condition in Eq.(12) still holds, even when the electronic wave functions are more complicated than plane waves. Consequently, the full electron-phonon Hamiltonian reduces to

$$H_{e-ph} = \sum_{\mathbf{q},\mathbf{k},\mathbf{L}} M_{\mathbf{q},\mathbf{L}} \alpha_{\mathbf{k}+\mathbf{q}+\mathbf{L},\mathbf{k}} a^{\dagger}_{\mathbf{q}+\mathbf{L}+\mathbf{k}} a_{\mathbf{k}} (b_{\mathbf{q}} + b^{\dagger}_{-\mathbf{q}}), \tag{14}$$

when Eqs.(11-13) are determined.

As is evident, this Hamiltonian contains a myriad of electron-phonon processes, some of which involve the electron's moving from one Brillouin zone to another, $\mathbf{L} \neq 0$. All such processes in which the electron wave vector is changed by $\mathbf{q} + \mathbf{L} + \mathbf{k}$ are called *Umklapp processes*. In German, *umklappen* means "to flip over". Normal processes refer to those in which momentum transfer does not result in an electron's changing Brillouin zones. In such cases, a phonon of wave vector $\mathbf{q}$ scatters an electron with momentum $\mathbf{k}$ and yields an electron state with wave vector $\mathbf{q} + \mathbf{k}$. Diagrams illustrating the various kinds of scattering processes are shown in Fig. (1).

We are interested primarily in the amplitude for emission and absorption. In emission, a phonon is created. Hence, only the $b^{\dagger}_{-\mathbf{q}}$ term

contributes. Likewise in absorption, a phonon is annihilated. For an emission process, the initial and final states must be of the form

$$|init\rangle = \left| n_{\mathbf{k}+\mathbf{q}}; N_{-\mathbf{q}}, N_{\mathbf{q}} \right\rangle \tag{15}$$

$$|efin\rangle = \left| n_{\mathbf{k}+\mathbf{q}} + 1, n_{\mathbf{k}} - 1; N_{-\mathbf{q}} + 1, N_{\mathbf{q}} \right\rangle. \tag{16}$$

The amplitude for emission involves the matrix elements

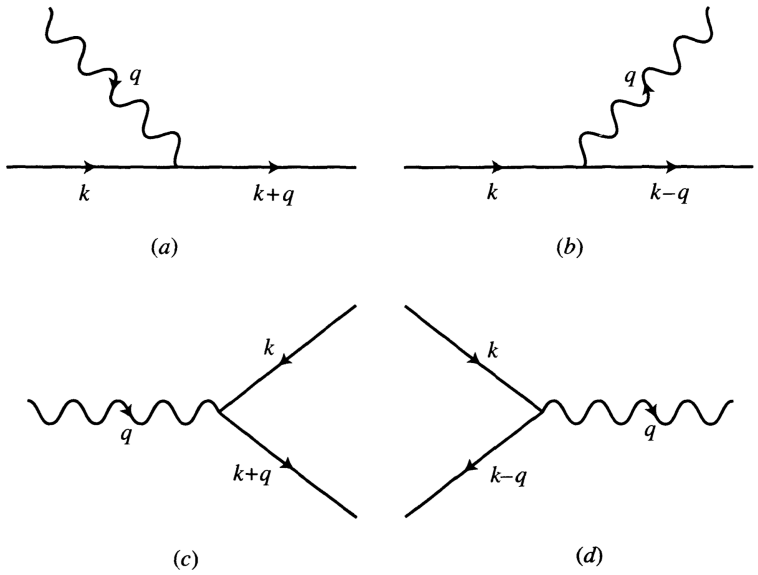

Figure 1: Electron-phonon scattering. A wavy line represents a phonon, and incoming and outgoing arrows represent electrons and holes, respectively. *(a)* and *(c)* represent absorption, whereas *(b)* and *(d)* correspond to emission of a phonon.

$$\langle fin|H_{e-ph}|init\rangle = \sum_{\mathbf{q},\mathbf{k}} M_{\mathbf{q}}\alpha_{\mathbf{k+q},\mathbf{k}} \langle fin|a^{\dagger}_{\mathbf{q+k}}a_{\mathbf{k}}b^{\dagger}_{-\mathbf{q}}|init\rangle\,. \tag{17}$$

Because $n_{\mathbf{k+q}}$ and $n_{\mathbf{k}}$ are restricted to be 1 or 0, $a_k\,|init\rangle$ is non-zero only if $n_{\mathbf{k}} = 1$. Likewise, $a^{\dagger}_{\mathbf{q+k}}\,|init\rangle$ will yield a non-zero result only if $1 - n_{\mathbf{q+k}} = 1$. Consequently,

$$\langle fin|H_{e-ph}|init\rangle = \sum_{\mathbf{q},\mathbf{k}} M_{\mathbf{q}}\alpha_{\mathbf{k+q},\mathbf{k}} \sqrt{(1 - n_{\mathbf{q+k}})n_{\mathbf{k}}(N_{-\mathbf{q}} + 1)}. \tag{18}$$

In the event that $n_{\mathbf{k}} = 1$ and $n_{\mathbf{q+k}} = 0$, the energy difference between the initial and final states is

$$\Delta E_{emis} = E_{fin} - E_{init} = E(\mathbf{q} + \mathbf{k}) - E(\mathbf{k}) + \hbar\omega_{\mathbf{q}}, \tag{19}$$

where E($\mathbf{k}$) is the energy of an electron state with momentum $\mathbf{k}$.

In the absorption process, the final state in this case is

$$|afin\rangle = \left|n_{\mathbf{k+q}} + 1, n_{\mathbf{k}} - 1; N_{-\mathbf{q}} - 1\right\rangle \tag{20}$$

As a consequence,

$$\langle afin|H_{e-ph}|init\rangle = \sum_{\mathbf{q},\mathbf{k}} M_{\mathbf{q}}\alpha_{\mathbf{k}+\mathbf{q},\mathbf{k}}\sqrt{(1-n_{\mathbf{q}+\mathbf{k}})n_{\mathbf{k}}N_{\mathbf{q}}}. \tag{21}$$

The energy difference here is

$$\Delta E_{abs} = E(\mathbf{k}+\mathbf{q}) - E(\mathbf{k}) - \hbar\omega_{\mathbf{q}}. \tag{22}$$

Applying Fermi's golden rule to the emission and absorption amplitudes yields

$$W^{abs}_{\mathbf{k}\rightarrow\mathbf{k}+\mathbf{q}} = \frac{2\pi}{\hbar}\langle M_{\mathbf{q}\alpha_{\mathbf{k}+\mathbf{q},\mathbf{k}}}\rangle^2 n_{\mathbf{k}}N_{\mathbf{q}}(1-n_{\mathbf{q}+\mathbf{k}})\delta(E(\mathbf{k}+\mathbf{q}) - E(\mathbf{k}) - \hbar\omega_{\mathbf{q}}) \tag{23}$$

and

$$W^{emis}_{\mathbf{k}\rightarrow\mathbf{k}+\mathbf{q}} = \frac{2\pi}{\hbar}\langle M_{\mathbf{q}}\alpha_{\mathbf{k}+\mathbf{q},\mathbf{k}}\rangle^2 n_{\mathbf{k}}(1-n_{\mathbf{q}+\mathbf{k}})\times(N_{-\mathbf{q}}+1)\delta(E(\mathbf{k}+\mathbf{q}) - E(\mathbf{k}) + \hbar\omega_{\mathbf{q}}) \tag{24}$$

for the emission and absorption rates, respectively. The δ-functions ensure that energy is conserved. For the sake of generality, we have included explicitly the electron occupation numbers, although $n_{\mathbf{k}} = 1$ and $n_{\mathbf{q}+\mathbf{k}} = 0$. It is customary at this stage of our calculation to replace the electron and phonon occupation numbers by their equilibrium Fermi-Dirac and Bose forms. This simplification is valid only if the electron-phonon system is in equilibrium before the transition occurs. We will find this simplification useful when we treat superconductivity.