

4 Phonons. Electron-phonon interaction. Attraction mediated by phonons

Refs: [AM] Chapter 23, [PC] Section 9.7.

Phonons are vibrations of a crystal lattice. They can be viewed as bosonic particles which propagate through the crystal and interact with electrons. In this section, we review some basic properties of phonons and show that interaction with phonons produces attraction between electrons (which is the mechanism of superconductivity in most superconductors).

4.1 Harmonic oscillators as free bosons

Any harmonic oscillator may be viewed as a single bosonic mode, which may be occupied by 0, 1, 2, etc. bosons. Consider the quantum Hamiltonian

$$H = \frac{p^2}{2m} + K \frac{q^2}{2} \quad (4.1.1)$$

with the operators p and q satisfying the canonical commutation relations $[p, q] = -i$ (Planck constant is put to 1, as usual). Then the operators

$$\begin{aligned} b &= \frac{1}{\sqrt{2}} \left[q(Km)^{1/4} + i \frac{p}{(Km)^{1/4}} \right], \\ b^+ &= \frac{1}{\sqrt{2}} \left[q(Km)^{1/4} - i \frac{p}{(Km)^{1/4}} \right] \end{aligned} \quad (4.1.2)$$

obey the canonical bosonic commutation relations

$$[b, b^+] = 1, \quad (4.1.3)$$

and the Hamiltonian takes the form

$$H = \omega \left(b^+ b + \frac{1}{2} \right) = \omega \left(n + \frac{1}{2} \right), \quad (4.1.4)$$

where $\omega = (K/m)^{1/2}$ is the oscillator frequency (= energy, once $\hbar = 1$) and n is the number of *bosons*.

4.2 Phonons

The definition of phonons is similar to the one-dimensional example above. In a crystal with N ions, the vibrations of the lattice can be parametrized by $3N$ coordinates (displacements of ions) and $3N$ momenta. Small vibrations can be described by a quadratic Hamiltonian, which is a $3N$ -dimensional version of (4.1.1). This Hamiltonian can be diagonalized, and its eigenmodes decoupled. Because of the translational symmetry of the lattice, the eigenmodes can be labeled by the wave vector (just like electron bands). If the crystal lattice has M atoms per unit cell, the number of bands (the number of phonon states for each k vector) equals $3M$.

The phonon Hamiltonian takes the quadratic form

$$H = \sum_{k,\alpha} \omega_{k,\alpha} b_{k,\alpha}^+ b_{k,\alpha} \quad (4.2.1)$$

(we have dropped the constant ground-state energy). The index α labels the phonon bands. At the level of the harmonic approximation, phonons do not interact. Anharmonic terms would correspond to phonon-phonon interactions.

There are three phonon modes which are special: the *acoustic* phonons. They correspond to slowly varying displacement of atoms and have a linear dispersion relation

$$\omega_k = c|k| \quad \text{as } k \rightarrow 0. \quad (4.2.2)$$

The energy of the acoustic phonons tends to zero as $k \rightarrow 0$. In this limit, all displacements are equal, which corresponds to displacing crystal as a whole, which obviously does not cost any energy. The sound velocities c for the longitudinal and transverse sounds are generally different and may also depend on the direction.

The phonons have energy bands which are periodic functions of k . They extend between 0 and some characteristic energy scale, the so called *Debye energy* ω_D . By the order of magnitude,

$$\omega_D \sim c/a_0 \quad (4.2.3)$$

(where a_0 is the lattice constant), which is much less than the Fermi energy $\varepsilon_F \sim v_F/a_0$. The typical Debye energy in a metal is between 100 K and 500 K (as opposed to the Fermi energy of about 10^4 K).

4.3 Specific heat of phonons

Except at very low temperatures, phonons give the main contribution to the specific heat. To calculate the specific heat of phonons exactly, one needs to know the distribution of phonon modes over energies [i.e., the *density of states* $\nu_{\text{ph}}(\omega)$].

For low-temperature specific heat (when only low-energy phonons are excited), the behavior of at $\omega \rightarrow 0$ matters, while for the high-temperature limit, it is important that the phonons have an upper cut-off in energy at $\omega \sim \omega_D$. The simplest approximation accurate in both limits is the *Debye theory*:

$$\nu_{\text{ph}}(\omega) = \begin{cases} C \omega^2, & \omega < \omega_D, \\ 0, & \omega > \omega_D \end{cases} \quad (4.3.1)$$

(see Fig. 15a). The constant C is fixed by the total number of modes

$$C \int_0^{\omega_D} \omega^2 d\omega = 3N \quad \Rightarrow \quad C = \frac{9N}{\omega_D^3}, \quad (4.3.2)$$

where N is the total number of atoms in the crystal. The specific heat of one bosonic mode with energy ω can be found as

$$c_V(\omega) = \frac{\partial E}{\partial T} = \omega \frac{\partial}{\partial T} \frac{1}{e^{\omega/T} - 1} = \frac{\omega^2}{T^2} \frac{e^{\omega/T}}{(e^{\omega/T} - 1)^2}. \quad (4.3.3)$$

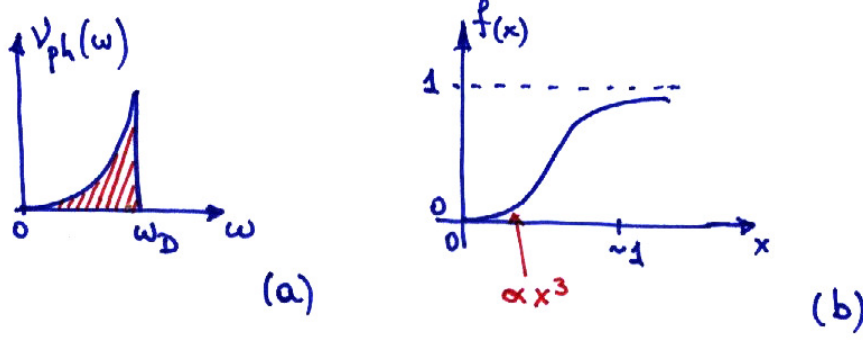


Figure 15: (a): Ansatz for $\nu_{ph}(\omega)$ in the Debye theory; (b): The form of the function $f(x)$ in Eq. (4.3.4).

So the total specific heat is

$$C_V = \int_0^\infty c_V(\omega) \nu_{ph}(\omega) d\omega = 3N f\left(\frac{T}{\omega_D}\right), \quad (4.3.4)$$

where

$$f(x) = 3x^3 \int_0^{1/x} \frac{y^4 e^y}{(e^y - 1)^2} dy \quad (4.3.5)$$

is a universal function (Fig. 15b).

This approximation describes a large number of different materials remarkably well (with one fitting parameter ω_D). At low temperatures, $C_V \propto T^3$ (the black-body specific heat), while at high temperatures $C_V \rightarrow 3N$ (the classical specific heat of $3N$ harmonic oscillators)

4.4 Electron-phonon interaction

For simplicity, we only discuss here interaction of electrons with acoustic phonons. Acoustic phonons correspond to a slowly (on the scale of a lattice constant) varying in space displacement of atoms $\mathbf{u}(x)$, which produces the charge $Z \operatorname{div} \mathbf{u}(x)$ per unit cell (Z is the charge of a single ion). This charge, in turn, results in an electric potential for the electrons. Taking into account screening (see Section 3.3), the electric potential is proportional to this charge, which finally results in the electron-phonon interaction

$$H_{e-ph} = \frac{\text{const}}{\nu a_0^3} \int d^3x a^+(x) a(x) \operatorname{div} \mathbf{u}(x), \quad (4.4.1)$$

where ν is the density of states at the Fermi level, a_0 is the lattice constant, and const is some numerical coefficient of order 1. Note that electrons are coupled only to *longitudinal* phonon modes (with the displacements along the k vector).

Next we rewrite the displacement $\mathbf{u}(x)$ in terms of the phonon creation and annihilation operators b_k and b_k^+ :

$$\mathbf{u}(x, t) = \int \frac{d^3q}{(2\pi)^3} \frac{a_0^{3/2}}{\sqrt{2M_i\omega_q}} (b_q e^{i(qr - \omega_q t)} + b_q^+ e^{-i(qr - \omega_q t)}) . \quad (4.4.2)$$

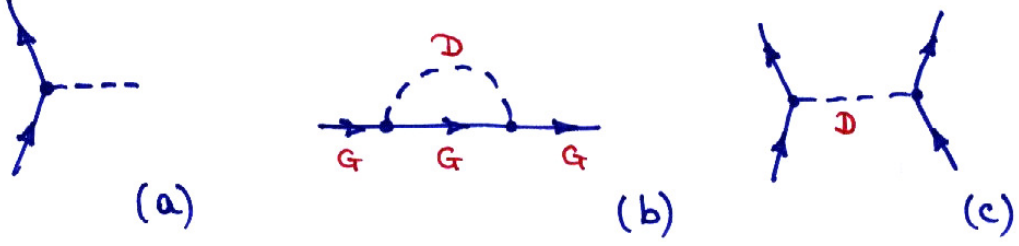


Figure 16: (a): the vertex corresponding to the electron-phonon interaction (4.4.5); (b): The lowest-order diagram describing the renormalization of the electron spectrum due to phonons; (c): The interaction between electrons mediated by phonons.

where M_i is the mass of an ion and ω_q is the phonon frequency at the wave vector q (derive this formula as a homework). The phonon creation and annihilation operators here are normalized as

$$[b_q, b_{q'}^+] = (2\pi)^3 \delta(q - q'). \quad (4.4.3)$$

It turns out to be convenient to define the phonon operator as

$$\varphi(x) = \int \frac{d^3q}{(2\pi)^3} \sqrt{\frac{\omega_q}{2}} (b_q e^{iqr} + b_q^+ e^{-iqr}), \quad (4.4.4)$$

which results in the electron-phonon interaction written in the simple form (we used the linear relation $\omega_q = c|q|$):

$$H_{\text{e-ph}} = g \int d^3x a^+(x) a(x) \varphi(x), \quad (4.4.5)$$

where g is an interaction constant (with the above definitions, $g \sim \nu^{-1/2}$ up to a numerical coefficient)

This electron-phonon interaction can now be incorporated into the diagrammatic approach as a triple vertex (Fig. 16a). One can further derive the Green's function for phonons and construct the perturbative diagrammatic series in the usual way. For example, the leading correction to the electron spectrum due to phonons is given by the diagram in Fig. 16b.

4.5 Green's function for phonons

Similarly to electrons, we define the Green's function for phonons as

$$D(x, t) = -iT \langle \varphi(x, t), \varphi(0, 0) \rangle. \quad (4.5.1)$$

(T denotes the time ordering). It can be easily computed at zero temperature. Using the definition (4.4.4), and the fact that there are no phonons at zero temperature, we find

$$D(x, t) = -i \int \frac{d^3q}{(2\pi)^3} \frac{\omega_q}{2} \begin{cases} e^{i(qx - \omega_q t)}, & t > 0, \\ e^{-i(qx - \omega_q t)}, & t < 0. \end{cases} \quad (4.5.2)$$

Performing the Fourier transform in time and space, we find the Green's function of phonons in the frequency-momentum representation:

$$D(q, \omega) = \frac{\omega_q}{2} \left(\frac{1}{\omega - \omega_q + i0} - \frac{1}{\omega + \omega_q - i0} \right) = \frac{\omega_q^2}{\omega^2 - \omega_q^2 + i0}. \quad (4.5.3)$$

4.6 Attraction between electrons mediated by phonons

We are now ready to show that interaction with phonons leads to attraction. This attraction appears in the second order of the perturbation theory as the phonon line in the diagram, see Fig. 16c.

For a formal derivation, expand the evolution operator with respect to the electron-phonon interaction:

$$U = e^{-i(H_0 + H_{\text{e-ph}})t} = U_0 + U_1 + U_2 + \dots \quad (4.6.1)$$

At the second order of the perturbation theory,

$$U_2 = \iint_{0 < t_1 < t_2 < t} dt_1 dt_2 e^{-iH_0(t-t_2)} (-iH_{\text{e-ph}}) e^{-iH_0(t_2-t_1)} (-iH_{\text{e-ph}}) e^{-iH_0 t_1}. \quad (4.6.2)$$

If we now substitute the electron-phonon interaction term (4.4.5) and perform the Wick contraction (= averaging) of the phonon operators, we arrive at

$$U_2 = U_0 \iint_{0 < t_1 < t_2 < t} dt_1 dt_2 \iint d^3x_1 d^3x_2 a^+(x_2, t_2) a(x_2, t_2) a^+(x_1, t_1) a(x_1, t_1) \times \\ \times (-i)g^2 D(x_2 - x_1, t_2 - t_1). \quad (4.6.3)$$

This equation has the same form as the first-order correction U_1 with the usual density-density interaction, except that this interaction is time dependent. The role of interaction is played by the phonon Green's function $D(x_2 - x_1, t_2 - t_1)$.

For superconductivity, the interaction averaged over time (or, equivalently, at low frequency) is important. This low-frequency effective interaction is

$$V_{\text{eff}} = D(\omega \rightarrow 0) = -g^2. \quad (4.6.4)$$

It has a negative sign, which means that it is attractive.

The physical meaning of this interaction is as follows. An electron distorts the crystal lattice (creates a positive charge around itself) which, in turn, attracts other electrons. This interaction is delayed: the characteristic time scale for phonons is ω_D^{-1} while electrons are much faster (their characteristic time scale is ε_F^{-1}). As a result, a moving electron leaves behind itself a positively charged track, which attract other electrons even after the original electron has moved away. This is also a reason why the attraction via phonons is not killed by the Coulomb repulsion of electrons: while the overall magnitudes of these interactions are of the same order, the Coulomb repulsion is instant, and the phonon attraction has a longer time scale and wins at low frequencies. An accurate treatment of this competition of the two interactions is technical and goes beyond the scope of this lecture: see, e.g., the original paper P. Morel and P. W. Anderson, Phys. Rev. **125**, 1263 (1962).

Problem Set 9

Problem 9.1

Compare the specific heat of phonons and electrons in a typical metal [as an example, think of potassium (K) with $\omega_D \sim 100\text{K}$ and $\varepsilon_F \sim 2 \cdot 10^4\text{K}$]:

(a) Consider first the high-temperature limit, $T \geq \omega_D$ (but still $T \ll \varepsilon_F$). In this limit, the phonon contribution is $c_{\text{phonon}} \approx 3N$. Assuming that there is one conduction electron per atom, estimate the relative contribution of electrons to the specific heat.

Hint: you should obtain the result $c_{\text{elec}}/c_{\text{phonon}} \sim (T/\varepsilon_F) \ll 1$.

(b) Consider now the limit of low temperatures, $T \ll \omega_D$, where the phonon specific heat is proportional to T^3 . Estimate the temperature T^* , below which the electron specific heat dominates over that of phonons.

Hint: you should find $T^* \sim \omega_D^{3/2} \varepsilon_F^{-1/2} \ll \omega_D$.

Problem 9.2

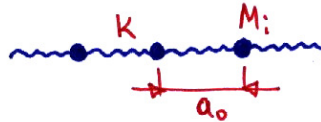
(a) Derive the coefficient in (4.4.1) up to a numerical coefficient of order one.

(b) Consider a one-dimensional model of a solid: a chain of points of mass M_i connected with springs of stiffness K (see Fig. below). The Hamiltonian reads

$$H = \sum_i \frac{p_i^2}{2M_i} + \sum_i K \frac{(x_i - x_{i+1})^2}{2}.$$

Treat this Hamiltonian as quantum-mechanical, find the spectrum and represent the vibrations as bosonic operators b_q and b_q^+ . Normalize these operators as in (4.4.3) and derive Eq. (4.4.2) for the displacement x_i .

(c) With the phonon operator defined as in (4.4.4), derive the coefficient g in (4.4.5) up to a numerical coefficient of order one and show that $g \sim \nu^{-1/2}$.



A one-dimensional model of a crystal lattice.