

Chapter 2

Phonons and Their Interactions

2.1 The Phonon–Phonon Interaction

Within the harmonic approximation, phonons are non-interacting and have an infinite lifetime. Including higher terms (anharmonic terms) in the expansion of the potential leads to an interaction between phonons. As a result, a phonon from a given state defined by the wave vector \mathbf{q} and the branch j of the dispersion spectrum $\omega_j(\mathbf{q})$ will decay into other phonons after a finite time. Phonon–phonon interactions involve different number of phonons in the interaction process.

In perturbation theory, the crystal potential is expanded as a power of displacement and the Hamiltonian may be written as:

$$H = H_0 + \lambda H_3 + \lambda^2 H_4 + \lambda^3 H_5 + \dots \quad (2.1)$$

where H_0 is the harmonic Hamiltonian and H_3, H_4, H_5, \dots are the perturbation terms involving three, four, five ... interacting phonons. The simplest case is the three-phonon interaction where a phonon decays to form two other phonons and vice-versa. The possible interactions are shown in Fig. 2.1. The Hamiltonian for three-phonon processes reads¹:

$$H_3 = \frac{1}{3!} \sum_{\mathbf{q}''} \sum_{jj''} \frac{\hbar^3/2}{2^{3/2} N^{1/2} \sqrt{\omega_j \omega_{\mathbf{q}''j'} \omega_{\mathbf{q}''j''}}} \phi(\mathbf{q}j, \mathbf{q}''j', \mathbf{q}''j'') \delta_{\mathbf{q}+\mathbf{q}''+\mathbf{G}} \times (a_{-\mathbf{j}}^\dagger + a_{\mathbf{q}j})(a_{-\mathbf{j}'}^\dagger + a_{\mathbf{q}''j'})(a_{-\mathbf{j}''}^\dagger + a_{\mathbf{q}''j''}) \quad (2.2)$$

where $\phi(\mathbf{q}j, \mathbf{q}''j', \mathbf{q}''j'')$ is the 3×3 matrix element, $\mathbf{q}, \mathbf{q}', \mathbf{q}''$ are the wave vectors of the three phonons involved in the process and \mathbf{G} is the reciprocal lattice vector. The δ -function guarantees momentum conservation in these processes. The last

¹ For a derivation of the Hamiltonian refer to [1, 2].

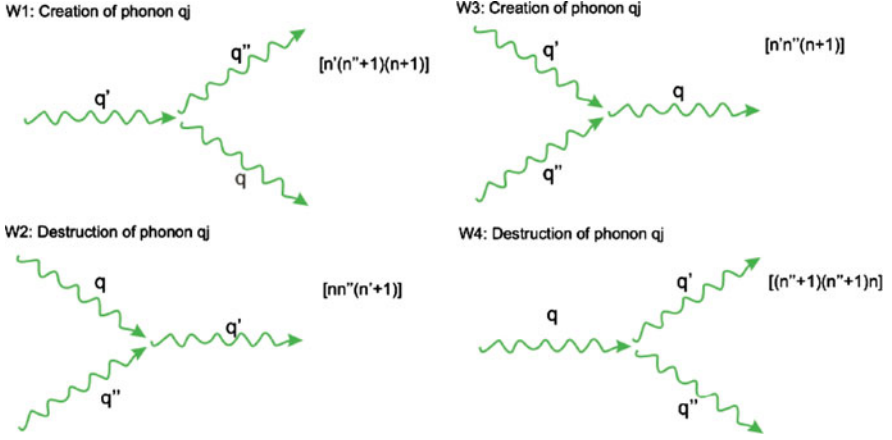


Fig. 2.1 Three-phonon interaction processes that may destroy or create the phonon $\mathbf{q}j$. Creation of a phonon in the process contributes to the transition probability by a factor $[(\hbar/2m\omega)(n+1)]^{1/2}$ while a phonon destruction contributes by $[(\hbar/2m\omega)(n)]^{1/2}$

three terms of Eq. 2.2 represent the different processes of creation and annihilation of the three phonons.

The probability per unit time, that a phonon in an initial state $|i\rangle$ with index $\mathbf{q}j$ will decay, as a result of one of the processes mentioned, into some other state $|f\rangle$ is given by the Fermi “Golden rule”:

$$W(i \rightarrow f) = \frac{2\pi}{\hbar} |\langle f | H_3 | i \rangle|^2 D_f(E) \quad (2.3)$$

where $D_f(E)$ is the density of the final states and H_3 is the three-phonon Hamiltonian of Eq. 2.2. The lifetime of this phonon $\mathbf{q}j$ is then defined as the reciprocal value of the decay rate. This rate is the sum of the rates of the processes where the phonon $\mathbf{q}j$ is created, minus the rate of the processes where the phonon $\mathbf{q}j$ is destroyed. Altogether it follows that the lifetime $\tau(\mathbf{q}j)$ is given by:

$$\begin{aligned} \frac{1}{\tau(\mathbf{q}j)} = & \frac{\pi}{16N} \sum_{\mathbf{q}'j', \mathbf{q}''j''} \frac{|\phi(\mathbf{q}j, \mathbf{q}'j', \mathbf{q}''j'')|^2}{\omega_{\mathbf{q}j}\omega_{\mathbf{q}'j'}\omega_{\mathbf{q}''j''}} \delta_{\mathbf{q}+\mathbf{q}'+\mathbf{q}'', \mathbf{G}} \\ & \times \{ [n'(n''+1)(n+1) - nn''(n'+1)] \times \delta(\omega_{\mathbf{q}} - \omega_{\mathbf{q}'} + \omega_{\mathbf{q}''}) \\ & + [n'n''(n+1) - n(n''+1)(n'+1)] \times \delta(\omega_{\mathbf{q}} - \omega_{\mathbf{q}'} - \omega_{\mathbf{q}''}) \} \end{aligned} \quad (2.4)$$

Each partial probability contains the square of the transition matrix element times a delta function which guarantees energy and momentum conservation. The squares of the matrix elements for the different processes differ only in the occupation numbers of the phonons n , n' , and n'' . Higher order phonon processes, involving four or more phonons, are more numerous and arise from higher orders of the perturbation theory as seen from Eq. 2.1. Nevertheless the strength for these

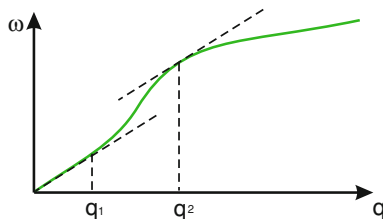


Fig. 2.2 Anomalous phonon dispersion, as is the case for liquid helium. Within the range $q_1 < q < q_2$, the phonon phase velocity, v_p , exceeds the sound velocity v_s and spontaneous decay is allowed. $v_s = \omega/q$ as $q \rightarrow 0$; $v_p = d\omega/dq$

interactions decreases as the number of phonons in the interaction process increases.

As the temperature tends to zero, due to the absence of thermal phonon population (n' and $n'' = 0$), the decay probabilities for up-conversion processes vanish. The intrinsic phonon lifetime (due to p – p interaction) is thus dominated by spontaneous down-conversion decay towards lower energy phonons (Fig. 2.1d). In the case of a normal phonon dispersion, it has been discussed that four-phonon interaction is the lowest order decay process [3]. Three-phonon decay processes are kinematically not allowed. For anomalous phonon dispersion, however, where the phonon phase velocity exceeds the sound velocity, collinear (i.e. wave vectors of the involved phonons are all along the same direction) intra-branch three-phonon decay processes for transverse phonons become kinematically allowed. This leads to a finite phonon lifetime even at zero temperature. The phonon spectrum of superfluid helium exhibits such an anomaly, and spontaneous phonon decay at very low temperatures is experimentally observed for phonons with $v_g > v_s$ [4, 5] (v_g and v_s are the group velocity and the sound velocity, respectively). Figure 2.2 shows such an anomalous phonon dispersion. Within the range $q_1 < q < q_2$, the phonon phase velocity, v_p , exceeds the sound velocity. Only phonons within this range can decay to lower-energy phonons and therefore exhibit a finite lifetime at zero temperature.

2.2 The Electron–Phonon Interaction

In the band model description, electrons in a solid are quasi-particles which occupy one-electron states. They are described by Bloch functions $|\mathbf{k}, \sigma\rangle$, where \mathbf{k} is the wave vector of the electron and σ is the spin.

In a perfect crystal, an electron propagates without scattering, however, the perfect periodicity is destroyed by the lattice vibrations of the atoms. These vibrations cause the electrons to have a certain probability of being scattered.

The electron–phonon interaction process induces the annihilation or creation of a phonon (\mathbf{q}, j) and a simultaneous excitation or de-excitation of the electron from

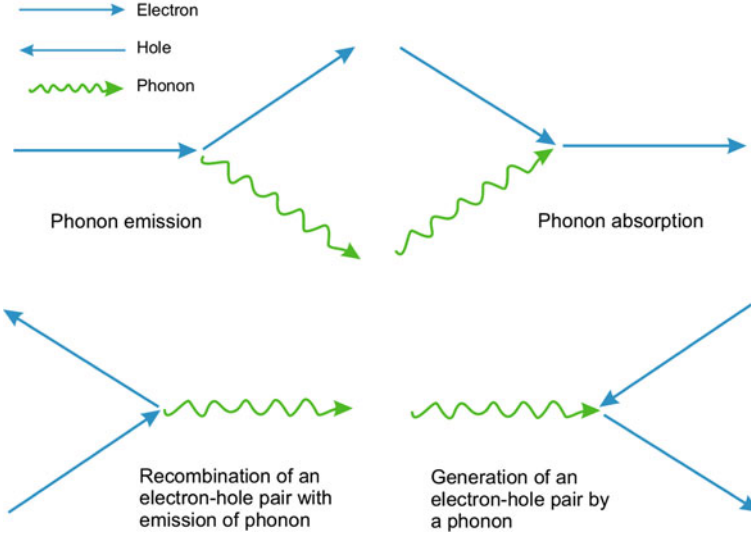


Fig. 2.3 The different possible electron–phonon interaction processes

state $|\mathbf{k}, \sigma\rangle$ to $|\mathbf{k} \pm \mathbf{q}, \sigma\rangle$. These two processes are illustrated in the top row of Fig. 2.3. Another two possible processes are illustrated in the second row of Fig. 2.3: recombination of an electron–hole pair with the creation of a phonon, and the creation of an electron–hole pair by the annihilation of a phonon. These four basic processes can be described quantum mechanically by a first-order perturbation calculation. The Hamiltonian of the electron–phonon interaction is²:

$$H_{e-p} = \sum_{\mathbf{k}, \mathbf{q}, j} g(\mathbf{k}_1, \mathbf{k}_2; \mathbf{q}, j) c_{\mathbf{k}_1 j}^\dagger c_{\mathbf{k}_2 j} (a_{-\mathbf{q}, j}^\dagger + a_{\mathbf{q}, j}) \quad (2.5)$$

where $c_{\mathbf{k}_1 j}^\dagger$ and $c_{\mathbf{k}_2 j}$ are the creation and annihilation operators for the quasi-particles with wave vectors $\mathbf{k}_1 = \mathbf{k} + \mathbf{q}$ and $\mathbf{k}_2 = \mathbf{k}$, respectively; $a_{\mathbf{q}, j}^\dagger$ and $a_{\mathbf{q}, j}$ are the creation and the annihilation operators of the phonon of energy $\omega_{\mathbf{q}, j}$ and wave vector \mathbf{q} . The latter two operators in the Hamiltonian mean that two interactions are possible, one in which a phonon with wave vector \mathbf{q} in branch j is created, and a second in which a phonon \mathbf{q}, j is annihilated. Both processes are accompanied by an electron transition from an initial state \mathbf{k}_1 into a final state \mathbf{k}_2 . The matrix element $g(\mathbf{k}_1, \mathbf{k}_2; \mathbf{q}, j)$ describes the electron–phonon coupling and is defined as:

$$g(\mathbf{k}_1, \mathbf{k}_2; \mathbf{q}, j) = -i\varepsilon(\mathbf{q}, j) \cdot \mathbf{q} V(\mathbf{q}) \quad (2.6)$$

² For more details and derivation of the Hamiltonian we point to the corresponding chapters in the books by Ziman [1], Grimvall [6], and Reissland [2].

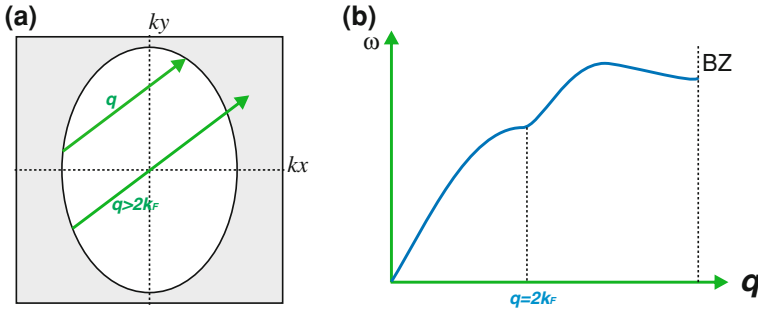


Fig. 2.4 **a** Schematic 2D Fermi surface. The *arrows* correspond to phonon wave vectors. **b** Phonon dispersion along \mathbf{q} . The *kink* corresponds to the Kohn anomaly at $q = 2k_F$

where $V(\mathbf{q})$ is the matrix element of the electron–phonon pseudopotential and $\varepsilon(\mathbf{q}, j)$ is the phonon polarisation. Due to the factor $\varepsilon(\mathbf{q}, j) \cdot \mathbf{q}$, transverse phonons in the first Brillouin zone will not interact with the electrons. However in higher Brillouin zones, due to *Umklapp* processes the factor $\varepsilon(\mathbf{q}, j) \cdot \mathbf{q} \neq 0$ in general.

2.2.1 Kohn Anomalies in the Phonon Dispersion of Metals

The coupling function (Eq. 2.6) refers to the scattering of a quasi-particle from a point \mathbf{k}_1 to a point \mathbf{k}_2 in momentum space with $\mathbf{q} = \mathbf{k}_1 - \mathbf{k}_2$. Energy and momentum conservation require that both \mathbf{k}_1 and \mathbf{k}_2 lie on the Fermi surface.³ This immediately introduces a restriction on the phonon wave vector \mathbf{q} : phonon wave vectors connecting nested parts of the Fermi surface will strongly interact with the electrons leading to a large phonon damping, whereas those which do not span the Fermi surface will not interact with the electrons. It has been pointed out by Kohn [7] that the interaction of phonons with the conduction electrons in a metal should cause anomalies in the phonon spectra. The phonon dispersion should exhibit kinks at wave vectors $\mathbf{q} + \mathbf{G} = 2\mathbf{k}_F$, where \mathbf{k}_F is the Fermi wave vector and \mathbf{G} is the reciprocal lattice vector. Figure 2.4a illustrates a schematic two-dimensional (2D) Fermi surface. Phonons with wave vector $\mathbf{q} + \mathbf{G} < 2\mathbf{k}_F$ (represented by the short arrow in Fig. 2.4a) can always excite quasi-particle quasi-hole pair since they span the Fermi surface. Their self-energy is therefore renormalized with respect to the bare phonon energy. For $\mathbf{q} + \mathbf{G} > 2\mathbf{k}_F$ this condition is not fulfilled and those phonons do not interact with the electrons. At $\mathbf{q} + \mathbf{G} = 2\mathbf{k}_F$ a discontinuity results in the momentum dependence of the electron–phonon interaction. This is reflected

³ This is due to the fact that the typical phonon energy is in the meV range which is three orders of magnitude smaller than the typical electron energy.

in the phonon dispersion illustrated schematically in Fig. 2.4b. The anomaly at $\mathbf{q} + \mathbf{G} = 2\mathbf{k}_F$ is the Kohn anomaly after Walter Kohn [7].

The strength of the Kohn anomaly depends on the joint density of occupied and unoccupied electronic states. If their quantity is large, conduction electrons may, become unstable with respect to a spatially inhomogeneous perturbation. To first order, the response of the electrons to such a perturbation is measured by the generalized susceptibility $\chi_{\mathbf{q}}$. Instability sets in when this quantity diverges. This happens in a nesting situation, that is, in a situation in which there are large areas of the Fermi surface which are parallel or nearly parallel. In two-dimensional systems, such instabilities usually lead to a charge- or spin-density wave ground state.

Highly accurate neutron measurements of $\omega(\mathbf{q})$ are required to reveal these anomalies. Such measurements were performed on various metals and indicate a structure of singularities that is consistent with the Fermi surface geometry. Figure 2.5 shows the phonon dispersion in elemental Pb along the $(\xi\xi 0)L$ branch [8] and the $(\xi\xi 0)T$ branches (measured on TRISP). Kohn anomalies can be seen in the dispersion. The locations of those anomalies correspond to diameter of the Fermi surface [10]. Similar Kohn anomalies have also been observed in the phonon dispersion of transition-metal dichalcogenides 2H-TaSe₂ and 2H-NbSe₂ [9]. Pronounced softening were detected by inelastic neutron scattering at $q = 0.2$ in both systems due to the quasi-two-dimensional nature of their Fermi surface which leads to a charge density wave ground state.

Figure 2.6 shows the phonon dispersion of the $(\xi\xi\xi)L$ branch in Pb_{1-x}Tl_x alloys [11]. Pure Pb exhibits a strong Kohn anomaly at $q \approx 0.42$ rlu. By doping Pb with

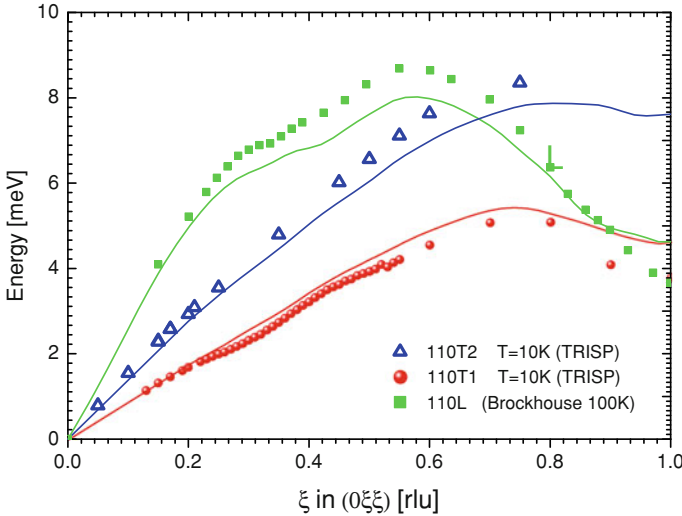
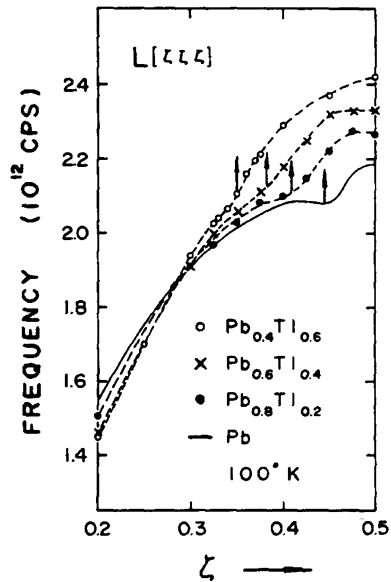


Fig. 2.5 Phonon dispersion of Pb along the $(\xi\xi 0)$ branch. Kohn anomalies are observed which are consistent with the Fermi surface geometry. The transverse branches (T_1 and T_2) were measured on TRIPS whereas the data for longitudinal branch is taken from Brockhouse [8]

Fig. 2.6 Dispersion curves for $\text{Pb}_{1-x}\text{Tl}_x$ alloys along the $(\xi\xi\xi)L$ branch. The lines are guide to the eye. The *arrows* indicate the location of the Kohn anomalies which, via doping Pb with Tl, progressively move to lower momenta due to change of the Fermi surface. Figure is taken from Ng et al. [11]



Tl (hole doping since Tl has one fewer electron), the Fermi surface shrinks. This is reflected in the location of the Kohn anomaly, which gradually moves to smaller wave vectors.

In the above figures, the phonon dispersion was plotted along a specific direction. In two or three dimensions, the locus of Kohn anomalies form a surface, the Kohn surface whose shape and strength reflect the geometry of the Fermi surface. For example, from Fig. 2.4a, the Kohn anomaly along k_x lies at a smaller wave vector than that along the k_y direction. The strengths of the anomalies also differ due to the different curvatures along those directions.

References

1. J.M. Ziman, *Electrons and Phonons*. (Oxford, London, 1962)
2. J.A. Reissland, *The Physics of Phonons*. (Wiley, Toronto, 1972)
3. A. Berke, J. Phys. C Solid State Phys. **21**, 2205 (1988)
4. H.J. Maris et al., Phys. Rev. Lett. **25**, 220 (1970)
5. L.P. Pitayevski et al., Phys. Rev. B **14**, 263 (1976)
6. G. Grimvall, *The Electrons-Phonons Interaction in Metals*, vol. XVI. (North Holland, 1980)
7. W. Kohn, Phys. Rev. Lett. **2**, 393 (1959)
8. B.N. Brockhouse, *Inelastic Scattering of Neutrons in Solids and Liquids*. (IAEA, Vienna, 1961)
9. D.E. Moncton et al., Phys. Rev. B **16**, 801 (1977)
10. R. Stedman et al., Phys. Rev. **163**, 567 (1967)
11. S.C. Ng et al., Solid State Comm. **5**, 79 (1967)

Electron-Phonon Interaction in Conventional and
Unconventional Superconductors

Aynajian, P.

2011, XII, 101 p., Hardcover

ISBN: 978-3-642-14967-2