Electron-Lattice Interaction

So far, we have focused on the electron problem, treating the ions as fixed in place at their equilibrium positions $\mathbf{R}_i^0$. In the context of the electron gas, we adopted an even simpler view of the ions, namely, that they provide a uniform background of compensating positive charge. To be able to describe the range of physics observed in a solid, we must invoke some realism into our treatment of ion motion. The coupling of electronic degrees of freedom with the motion of the ions is the electron-phonon problem. Phonons in a solid arise from collective motion of the ions. Such motion is quantized and fundamentally responsible for 1) polaron formation, 2) the electron attraction in superconductivity, and 3) the temperature dependence of the resistivity in metals. In this lectures, we focus on the general formulation of the electron-phonon problem and its subsequent application to the low-temperature resistivity in metals.

1 Harmonic Chain

We begin with a brief review of a 1d chain of N atoms joined by harmonic springs. Let x_i denote the deviation of each oscillator from its equilibrium position, ω the frequency of oscillation of each spring, and M the mass of each atom. The total Hamiltonian for this harmonic chain is

$$H = \sum_i \frac{P_i^2}{2M} + \frac{M\omega^2}{2}\sum_i (x_i - x_{i+1})^2. \tag{1}$$

We diagonalize this Hamiltonian by Fourier transforming the momentum

$$P_n = \frac{1}{\sqrt{N}}\sum_k e^{\imath kna} P_k \tag{2}$$

and the displacement operators

$$x_n = \frac{1}{\sqrt{N}}\sum_k e^{\imath kna} x_k, \tag{3}$$

where a is a lattice constant. By noting that

$$\sum_n P_n^2 = \sum_k P_k P_{-k} \tag{4}$$

and

$$\sum_n x_n x_{n+m} = \sum_k x_k x_{-k} e^{-\imath kma}, \tag{5}$$

we rewrite the Hamiltonian in k-space:

$$H = \frac{1}{2M} \sum_k P_k P_{-k} + \frac{M}{2} \sum_k \omega_k^2 x_k x_{-k}, \tag{6}$$

where $\omega_k^2 = 2\omega^2(1 - coska) = 4\omega^2 \sin^2 ka/2$. As a consequence, the $k = 0$ mode costs no energy to excite. This is a defining feature of acoustic phonons. The $k = 0$ mode corresponds to a uniform translation of the ions. By translational invariance, such a transformation cannot change the energy. Such long-wavelength bosonic excitations which cost no energy are called Goldstone modes. In magnetic systems, such as ferro-magnets and antiferromagnets, analogous long-wavelength excitations exist, which at $k = 0$ cost no energy.Such excitations, known as spin waves or magnons, constitute the low-energy excitations in magnetic systems and hence determine the magnetic contribution to the specific heat, for example.

Let us define new operators

$$\tilde{Q}_k = x_k \left(\frac{M\omega_k}{2\hbar} \right)^{1/2} \tag{7}$$

and

$$\tilde{P}_k = \frac{P_k}{(2M\omega_k\hbar)^{1/2}}, \tag{8}$$

which allow us to recast H in the suggestive form

$$H = \sum_k \hbar\omega_k [\tilde{P}_k \tilde{P}_{-k} + \tilde{Q}_k \tilde{Q}_{-k}]. \tag{9}$$

We can factorize H once we define the creation

$$b_k^\dagger = (\tilde{Q}_{-k} - i\tilde{P}_k) \tag{10}$$

and annihilation

$$b_k = (\tilde{Q}_k + i\tilde{P}_{-k}) \tag{11}$$

operators. The commutation relations obeyed by b_k and $b_k^\dagger$,

$$[b_k^\dagger, b_{k'}] = -\delta_{kk'}, \tag{12}$$

follow from the canonical commutator

$$[\tilde{P}_k, \tilde{Q}_k] = -\frac{i}{2}. \tag{13}$$

The factorized Hamiltonian takes on the familiar oscillator form

$$H = \sum_k \hbar\omega_k\Big(b_k^\dagger b_k + \frac{1}{2}\Big), \tag{14}$$

which is indicative of a collection of bosons. The time dependence of the $b_k's$,

$$b_k(t) = b_k(t=0)e^{-\imath\omega_k t}, \tag{15}$$

is obtained by solving the Heisenberg equations of motion,

$$-i\hbar\dot{b}_k = [H, b_k] = -\hbar\omega_k b_k. \tag{16}$$

The operators $b_k^\dagger(t)$ create a collective lattice distortion with frequency ω_k at time t. The spatial resolution of this distortion is given by solving Eqs. (10) and (11) for x_k

$$\begin{aligned} x_k(t) &= \frac{1}{2}\Big(\frac{2\hbar}{M\omega_k}\Big)^{1/2}(b_k(t) + b_{-k}^\dagger(t)) \\ &= \Big(\frac{\hbar}{2M\omega_k}^{1/2}(b_k e^{-\imath\omega_k}t + b_{-k}^\dagger e^{\imath\omega_k}t)\Big) \end{aligned} \tag{17}$$

and then Fourier transforming

$$x_\ell(t) = \sum_k \Big(\frac{\hbar}{2MN\omega_k}\Big)^{1/2}(b_k e^{-i\omega_k t} + b_{-k}^\dagger e^{i\omega_k t})e^{ik\ell a}. \tag{18}$$

This expression for $x_l(t)$ tells us the amplitude of the lattice vibration on site l at time t. The sum over k is restricted to the first Brillouin zone.