

Chapter 2

Electron–Phonon Interaction

The electron–phonon interaction is important not only in creating the phonon scattering of the electrons but also in the formation of Cooper pairs. This interaction is indeed the cause of the superconductivity. The Fröhlich Hamiltonian is derived. A phonon exchange can generate an attraction between a pair of electrons.

2.1 Phonons and Lattice Dynamics

In this section, we will review a general theory of the heat capacity based on lattice dynamics.

Let us take a crystal composed of N atoms. The potential energy V depends on the configuration of N atoms, $(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$. We regard this energy V as a function of the *displacements* of the atoms,

$$\mathbf{u}_j \equiv \mathbf{r}_j - \mathbf{r}_j^{(0)}, \quad (2.1)$$

measured from the equilibrium positions $\mathbf{r}_j^{(0)}$. Let us expand the potential $V = V(\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_N) \equiv V(u_{1x}, u_{1y}, u_{1z}, u_{2x}, \dots)$ in terms of small displacements $\{u_{j\mu}\}$:

$$V = V_0 + \sum_j \sum_{\mu=x,y,z} u_{j\mu} \left[\frac{\partial V}{\partial u_{j\mu}} \right]_0 + \frac{1}{2} \sum_j \sum_{\mu} \sum_k \sum_{\mu} u_{j\mu} u_{k\mu} \left[\frac{\partial^2 V}{\partial u_{j\mu} \partial u_{k\mu}} \right]_0 + \dots, \quad (2.2)$$

where all partial derivatives are evaluated at $\mathbf{u}_1 = \mathbf{u}_2 = \dots = 0$, which is indicated by subscripts 0. We may set the constant V_0 equal to zero with no loss of rigor. By assumption, the lattice is stable at the equilibrium configuration. Then the potential energy V must have a minimum, requiring that all first-order derivatives vanish:

$$\left[\frac{\partial V}{\partial u_{j\mu}} \right]_0 = 0. \quad (2.3)$$

For small oscillations we may keep terms of the second order in $u_{j\mu}$ only. We then have

$$V \simeq V' \equiv \sum_j \sum_\mu \sum_k \sum_v \frac{1}{2} A_{j\mu kv} u_{j\mu} u_{kv}, \quad (2.4)$$

$$A_{j\mu kv} \equiv \left[\frac{\partial^2 V}{\partial u_{j\mu} \partial u_{kv}} \right]_0. \quad (2.5)$$

The prime (') on V indicating the *harmonic approximation*, will be dropped hereafter. The kinetic energy of the system is

$$T \equiv \sum_j \frac{m}{2} \dot{r}_j^2 = \sum_j \frac{m}{2} \dot{u}_j^2 \equiv \sum_j \sum_\mu \frac{m}{2} \dot{u}_{j\mu}^2. \quad (2.6)$$

We can now write down the Lagrangian $L \equiv T - V$ as

$$L = \sum_j \sum_\mu \frac{m}{2} \dot{u}_{j\mu}^2 - \sum_j \sum_\mu \sum_k \sum_v \frac{1}{2} A_{j\mu kv} u_{j\mu} u_{kv}. \quad (2.7)$$

This Lagrangian L in the harmonic approximation is quadratic in $u_{j\mu}$ and $\dot{u}_{j\mu}$. According to theory of the *principal-axis transformation* [1], we can transform the Hamiltonian (total energy) $H = T + V$ for the system into the sum of the energies of the normal modes of oscillations:

$$H = \sum_{\kappa=1}^{3N} \frac{1}{2} (P_\kappa^2 + \omega_\kappa^2 Q_\kappa^2), \quad (2.8)$$

where $\{Q_\kappa, P_\kappa\}$ are the normal coordinates and momenta, and $\{\omega_\kappa\}$ are normal-mode frequencies. Note that there are exactly $3N$ normal modes.

Let us first calculate the heat capacity by means of classical statistical mechanics. This Hamiltonian H is quadratic in canonical variables (Q_κ, P_κ) . Hence the equipartition theorem holds. We multiply the average thermal energy for each mode, $k_B T$, by the number of modes, $3N$, and obtain $3Nk_B T$ for the average energy $\langle H \rangle$. Differentiating this $3Nk_B T$ with respect to T , we obtain $3Nk_B$ for the heat capacity, which is in agreement with Dulong–Petit’s law: $C = 3R$. It is interesting to observe that we obtained this result without knowing the actual distribution of normal-mode frequencies. The fact that there are $3N$ normal modes played an important role.

Let us now use quantum theory and calculate the heat capacity based on Equation (2.8). The energy eigenvalues of the Hamiltonian H are given by

$$E[\{n_k\}] = \sum_\kappa \left(\frac{1}{2} + n_\kappa \right) \hbar \omega_\kappa, \quad n_\kappa = 0, 1, 2, \dots \quad (2.9)$$

We can interpret Equation (2.9) in terms of *phonons* as follows: the energy of the lattice vibrations is characterized by the set of the *numbers of phonons* $\{n_\kappa\}$ in the normal modes $\{\kappa\}$. Taking the canonical-ensemble average of Equation (2.9), we obtain

$$\langle E[\{n\}] \rangle = \sum_{\kappa} \left[\frac{1}{2} + \langle n_\kappa \rangle \right] \hbar \omega_\kappa = \sum_{\kappa} \left[\frac{1}{2} + f_0(\hbar \omega_\kappa) \right] \hbar \omega_\kappa \equiv E(T), \quad (2.10)$$

where

$$f_0(\epsilon) \equiv \frac{1}{\exp(\epsilon/k_B T) - 1} \quad (2.11)$$

is the *Planck distribution function*.

The normal-modes frequencies $\{\omega_\kappa\}$ depend on the normalization volume V , and they are densely populated for large V . In the bulk limit we may convert the sum over the normal modes into a frequency integral, and obtain

$$E(T) = E_0 + \int_0^\infty d\omega \hbar \omega f_0(\hbar \omega) \mathcal{D}(\omega), \quad (2.12)$$

$$E_0 \equiv \frac{1}{2} \int_0^\infty d\omega \hbar \omega \mathcal{D}(\omega), \quad (2.13)$$

where $\mathcal{D}(\omega)$ is the *density of states* (modes) in *angular frequency* defined such that

$$\text{Number of modes in the interval } (\omega, \omega + d\omega) \equiv \mathcal{D}(\omega) d\omega. \quad (2.14)$$

The constant E_0 represents a temperature-independent zero-point energy.

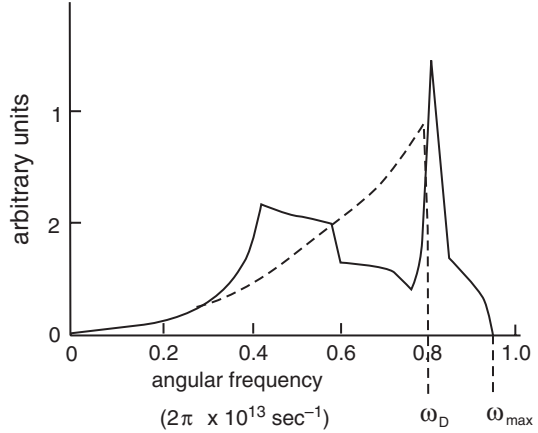
Differentiating $E(T)$ with respect to T , we obtain for the heat capacity at constant volume:

$$C_V = \left[\frac{\partial E}{\partial T} \right]_V = \int_0^\infty d\omega \hbar \omega \frac{\partial f_0(\hbar \omega)}{\partial T} \mathcal{D}(\omega). \quad (2.15)$$

This expression was obtained under the harmonic approximation only, which is expected to be valid at very low temperatures.

To proceed further, we have to know the density of normal modes, $\mathcal{D}(\omega)$. To find the set of characteristic frequencies $\{\omega_\kappa\}$ requires solving an algebraic equation of $3N$ -th order, and we need the frequency distribution for large N . This is not a simple matter. In fact, a branch of mathematical physics whose principal aim is to find the frequency distribution is called *lattice dynamics*. Figure 2.1 represents a result obtained by Walker [2] after the analysis of the X-ray scattering data for aluminum, based on lattice dynamics. Some remarkable features of the curve are

Fig. 2.1 The density of normal modes in the angular frequency for aluminum. The *solid curve* represents the data deduced from X-ray scattering measurements due to Walker [2]. The *broken lines* indicate the Debye distribution with $\Theta_D = 328$ K



(A) At low frequencies

$$D(\omega) \propto \omega^2. \quad (2.16)$$

(B) There exists a maximum frequency ω_{\max} such that

$$D(\omega) = 0 \quad \text{for} \quad \omega \geq \omega_{\max}. \quad (2.17)$$

(C) A few sharp peaks, called *van Hove singularities* [3], exist below ω_{\max} .

The feature (A) is common to all crystals. The low frequency modes can be described adequately in terms of longitudinal and transverse elastic waves. This region can be represented very well by the Debye's continuum model [4], indicated by the broken line and discussed in Book 1, Section 2.2. The feature (B) is connected with the lattice structure. Briefly, no normal modes of extreme short wavelengths (extreme high frequencies) exist. Hence there is a limit frequency ω_{\max} . The sharp peaks, feature (C), were first predicted by van Hove [3] on topological grounds, and these peaks are often referred to as *van Hove singularities*.

The cause of superconductivity lies in the electron–phonon interaction [5]. The microscopic theory can be formulated in terms of the generalized BCS Hamiltonian [5], where all phonon variables are eliminated. In this sense the details of lattice dynamics are secondary to our main concern (superconductivity). The following point, however, is noteworthy. All lattice dynamical calculations start with a real crystal lattice. For example, to treat aluminum, we start with an fcc lattice having empirically known lattice constants. The equations of motion for a set of ions are solved under the assumption of a periodic lattice-box boundary condition. Thus, the k -vectors used in lattice dynamics and Bloch electron dynamics are the same. The domain of the k -vectors can be restricted to the same first Brillouin zone. Colloquially speaking, phonons (bosons) and electrons (fermions) live together in the same Brillouin zone, which is equivalent to say that electrons and phonons share the same house (crystal

lattice). This affinity between electrons and phonons makes the conservation of momentum in the electron–phonon interaction physically meaningful. Thus, the fact that the electron–phonon interaction is the cause of superconductivity is not accidental.

2.2 Electron–Phonon Interaction

A crystal lattice is composed of a regular arrays of ions. If the ions move, then the electrons must move in a changing potential field. Fröhlich proposed an interaction Hamiltonian, which is especially suitable for transport and superconductivity problems. In the present section we derive the Fröhlich Hamiltonian [6, 7].

Let us consider a simple cubic (sc) lattice. The normal modes of oscillations for a solid are longitudinal and transverse running waves characterized by wave vector \mathbf{q} and frequency ω_q . A longitudinal wave proceeding in the crystal axis x , which is represented by

$$u_q \exp(-i\omega_q t + i\mathbf{q} \cdot \mathbf{r}) = u_q \exp(-i\omega_q t + iqx), \quad (2.18)$$

where u_q is the displacement in the x -direction. The wavelength $\lambda \equiv 2\pi/q$ is greater than twice the lattice constant a_0 . The case: $\lambda = 12a_0$ is shown in Fig. 2.2.

If we imagine a set of parallel plates containing a great number of ions fixed in each plate, then we have a realistic picture of the lattice vibration mode. From Fig. 2.2 we see that the density of ions changes in the x -direction. Hence, the longitudinal modes are also called the *density-wave* modes. The transverse wave mode can also be pictured from Fig. 2.2 by imagining a set of parallel plates containing a great number of ions fixed in each plate and assuming the transverse displacements of the plates. Notice that this mode generates no charge-density variation.

The Fermi velocity v_F in a typical metal is of the order 10^6 ms^{-1} while the speed of sound is of the order 10^3 ms^{-1} . The electrons are likely to move quickly to negate any electric field generated by the density variations associated with the lattice wave. In other words, the electrons may follow the lattice waves instantly. Given a traveling normal wave mode in Equation (2.18), we may assume an electron density deviation of the form:

$$C_q \exp(-i\omega_q t + i\mathbf{q} \cdot \mathbf{r}). \quad (2.19)$$

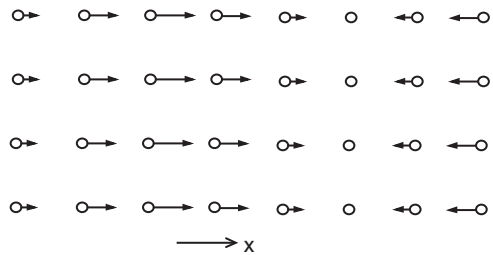


Fig. 2.2 A longitudinal wave proceeding in the x -direction; $\lambda = 12a_0$

Since electrons follow phonons immediately for all ω_q , the coefficient C_q can be regarded as independent of ω_q . If we further assume that the deviation is linear in the scalar product $\mathbf{u}_q \cdot \mathbf{q} = qu_q$ and again in the electron density $n(\mathbf{r})$, we obtain

$$C_q = A_q qu_q n(\mathbf{r}). \quad (2.20)$$

This is called the *deformation potential approximation*. The dynamic response factor A_q is necessarily complex since the traveling wave is represented by the exponential form in Equation (2.19). There is a time delay between the field (cause) and the density variation (result), and hence there is an exponential phase factor change. Complex conjugation of Equation (2.19) yields $C_q^* \exp(i\omega_q t - i\mathbf{q} \cdot \mathbf{r})$. Using this form we can reformulate the electron's response, but the physics must be the same. From this consideration we obtain (Problem 2.2.1)

$$A_q = A_{-q}^*. \quad (2.21)$$

The classical displacement u_q changes, following the harmonic equation of motion:

$$\ddot{u}_q + \omega_q^2 u_q = 0. \quad (2.22)$$

Let us write the corresponding Hamiltonian for each mode as

$$H = \frac{1}{2}(p^2 + \omega^2 q^2), \quad q \equiv u, \quad p \equiv \dot{q}, \quad \omega_q \equiv \omega, \quad (2.23)$$

where we dropped the mode index \mathbf{q} . If we assume the same quantum Hamiltonian H and the quantum condition:

$$[q, p] = i\hbar, \quad [q, q] = [p, p] = 0, \quad (2.24)$$

the quantum description of a harmonic oscillator is complete. The equations of motion are

$$\dot{q} = \frac{1}{i\hbar}[q, H] = p, \quad \dot{p} = \frac{1}{i\hbar}[p, H] = -\omega^2 q, \quad (2.25)$$

(Problem 2.2.2).

We introduce the dimensionless complex dynamical variables:

$$a^\dagger \equiv (2\hbar\omega)^{-1/2}(p + i\omega q), \quad a \equiv (2\hbar\omega)^{-1/2}(p - i\omega q). \quad (2.26)$$

Using the last two equations, we obtain

$$\dot{a}^\dagger \equiv (2\hbar\omega)^{-1/2}(-\omega^2 q + i\omega p) = i\omega a^\dagger, \quad \dot{a} = -i\omega a. \quad (2.27)$$

We can express (q, p) in terms of (a^\dagger, a) :

$$q = -i(\hbar/2\omega)^{1/2}(a^\dagger - a), \quad p = (\hbar\omega/2)^{1/2}(a^\dagger + a). \quad (2.28)$$

Thus, we may work entirely in terms of (a^\dagger, a) . After straightforward calculations, we obtain (Problem 2.2.3)

$$\begin{aligned} \hbar\omega a^\dagger a &= (2)^{-1}(p + i\omega q)(p - i\omega q) \\ &= (2)^{-1}[p^2 + \omega^2 q^2 + i\omega(qp - pq)] = H - \frac{1}{2}\hbar\omega, \\ \hbar\omega aa^\dagger &= H + \frac{1}{2}\hbar\omega, \end{aligned} \quad (2.29)$$

$$aa^\dagger - a^\dagger a \equiv [a, a^\dagger] = 1, \quad (2.30)$$

$$H = \frac{1}{2}\hbar\omega(a^\dagger a + aa^\dagger) = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) \equiv \hbar\omega \left(n + \frac{1}{2} \right). \quad (2.31)$$

The operators (a^\dagger, a) satisfy the *Bose commutation rules*, Equation (2.30). We can therefore use second quantization, which is summarized in Appendix A, Sections A.1 and A.2, and obtain

- Eigenvalues of $n \equiv a^\dagger a$: $n' = 0, 1, 2, \dots$ [see Equation (A.1)]
- Vacuum ket $|\phi\rangle$: $a|\phi\rangle = 0$ [see Equation (A.14)]
- Eigenkets of n : $|\phi\rangle, a^\dagger|\phi\rangle, (a^\dagger)^2|\phi\rangle, \dots$ having the eigenvalues $0, 1, 2, \dots$ [see Equation (A.16)]
- Eigenvalues of H : $\frac{1}{2}\hbar\omega, \frac{3}{2}\hbar\omega, \frac{5}{2}\hbar\omega, \dots$

In summary, the quantum Hamiltonian and the quantum states of a harmonic oscillator can be simply described in terms of the bosonic second quantized operators (a, a^\dagger) .

We now go back to the case of the lattice normal modes. Each normal mode corresponds to a harmonic oscillator characterized by (\mathbf{q}, ω_q) . The displacements $u_{\mathbf{q}}$ can be expressed as

$$u_{\mathbf{q}} = i \left(\frac{\hbar}{2\omega_q} \right)^{1/2} (a_{\mathbf{q}} - a_{\mathbf{q}}^\dagger), \quad (2.32)$$

where $(a_{\mathbf{q}}, a_{\mathbf{q}}^\dagger)$ are operators satisfying the *Bose commutation rules*:

$$\boxed{[a_{\mathbf{q}}, a_{\mathbf{p}}^\dagger] \equiv a_{\mathbf{q}}a_{\mathbf{p}}^\dagger - a_{\mathbf{p}}^\dagger a_{\mathbf{q}} = \delta_{\mathbf{pq}}, \quad [a_{\mathbf{q}}, a_{\mathbf{p}}] = [a_{\mathbf{q}}^\dagger, a_{\mathbf{p}}^\dagger] = 0.} \quad (2.33)$$

We can express the electron density (field) by

$$n(\mathbf{r}) = \psi^\dagger(\mathbf{r})\psi(\mathbf{r}), \quad (2.34)$$

where $\psi(\mathbf{r})$ and $\psi^\dagger(\mathbf{r})$ are *annihilation* and *creation electron field operators*, respectively, satisfying the following *Fermi anticommutation rules*:

$$\begin{aligned} \{\psi(\mathbf{r}), \psi^\dagger(\mathbf{r}')\} &\equiv \psi(\mathbf{r})\psi^\dagger(\mathbf{r}') + \psi^\dagger(\mathbf{r}')\psi(\mathbf{r}) = \delta^{(3)}(\mathbf{r} - \mathbf{r}'), \\ \{\psi(\mathbf{r}), \psi(\mathbf{r}')\} &= \{\psi^\dagger(\mathbf{r}), \psi^\dagger(\mathbf{r}')\} = 0. \end{aligned} \quad (2.35)$$

The field operators ψ (ψ^\dagger) can be expanded in terms of the momentum-state electron operators $c_{\mathbf{k}}$ ($c_{\mathbf{k}}^\dagger$):

$$\psi(\mathbf{r}) = \frac{1}{(V)^{1/2}} \sum_{\mathbf{k}} \exp(i\mathbf{k} \cdot \mathbf{r}) c_{\mathbf{k}}, \quad \psi^\dagger(\mathbf{r}) = \frac{1}{(V)^{1/2}} \sum_{\mathbf{k}'} \exp(-i\mathbf{k}' \cdot \mathbf{r}) c_{\mathbf{k}'}^\dagger, \quad (2.36)$$

where operators c , c^\dagger satisfy the *Fermi anticommutation rules*:

$$\boxed{\{c_{\mathbf{k}}, c_{\mathbf{k}'}^\dagger\} \equiv c_{\mathbf{k}} c_{\mathbf{k}'}^\dagger + c_{\mathbf{k}'}^\dagger c_{\mathbf{k}} = \delta_{\mathbf{k}, \mathbf{k}'}^{(3)}, \quad \{c_{\mathbf{k}}, c_{\mathbf{k}'}\} = \{c_{\mathbf{k}}^\dagger, c_{\mathbf{k}'}^\dagger\} = 0.} \quad (2.37)$$

Let us now construct an interaction Hamiltonian H_F , which has the dimensions of an energy *and* which is Hermitian. We propose

$$H_F = \int d^3r \sum_{\mathbf{q}} \frac{1}{2} [A_{\mathbf{q}} q u_{\mathbf{q}} \exp(i\mathbf{q} \cdot \mathbf{r}) \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}) + h.c.], \quad (2.38)$$

where *h.c.* denotes the *Hermitian conjugate*. Using Equations (2.20), (2.32) and (2.36), we can re-express Equation (2.38) as (Problem 2.2.3):

$$H_F = \sum_{\mathbf{k}} \sum_{\mathbf{q}} \frac{1}{2} (V_{\mathbf{q}} c_{\mathbf{k}+\mathbf{q}}^\dagger c_{\mathbf{k}} a_{\mathbf{q}} + h.c.), \quad V_{\mathbf{q}} \equiv A_{\mathbf{q}} (\hbar/2\omega_{\mathbf{q}})^{1/2} i q. \quad (2.39)$$

This is the *Fröhlich Hamiltonian*. Electrons describable in terms of $c_{\mathbf{k}}$ are now coupled with phonons describable in terms of $a_{\mathbf{q}}$. The term

$$V_{\mathbf{q}} c_{\mathbf{k}+\mathbf{q}}^\dagger c_{\mathbf{k}} a_{\mathbf{q}} \quad (V_{\mathbf{q}}^* c_{\mathbf{k}}^\dagger c_{\mathbf{k}+\mathbf{q}} a_{\mathbf{q}}^\dagger) \quad (2.40)$$

can be pictured as an interaction process in which a phonon is absorbed (emitted) by an electron as represented by the Feynman diagram [8, 9] in Fig. 2.3 (a) [(b)]. Note: At each vertex the momentum is conserved. The Fröhlich Hamiltonian H_F is applicable for the longitudinal phonons only. As noted earlier, the transverse lattice normal modes generate no charge density variations, making the interaction negligible.

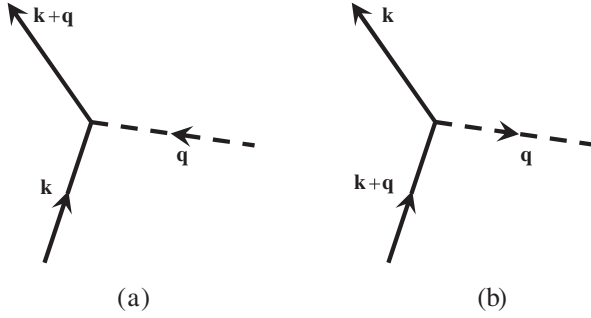


Fig. 2.3 Feynman diagrams representing (a) absorption and (b) emission of a phonon by an electron

Problem 2.2.1. Prove Equation (2.21).

Problem 2.2.2. Verify Equation (2.27).

Problem 2.2.3. Verify Equation (2.31).

Problem 2.2.4. Verify Equation (2.37).

2.3 Phonon–Exchange Attraction

By exchanging a phonon, a pair of electrons can gain attraction under a certain condition. We treat this effect in this section by using the many-body perturbation method [10, 11].

Let us consider an *electron–phonon system* characterized by

$$\begin{aligned}
 H &= \sum_{\mathbf{k}} \sum_s \epsilon_k c_{\mathbf{k}s}^\dagger c_{\mathbf{k}s} + \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} \left(\frac{1}{2} + a_{\mathbf{q}}^\dagger a_{\mathbf{q}} \right) \\
 &\quad + \lambda \sum_{\mathbf{k}} \sum_s \sum_{\mathbf{q}} \frac{1}{2} \left(V_{\mathbf{q}} a_{\mathbf{q}} c_{\mathbf{k}+\mathbf{q}s}^\dagger c_{\mathbf{k}s} + h.c. \right) \\
 &\equiv H_{el} + H_{ph} + \lambda H_F \equiv H_0 + \lambda V, \quad (V \equiv H_F) \quad (2.41)
 \end{aligned}$$

where the three sums represent: the total electron kinetic energy (H_{el}), the total phonon energy (H_{ph}), and the Fröhlich interaction Hamiltonian H_F , [see Equation (2.39)].

For comparison we consider an *electron gas system* characterized by the Hamiltonian

$$H_c = \sum_{\mathbf{k}} \sum_s \epsilon_k c_{\mathbf{k}s}^\dagger c_{\mathbf{k}s} + \frac{1}{2} \sum_{\mathbf{k}_1 s_1} \cdots \sum_{\mathbf{k}_4 s_4} \langle 3, 4 | v_c | 1, 2 \rangle c_4^\dagger c_3^\dagger c_1 c_2 \equiv H_{el} + V_c, \quad (2.42)$$

$$\begin{aligned}
 \langle 3, 4 | v_c | 1, 2 \rangle &\equiv \langle \mathbf{k}_3 s_3, \mathbf{k}_4 s_4 | v_c | \mathbf{k}_1 s_1, \mathbf{k}_2 s_2 \rangle \\
 &= \frac{4\pi e^2 k_0}{V} \frac{1}{q^2} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4} \delta_{\mathbf{k}_1 - \mathbf{k}_3, \mathbf{q}} \delta_{s_3 s_1} \delta_{s_4 s_2}.
 \end{aligned} \quad (2.43)$$

The elementary interaction process can be represented by the diagram in Fig. 2.4. The wavy horizontal line represents the instantaneous Coulomb interaction v_c . The net momentum of a pair of electrons is conserved:

$$\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4, \quad (2.44)$$

represented by the Kronecker's delta in Equation (2.43). Physically, the Coulomb force between a pair of electrons is an internal force, and hence it cannot change the net momentum.

We wish to find an *effective* Hamiltonian v_e between a pair of electrons generated by a phonon exchange. If we look for this v_e in the second order in the coupling constant λ , then the likely candidates are represented by two Feynman diagrams in Fig. 2.5. Here, the time is measured upward. (Historically, Feynman represented the elementary interaction processes by diagrams. Diagram representation is widely

Fig. 2.4 The Coulomb interaction represented by the horizontal wavy line generates the change in the momenta of two electrons

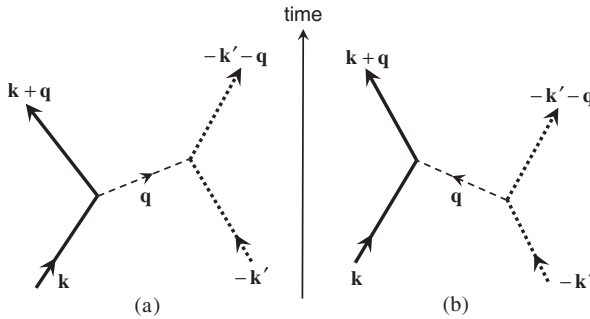
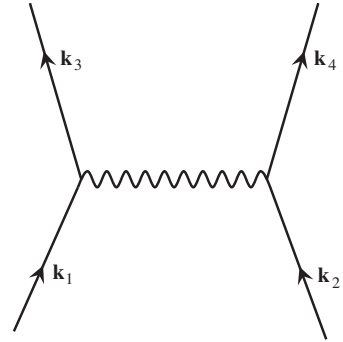


Fig. 2.5 A one-phonon-exchange process generates the change in the momenta of two electrons similar to that caused by the Coulomb interaction

used in quantum field theory [8, 9].) In the diagrams in Fig. 2.5, we follow the motion of two electrons. We may therefore consider a system of two electrons and obtain the effective Hamiltonian v_e through a study of the evolution of two-body density operator ρ_2 . Hereafter, we shall drop the subscript 2 on ρ indicating two-body system.

The system-density operator $\rho(t)$ changes in time, following the *quantum Liouville equation*:

$$i\hbar \frac{\partial \rho(t)}{\partial t} = [H, \rho] \equiv \mathcal{H}\rho. \quad (2.45)$$

We assume the Hamiltonian H in Equation (2.41) and study the time evolution of $\rho(t)$, using quantum many-body perturbation theory. Here, we sketch only the important steps; more detailed calculations were given in Fujita–Godoy’s book, *Quantum Statistical Theory of Superconductivity* [10, 11].

Let us introduce a *quantum Liouville operator*

$$\mathcal{H} \equiv \mathcal{H}_0 + \lambda \mathcal{V}, \quad (2.46)$$

which generates a commutator upon acting on ρ , see Equation (2.45). We assume that the initial-density operator ρ_0 for the electron–phonon system can be factorized as

$$\rho_0 = \rho_{\text{electron}} \rho_{\text{phonon}}, \quad (2.47)$$

which is reasonable at 0 K, where there are no real phonons and only virtual phonons are involved in the dynamical processes. We can then choose

$$\rho_{\text{phonon}} = |0\rangle \langle 0|, \quad (2.48)$$

where $|0\rangle$ is the vacuum-state ket for phonons:

$$a_{\mathbf{q}} |0\rangle = 0 \quad \text{for any } \mathbf{q}. \quad (2.49)$$

The phonon vacuum average will be denoted by an upper bar or by angular brackets:

$$\bar{\rho}(t) \equiv \langle 0 | \rho(t) | 0 \rangle \equiv \langle \rho(t) \rangle_{av}. \quad (2.50)$$

Using a time-dependent perturbation theory and taking a phonon-average, we obtain from Equation (2.45)

$$\frac{\partial \bar{\rho}(t)}{\partial t} = -\frac{\lambda^2}{\hbar^2} \int_0^t d\tau \langle \mathcal{V} \exp(-i\tau \hbar^{-1} \mathcal{H}_0) \mathcal{V} \rho(t-\tau) \rangle_{av}. \quad (2.51)$$

In the *weak-coupling approximation*, we may calculate the phonon-exchange effect to the lowest (second) order in λ and obtain

$$\lambda^2 \langle \mathcal{V} \exp(-i\tau \hbar^{-1} \mathcal{H}_0) \mathcal{V} \rho(t - \tau) \rangle = \lambda^2 \langle \mathcal{V} \exp(-i\tau \hbar^{-1} \mathcal{H}_0) \mathcal{V} \rangle_{av} \bar{\rho}(t - \tau). \quad (2.52)$$

Using the Markoffian approximation we may replace $\bar{\rho}(t - \tau)$ by $\bar{\rho}(t)$ and take the upper limit t of the τ -integration to ∞ . Using these two approximations, we obtain from Equation (2.51)

$$\frac{\partial \bar{\rho}(t)}{\partial t} = i\lambda^2 \hbar^{-1} \lim_{a \rightarrow 0} \langle \mathcal{V} (\mathcal{H}_0 - ia)^{-1} \mathcal{V} \rangle_{av} \bar{\rho}(t), \quad a > 0. \quad (2.53)$$

Let us now take momentum-state matrix elements of Equation (2.53). The lhs is

$$\frac{\partial}{\partial t} \langle \mathbf{k}_1 s_1, \mathbf{k}_2 s_2 | \rho(t) | \mathbf{k}_3 s_3, \mathbf{k}_4 s_4 \rangle \equiv \frac{\partial}{\partial t} \rho(1, 2; 3, 4, t), \quad (2.54)$$

where we dropped the upper bar indicating the phonon vacuum average. The rhs requires more sophisticated computations due to the Liouville operators $(\mathcal{V}, \mathcal{H}_0)$. After lengthy but straightforward calculations, we obtain from Equation (2.53)

$$\begin{aligned} \frac{\partial}{\partial t} \rho(1, 2; 3, 4, t) = & \sum_{\mathbf{k}_5 s_5} \sum_{\mathbf{k}_6 s_6} -i\hbar^{-1} [\langle 1, 2 | v_e | 5, 6 \rangle \rho_2(5, 6; 3, 4, t) \\ & - \langle 5, 6 | v_e | 3, 4 \rangle \rho_2(1, 2; 5, 6, t)], \end{aligned} \quad (2.55)$$

$$\langle 3, 4 | v_e | 1, 2 \rangle \equiv |V_q|^2 \frac{\hbar \omega_q}{(\epsilon_3 - \epsilon_1)^2 - \hbar^2 \omega_q^2} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4} \delta_{\mathbf{k}_3 - \mathbf{k}_1, \mathbf{q}} \delta_{s_3 s_1} \delta_{s_4 s_2}. \quad (2.56)$$

Kronecker's delta $\delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4}$ in Equation (2.56) means that the net momentum is conserved, since the phonon exchange is an internal interaction.

For comparison, consider the electron-gas system. The two-electron density matrix ρ_c for this system changes, following

$$\begin{aligned} \frac{\partial}{\partial t} \rho_c(1, 2; 3, 4, t) = & \sum_{\mathbf{k}_5 s_5} \sum_{\mathbf{k}_6 s_6} -i\hbar^{-1} [\langle 1, 2 | v_c | 5, 6 \rangle \rho_c(5, 6; 3, 4, t) \\ & - \langle 5, 6 | v_c | 3, 4 \rangle \rho_c(1, 2; 5, 6, t)], \end{aligned} \quad (2.57)$$

which is of the same form as Equation (2.55). The only differences are in the interaction matrix elements. Comparison between Equations (2.43) and (2.56) yields

$$\frac{4\pi e^2 k_0}{V} \frac{1}{q^2} \quad (\text{Coulomb interaction}), \quad (2.58)$$

$$|V_q|^2 \frac{\hbar\omega_q}{(\epsilon_{\mathbf{k}_1+\mathbf{q}} - \epsilon_{\mathbf{k}_1})^2 - \hbar^2\omega_q^2} \quad (\text{phonon-exchange interaction}). \quad (2.59)$$

In our derivation, the weak-coupling and the Markoffian approximations were used. The Markoffian approximation is justified in the steady state condition in which the effect of the duration of interaction can be neglected. The electron mass is four orders of magnitude smaller than the lattice-ion mass, and hence the coupling between the electron and ionic motion must be small by the mass mismatch. Thus, expression (2.59) is highly accurate for the effective phonon-exchange interaction at 0 K. This expression has remarkable features. First, the interaction depends on the phonon energy $\hbar\omega_q$. Second, the interaction depends on the electron energy difference $\epsilon_{\mathbf{k}_1+\mathbf{q}} - \epsilon_{\mathbf{k}_1}$ before and after the transition. Third, if

$$|\epsilon_{\mathbf{k}_1+\mathbf{q}} - \epsilon_{\mathbf{k}_1}| < \hbar\omega_q, \quad (2.60)$$

then the effective interaction is *attractive*. Fourth, the attraction is greatest when $\epsilon_{\mathbf{k}_1+\mathbf{q}} - \epsilon_{\mathbf{k}_1} = 0$, that is, when the phonon momentum \mathbf{q} is parallel to the constant-energy (Fermi) surface. A bound electron-pair, called a *Cooper pair*, may be formed by the phonon-exchange attraction, which was shown in 1956 by Cooper [12].

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