FIP10601 – Text 17

Electron-phonon interaction

So far, our study of solids was restricted to electronic degrees of freedom, treating the *lattice* (ensemble of periodically arranged ions) as absolutely rigid. Although this is a reasonable approximation in many cases, it is known that degrees of freedom related to ion movements play an important role in various phenomena. In addition to direct effects of these movements (e.g., specific heat and thermal conductivity of insulating solids), we have already mentioned lattice-vibration effects on electronic transport as well as their role in Fermi-liquid instabilities, which will be addressed later on. In this Text we briefly review the description of lattice vibrations, and introduce them into the many-body formalism that we have been using to deal with electrons in solids.

Lattice vibrations (short review)

Based on the very narrow lines characteristically observed in X-ray diffraction spectra of crystalline solids, the starting hypothesis is that ion motion consists of small-amplitude oscillations around the equilibrium positions that define the crystal structure. These oscillations are commonly called *lattice vibrations*. Because interactions keep ions connected to one another, such vibrations are **collective motions**, and should be analyzed in the context of *normal modes* of the whole system.

The instantaneous position of a given ion can be written as

$$\mathbf{r}_i(t) \equiv \mathbf{R}_i + \boldsymbol{u}_i(t) \ , \tag{1}$$

in terms of its equilibrium position $\mathbf{R}_i$ (which is a lattice vector in monoatomic lattices) and the displacement $\boldsymbol{u}_i$. Thus, the total kinetic energy of the atoms is

$$T = \frac{1}{2} M \sum_i \dot{u}_i^2 \ . \tag{2}$$

The assumption of small amplitude of oscillations leads to the **harmonic approximation**. It consists in expanding the potential energy (here denoted by Φ) in powers of the ionic displacements $\boldsymbol{u}_i$, keeping only the quadratic term, which is the first non null if we choose the zero of energy at the equilibrium configuration.

A Fourier representation of the displacements defines *normal coordinates* $Q_{\mathbf{k}}$ such that

$$u_i^\alpha(t) = \frac{1}{\sqrt{NM}} \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}^\alpha Q_{\mathbf{k}}(t)\, \mathrm{e}^{\mathrm{i}\mathbf{k}.\mathbf{R}_i} \ , \tag{3}$$

where N is the number of primitive cells, M is the mass of an ion, and $\epsilon_{\mathbf{k}}^{\alpha}$ ($\alpha = x, y, z$) are the components of a *polarization* vector $\boldsymbol{\epsilon}_{\mathbf{k}}$, of unit length. Note that $Q_{\mathbf{k}}$ may be complex, but $Q_{\mathbf{k}}^{*} = Q_{-\mathbf{k}}$ because the displacements u_i^{α} are real.

The **classical** equations of motion in terms of normal coordinates are

$$\ddot{Q}_{\mathbf{k}}\epsilon_{\mathbf{k}}^{\alpha} = -Q_{\mathbf{k}} \sum_{\beta} D_{\alpha\beta}(\mathbf{k})\epsilon_{\mathbf{k}}^{\beta} \ , \tag{4}$$

where

$$D_{\alpha\beta}(\mathbf{k}) \equiv \frac{1}{M} \sum_{j} \Phi_{ij}^{\alpha\beta} \, \mathrm{e}^{-\mathrm{i}\,\mathbf{k}.(\mathbf{R}_i - \mathbf{R}_j)} \tag{5}$$

and

$$\Phi_{ij}^{\alpha\beta} \equiv \left(\frac{\partial^2 \Phi}{\partial u_i^{\alpha} \partial u_j^{\beta}} \right)_0 \tag{6}$$

These equations describe harmonic vibrations of a system of particles coupled by elastic forces, with $\Phi_{ij}^{\alpha\beta}$ playing the role of *spring constants*. Introducing the time Fourier transform,

$$Q_{\mathbf{k}}(t) = \int_{-\infty}^{\infty} \mathrm{d}\omega \, Q_{\mathbf{k}}(\omega) \, \mathrm{e}^{-\mathrm{i}\omega t} \ , \tag{7}$$

we can write a matrix version of Eq. (4) as

$$\boldsymbol{D}(\mathbf{k}) \cdot \boldsymbol{\epsilon}_{\mathbf{k}\mu} = \omega_{\mu}^2(\mathbf{k}) \, \boldsymbol{\epsilon}_{\mathbf{k}\mu} \ . \tag{8}$$

This is an eigenvalue equation for the matrix $\boldsymbol{D}(\mathbf{k})$. The frequencies $\omega_{\mu}(\mathbf{k})$ correspond to *normal modes* of lattice vibration, with definite wavelengths. For each wavevector $\mathbf{k}$ the subscript μ identifies eigenvalues in different *branches* of the frequency spectrum, since the values of $\mathbf{k}$ are essentially continuous for a sufficiently large system. For monoatomic lattices, $\boldsymbol{D}(\mathbf{k})$ is a 3×3 matrix, and the three branches are *acoustic*, i.e., $\omega_{\mu}(\mathbf{k}) \to 0$ when $k \to 0$. Lattices with more than one ion per primitive cell additionally have *optical* branches, with finite frequency in the long-wavelength limit. A generic vibration state of the lattice can be decomposed into independent normal modes.

Introducing the canonically conjugate momenta

$$P_{\mathbf{k}\mu} = \frac{\partial L}{\partial \dot{Q}_{\mathbf{k}\mu}} = \dot{Q}_{\mathbf{k}\mu}^{*} \ , \tag{9}$$

where $L = T - \Phi$ is the Lagrangian, we obtain the classical Hamiltonian for lattice vibrations,

$$\mathcal{H} = \frac{1}{2} \sum_{\mathbf{k},\,\mu} \left[P_{\mathbf{k}\mu}^{*} P_{\mathbf{k}\mu} + \omega_{\mu}^2(\mathbf{k}) Q_{\mathbf{k}\mu}^{*} Q_{\mathbf{k}\mu} \right] \ . \tag{10}$$

Quantization

This is a typical case of *canonical quantization*. We just reinterpret the conjugate variables as operators obeying canonical commutation relations (not omitting $\hbar$),

$$[Q_{\mathbf{k}\mu}, P_{\mathbf{k}'\mu'}] = \mathrm{i}\hbar\, \delta_{\mathbf{k}\mathbf{k}'}\delta_{\mu\mu'} \ . \tag{11}$$

Complex conjugates correspond to Hermitian conjugates (or adjoints), $Q^\dagger_{\mathbf{k}\mu}$ and $P^\dagger_{\mathbf{k}\mu}$, obeying the conditions $Q^\dagger_{\mathbf{k}\mu} = Q_{-\mathbf{k},\mu}$ and $P^\dagger_{\mathbf{k}\mu} = P_{-\mathbf{k},\mu}$.

Phonons

It is now convenient to introduce the following operator and its Hermitian conjugate:

$$\begin{aligned} a_{\mathbf{k}\mu} &\equiv \frac{1}{\sqrt{2\hbar\omega_\mu(\mathbf{k})}}\left[\omega_\mu(\mathbf{k})Q_{\mathbf{k}\mu} + \mathrm{i}\,P^\dagger_{\mathbf{k}\mu}\right] , \\ a^\dagger_{\mathbf{k}\mu} &= \frac{1}{\sqrt{2\hbar\omega_\mu(\mathbf{k})}}\left[\omega_\mu(\mathbf{k})Q^\dagger_{\mathbf{k}\mu} - \mathrm{i}\,P_{\mathbf{k}\mu}\right] . \end{aligned} \tag{12}$$

Inverting these relations and replacing into the Hamiltonian, we obtain

$$H = \sum_{\mathbf{k},\,\mu} \hbar\omega_\mu(\mathbf{k})\left[a^\dagger_{\mathbf{k}\mu}a_{\mathbf{k}\mu} + \frac{1}{2}\right] \ . \tag{13}$$

It is easy to show that the operators $a^\dagger_{\mathbf{k}\mu}$ and $a_{\mathbf{k}\mu}$ satisfy commutation relations of (respectively) creation and annihilation boson operators,

$$[a_{\mathbf{k}\mu}, a^\dagger_{\mathbf{k}'\mu'}] = \delta_{\mathbf{k}\mathbf{k}'}\delta_{\mu\mu'} \ . \tag{14}$$

Thus, besides the additive *zero-point energy*, Eq. (13) can be viewed as the Fock-space Hamiltonian of a *gas of bosons*, each boson carrying an energy quantum $\hbar\omega_\mu(\mathbf{k})$, corresponding to a lattice-vibration excitation of wavevector $\mathbf{k}$ on branch μ. These bosons are called *phonons*.

The well known Bose-Einstein statistics can be applied to phonons, allowing to determine, for example, the low-temperature specific-heat as $c_V = \text{const.} \times T^3$, which is confirmed in experiments. The reference temperature here is the *Debye temperature*, $\Theta_D = \hbar\omega_D/k_B$, defined within the Debye model (linear relationship between frequency and wavevector), in terms of the *Debye frequency* ω_D, which is comparable in magnitude to the maximum frequency of acoustic branches. Θ_D is typically two orders of magnitude smaller than the Fermi temperature in metals.

Electron-phonon interaction

Effects of lattice vibrations on electrons (and vice-versa) have their origin on the interaction between electrons and ions, included in the generic Hamiltonian of Text 1 as

$$\mathcal{H}_{\text{el-ion}} = \sum_{i,l} V(\mathbf{r}_l - \mathbf{r}_i) \ , \tag{15}$$

where the subscripts i and l refer to ions and electrons, respectively. $V(\mathbf{r}_l - \mathbf{r}_i)$ is essentially a Coulomb potential with screening corrections.

We now expand $V(\mathbf{r}_l - \mathbf{r}_i)$ in powers of the displacements $\boldsymbol{u}_i$, defined in Eq. (1),

$$V(\mathbf{r}_l - \mathbf{R}_i - \boldsymbol{u}_i) = V(\mathbf{r}_l - \mathbf{R}_i) - \boldsymbol{u}_i \cdot \left(\frac{\partial V(\mathbf{r})}{\partial \mathbf{r}}\right)_{\mathbf{r}=\mathbf{r}_l - \mathbf{R}_i} + \dots \tag{16}$$

The first term on the r.h.s., when summed over the ionic equilibrium positions, gives the periodic potential to which electrons are subjected. This term is therefore taken into account in the independent-electron energies $\varepsilon(\mathbf{k})$. The remaining terms involve ionic displacements, and can be interpreted as *electron-phonon interaction*. We will keep only the lowest-order one, which in this case is **linear** in $\boldsymbol{u}_i$.

Going back to the above-mentioned generic Hamiltonian of electrons and ions (Text 1),

$$\mathcal{H} = \mathcal{H}_{\text{el}} + \mathcal{H}_{\text{ion}} + \mathcal{H}_{\text{el-ion}} \ , \tag{17}$$

we have that:

(i) summing $\mathcal{H}_{\text{el}}$ (electron's kinetic energy and e-e interaction) with the **equilibrium part** of $\mathcal{H}_{\text{el-ion}}$ reproduces the electronic Hamiltonian that we have studied via many-body methods;

(ii) $\mathcal{H}_{\text{ion}}$ in the harmonic approximation yields the free-phonon Hamiltonian of Eq. (13);

(iii) the part of $\mathcal{H}_{\text{el-ion}}$ involving ionic displacements (in first order) generates the electron-phonon interaction Hamiltonian

$$\mathcal{H}_{\text{el-ph}} = -\sum_{i,l} \boldsymbol{u}_i \cdot \left[\nabla V(\mathbf{r})\right]_{\mathbf{r}=\mathbf{r}_l - \mathbf{R}_i} \ . \tag{18}$$

So, we have now a complete Hamiltonian of a **system of electrons and phonons** to model a crystalline metal.

Second quantization

As we did for the other parts of the Hamiltonian, we should write $\mathcal{H}_{\text{el}-\text{ph}}$ in second quantization, that is, in terms of creation and annihilation operators of both electrons and phonons. First, using Eq. (3), we express the displacements $\boldsymbol{u}_i$ in terms of the generalized coordinates $Q_{\mathbf{k}\mu}$. We then write the latter as

$$Q_{\mathbf{k}\mu} = \sqrt{\frac{\hbar}{2\omega_\mu(\mathbf{k})}}\,(a_{\mathbf{k}\mu} + a^\dagger_{-\mathbf{k},\mu})\ , \tag{19}$$

which can be readily checked from Eqs. (12), and the fact that $Q^\dagger_{-\mathbf{k}\mu} = Q_{\mathbf{k}\mu}$.

On the other hand, we can use the Fourier representation of the electron-ion potential,

$$V(\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_{\mathbf{q}} V(\mathbf{q})\,\mathrm{e}^{\mathrm{i}\mathbf{q}.\mathbf{r}}\ , \tag{20}$$

to obtain

$$\nabla V(\mathbf{r}) = \frac{i}{\sqrt{N}}\sum_{\mathbf{q}} \mathbf{q}V(\mathbf{q})\,\mathrm{e}^{\mathrm{i}\mathbf{q}.\mathbf{r}}\ . \tag{21}$$

With this, we have

$$\mathcal{H}_{\text{el}-\text{ph}} = -\frac{\mathrm{i}}{\sqrt{M}}\frac{1}{N}\sum_{i,l}\sum_{\mathbf{k},\mathbf{q},\mu} V(\mathbf{q})\sqrt{\frac{\hbar}{2\omega_\mu(\mathbf{k})}}\,(a_{\mathbf{k}\mu} + a^\dagger_{-\mathbf{k},\mu})\,\boldsymbol{\epsilon}_{\mathbf{k}\mu}\cdot\mathbf{q}\,\mathrm{e}^{\mathrm{i}\mathbf{q}.\mathbf{r}_l}\,\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{q}).\mathbf{R}_i}\ . \tag{22}$$

The sum over i is simply

$$\frac{1}{N}\sum_i \mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{q}).\mathbf{R}_i} = \delta_{\mathbf{k}\mathbf{q}}\ , \tag{23}$$

while the scalar product $\boldsymbol{\epsilon}_{\mathbf{q}\mu}\cdot\mathbf{q}$ selects only the longitudinal polarization, thus eliminating the sum over phonon branches (which allows to drop the subscript μ).

With respect to electronic degrees of freedom, we have a **single-particle** potential, for which the second quantization rule is to take the matrix element between two $\mathbf{k}$-states multiplied by a creation operator into the final state and an annihilation operator from the initial one. The only part that depends on electron coordinates in Eq. (22) is the exponential $\exp(\mathrm{i}\,\mathbf{q}.\mathbf{r}_l)$. Using plane waves instead of Bloch states (as we have been doing), yields the matrix element

$$\langle\mathbf{k}'|\mathrm{e}^{\mathrm{i}\mathbf{q}.\mathbf{r}}|\mathbf{k}\rangle = \frac{1}{V}\int \mathrm{d}^3r\,\mathrm{e}^{\mathrm{i}(\mathbf{k}+\mathbf{q}-\mathbf{k}').\mathbf{r}} = \delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}}\ . \tag{24}$$

Equation (22) can then be written in the simple form

$$\mathcal{H}_{\text{el}-\text{ph}} = \sum_{\mathbf{k}\mathbf{q}\sigma}\Gamma(\mathbf{q})\,(a_{\mathbf{q}} + a^\dagger_{-\mathbf{q}})\,c^\dagger_{\mathbf{k}+\mathbf{q},\sigma}c_{\mathbf{k}\sigma}\ , \tag{25}$$

where

$$\Gamma(\mathbf{q}) \equiv -\frac{\mathrm{i}}{\sqrt{M}}\, \boldsymbol{\epsilon}_{\mathbf{q}} \cdot \mathbf{q}\, V(\mathbf{q}) \sqrt{\frac{\hbar}{2\omega(\mathbf{q})}}\ . \tag{26}$$

In spite of the i factor in the above equation, $\mathcal{H}_{\mathrm{el-ph}}$ is Hermitian. This can be easily verified taking into account that $\omega(-\mathbf{q}) = \omega(\mathbf{q})$, and that, due to the fact that $\boldsymbol{u}_i$ and $V(\mathbf{r})$ are real, $\boldsymbol{\epsilon}_{-\mathbf{q}} = \boldsymbol{\epsilon}_{\mathbf{q}}$ and $V(-\mathbf{q}) = V^*(\mathbf{q})$, which imply that $\Gamma^*(\mathbf{q}) = \Gamma(-\mathbf{q})$. The structure of Eq. (25) allows to interpret the electron-phonon (el-ph) interaction as a scattering of an electron by *absorption* or *emission* of a phonon.

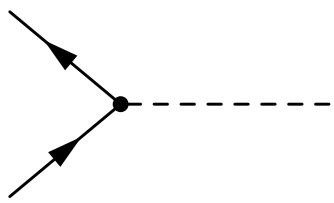
Putting it all together, the complete second-quantization Hamiltonian of electrons and phonons reads

$$\begin{aligned}\mathcal{H} \;=\; & \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \hbar\omega(\mathbf{q}) \left[a^\dagger_{\mathbf{q}} a_{\mathbf{q}} + \frac{1}{2} \right] \\ & + \frac{1}{2} \sum_{\substack{\mathbf{k}\mathbf{k}'\mathbf{q} \\ \sigma\sigma'}} U(\mathbf{q})\, c^\dagger_{\mathbf{k}+\mathbf{q},\sigma}\, c^\dagger_{\mathbf{k}'-\mathbf{q},\sigma'}\, c_{\mathbf{k}'\sigma'}\, c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{q}\sigma} \Gamma(\mathbf{q})\, (a_{\mathbf{q}} + a^\dagger_{-\mathbf{q}})\, c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} c_{\mathbf{k}\sigma}\ . \end{aligned} \tag{27}$$

At this point, it is worth noticing that the Green's function formalism can be extended to include the el-ph interaction. The first line in Eq. (27) is the non-interacting Hamiltonian, while the second line, containing all interactions, can be viewed as the perturbation part. We can then define a (Matsubara) phonon Green's function,

$$\tilde{\mathcal{D}}_{\mathbf{q}}(\tau) = -\langle \hat{T}\, a_{\mathbf{q}}(\tau)\, a^\dagger_{\mathbf{q}}(0) \rangle\ . \tag{28}$$

Its zeroth-order version is usually represented by a **dashed line** in a diagrammatic formalism, with the el-ph interaction vertex corresponding to the diagram below.



It is easy to see that phonon lines will connect internal vertices in electron Green's function diagrams in much the same way as Coulomb-interaction lines. This means that contributions of el-ph interaction may be worked out along the general scheme of evaluating the electron self-energy. Conversely, electronic polarization parts will renormalize the phonon Green's function, resulting, for instance, in modified phonon frequencies. We will not develop this approach in further detail. Instead, in Text 18 we will use the explicit form of electron-phonon interaction derived here to investigate phonon effects on electronic properties in two distinct regimes.