Contents

Reading:

1. Ch. 26, Ashcroft & Mermin
2. Ch. 7, Kittel

4 Electron-phonon interaction

4.1 Hamiltonian

The subtle interplay of electrons and phonons was explained in the 50's by some of the earliest practitioners of quantum many-body theory, leading eventually to an understanding of the mechanism underlying superconductivity. Recall that the ions in a metal have two basic effects on the electronic states: 1) the *static* ionic lattice provides a periodic potential in which conduction electrons must move, leading to the evolution of plane wave states in the Fermi gas into Bloch waves in the crystal, and 2) the scattering of electrons by lattice *vibrations*, and vice versa. The first effect will be ignored here, as we are essentially interested in long-wavelength phenomena, where the differences between proper calculations using Bloch waves and simpler ones using plane waves are negligible. It suffices then to consider the phonons in a lattice interacting with a Fermi gas in which the most important effects of the long-range Coulomb interaction have been accounted for. *Without* the Coulomb interaction, the phonon frequencies are just those we would get from a classical model of balls of mass M (ionic mass) connected by springs. For a 3D solid with 1 atom per unit cell, there are 3N normal modes comprising 3 *acoustic* phonon branches ω_k^λ. When one includes the long-range Coulomb interaction but neglects the electron-phonon coupling, one finds

that the longitudinal acoustic mode has been lifted to the ionic plasma frequency, $\omega_{pl}^{ion} \simeq (4\pi Z^2 e^2 n/M)^{1/2}$. The terms of the Goldstone theorem which insists on the existence of an acoustic mode for each spontaneously broken continuous symmetry are violated by the long-range nature of the Coulomb force, and the sloshing back and forth of the ion "fluid" at ω_{pl}^{ion} occurs for the same reason and at the same frequency (up to the mass difference) that it does in the electron case. At this point we are seriously worried that we don't understand how acoustic phonons ever exist in charged systems. If one now includes the electron- phonon coupling, however, the electronic medium screens the long-range Coulomb interaction, leading to a finite interaction length and the recovery of the Goldstone (acoustic) mode.

Let's give a brief overview of where we're going. I first want to get to the point where we can write down the full Hamiltonian for the problem. We want to show that it makes sense to write the Hamiltonian describing the electron-phonon system as

$$H = H_{el}^0 + H_{ph}^0 + H_{coul} + H_{int}, \tag{1}$$

where

$$H_{el}^0 = \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} \tag{2}$$

$$H_{ph}^0 = \sum_{k\lambda} \omega_{k\lambda} (a_{k\lambda}^\dagger a_{k\lambda} + \frac{1}{2}) \tag{3}$$

$$H_{Coul} = \frac{1}{2} \sum_{\substack{kk'q \\ \sigma\sigma'}} V(q) c_{k'+q\sigma'}^\dagger c_{k\sigma}^\dagger c_{k+q\sigma} c_{k'\sigma'} \tag{4}$$

$$H_{int} = \sum_{kk'\sigma\lambda} g_{kk'} c_{k\sigma}^\dagger c_{k'\sigma} (a_{-q\lambda}^\dagger + a_{q\lambda}) \tag{5}$$

where $a_{k\lambda}^\dagger$ creates a phonon with wave vector $q \equiv k' - k$ and polarization λ, and $g_{kk'} \propto M^{-1/2}$ is the bare electron-phonon

coupling. The unperturbed phonon Hamiltonian H_{ph} is of course just the sum of 3N independent harmonic oscillators in 2nd quantized form, and the bare Coulomb matrix element in H_{Coul} is $V(q) = 4\pi e^2/q^2$. The derivation of the electron-phonon Hamiltonian H_{int} and its quantization is relatively straightforward, and I will sketch it here.

4.1.1 Derivation of e^--ph coupling

Assume the ion is located at position $\mathbf{R}_i$, at a displacement $\mathbf{u}_i$ from its equilibrium position $\mathbf{R}_i^0$. If the potential of the ion is assumed to be rigid, the interaction energy of the electronic charge density with the ions is simply[1]

$$H_{int} = \sum_{i\sigma} \int d^3r \psi_\sigma^\dagger(\mathbf{r})\psi_\sigma(\mathbf{r})V(\mathbf{r}-\mathbf{R}_i). \tag{6}$$

For small amplitude vibrations, we can expand in powers of $\mathbf{u}_i$:

$$\begin{aligned} H_{int} &= \sum_{i\sigma} \int d^3r \psi_\sigma^\dagger(\mathbf{r})\psi_\sigma(\mathbf{r})V(\mathbf{r}-\mathbf{R}_i^0) \\ &\quad + \sum_{i\sigma} \int d^3r \psi_\sigma^\dagger(\mathbf{r})\psi_\sigma(\mathbf{r})\mathbf{u}_i \cdot \nabla_{\mathbf{R}_i} V(\mathbf{r}-\mathbf{R}_i)|_{\mathbf{R}_i^0} + \ldots \end{aligned} \tag{7}$$

Now expand the field operators ψ_σ in terms of Bloch waves:

$$\psi(\mathbf{r}) = \sum_{\mathbf{k}} c_{\mathbf{k}\sigma}\phi_{\mathbf{k}}(\mathbf{r}), \tag{8}$$

where

$$\phi_{\mathbf{k}\sigma}(\mathbf{r}+\mathbf{R}_i^0) = e^{i\mathbf{k}\cdot\mathbf{R}_i^0}\phi_{\mathbf{k}}(\mathbf{r}) \tag{9}$$

so the quantity which appears in Eq. (7) may be recast by performing a shift by a Bravais lattice vector and using the periodicity

[1]This is for a Bravais lattice. If there is a basis one has to be a bit careful about labelling the lattice sites with additional intracell indices, i.e. $\mathbf{R}_{i\alpha}, \alpha = 1 \ldots m$, where m is number of atoms/cell.

of $\nabla_{\mathbf{R}_i^0} V(\mathbf{r} - R_i^0)$,

$$\begin{aligned}
&\int d^3r \phi^*_{\mathbf{k}'\sigma}(\mathbf{r}) \phi_{\mathbf{k}\sigma}(\mathbf{r}) \nabla_{\mathbf{R}_i^0} V(\mathbf{r} - \mathbf{R}_i^0) \\
&\quad = \int d^3r \phi^*_{\mathbf{k}'\sigma}(\mathbf{r} + \mathbf{R}_j^0) \phi_{\mathbf{k}\sigma}(\mathbf{r} + R_j^0) \nabla_{\mathbf{R}_i^0} V(\mathbf{r} - \mathbf{R}_i^0) \\
&\quad = e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j^0} \underbrace{\int d^3r \phi^*_{\mathbf{k}'\sigma}(\mathbf{r}) \phi_{\mathbf{k}\sigma}(\mathbf{r}) \nabla_{\mathbf{R}_i^0} V(\mathbf{r} - \mathbf{R}_i^0)}_{\mathbf{W}_{\mathbf{k}\mathbf{k}'}} \qquad (10) \qquad (11)
\end{aligned}$$

Now let us 2nd-quantize the displacement $\mathbf{u}$ as we did when we were discussing the isolated phonon system,[2]

$$\mathbf{u}_i(t) = \frac{1}{\sqrt{NM}} \sum_{\mathbf{k}\lambda} Q(\mathbf{k}, t) \mathbf{e}^\lambda(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{R}_i^0} \qquad (13)$$

with

$$Q_\lambda(\mathbf{q}) = \frac{1}{\sqrt{2\omega_\lambda(\mathbf{q})}} \left(a_\lambda(\mathbf{q}) + a^\dagger_\lambda(-\mathbf{q}) \right) \qquad (14)$$

so interaction Hamiltonian can be rewritten

$$\begin{aligned}
H_{int} &= \sum_{\mathbf{k}\mathbf{k}'\sigma} c^\dagger_{\mathbf{k}'\sigma} c_{\mathbf{k}\sigma} \sum_j \mathbf{W}_{\mathbf{k}\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_j^0} \frac{1}{\sqrt{NM}} \times \\
&\quad \times \sum_{\mathbf{q}\lambda} Q_\lambda(\mathbf{q}) \mathbf{e}^\lambda(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{R}_j^0} \\
&= \sum_{\mathbf{k}\mathbf{k}'\sigma} \sum_\lambda c^\dagger_{\mathbf{k}'\sigma} c_{\mathbf{k}\sigma} \left(\mathbf{W}_{\mathbf{k}\mathbf{k}'} \cdot \mathbf{e}^\lambda(\mathbf{q}) \right) Q_\lambda(\mathbf{q}) \sqrt{\frac{N}{M}} \\
&\equiv \sum_{\mathbf{k}\mathbf{k}'\sigma\lambda} g_{\mathbf{k}\mathbf{k}'\lambda} c^\dagger_{\mathbf{k}'\sigma} c_{\mathbf{k}\sigma} \left(a_\lambda(\mathbf{q}) + a^\dagger_\lambda(-\mathbf{q}) \right) \qquad (15)
\end{aligned}$$

[2]Before we dealt primarily with the 1D chain, so I supressed the polarization indices. It is important to recall that in a 3 dimensional system there are 3N normal modes (3mN if there are m atoms per unit cell). For each value of $\mathbf{k}$ there are 3 acoustic (optical only if there are add'l atoms per unit cell requiring index α) modes denoted by different values of the branch index λ. The vectors $\mathbf{e}^\lambda(\mathbf{k})$ are the polarization vectors of the modes and satisfy the orthogonality condition

$$\sum_\alpha \mathbf{e}^\lambda_\alpha(\mathbf{k}) \cdot e^{\lambda'}_\alpha(\mathbf{k}) = \delta_{\lambda\lambda'} \qquad (12)$$

where now $\mathbf{q}$ due to momentum conservation (δ-function from summing over j) is to be interpreted as

$$\mathbf{q} = \mathbf{k} - \mathbf{k}' + \mathbf{G} \tag{16}$$

with G is a vector of reciprocal lattice (arose because $\mathbf{q}$ was defined to lie in 1st B-zone). The electron-phonon coupling constant is

$$g_{\mathbf{k}\mathbf{k}'\lambda} = \left(\mathbf{W}_{\mathbf{k}\mathbf{k}'} \cdot \mathbf{e}^{\lambda}(\mathbf{q})\right) \sqrt{\frac{N}{2M\omega_{pl}^{ion}(\mathbf{q})}} \tag{17}$$

The final result, then, is that an electron in state $\mathbf{k}, \sigma$ can undergo a scattering process with amplitude $g_{\mathbf{k}\mathbf{k}'}$, ending up in final state $\mathbf{k}', \sigma$ by absorption (emission) of a phonon of momentum $\mathbf{q}$. This form is useful, but calculating $g_{\mathbf{k}\mathbf{k}'}$ from first principles is difficult because V is poorly known.

4.1.2 Jellium model

We can get some dimensionally reasonable results in the so-called "jellium" model, where the ions are represented as a featureless, positively charged elastic continuum,[3] we will simply replace the eigenfrequencies $\omega_{k\lambda}$ of the neutral system by the constant ω_{pl}^{ion} according to the arguments given above. Again we expand the crystal potential $V(r - R_j)$ around the equilibrium sites R_i^0. The dispacements $\mathbf{u}(\mathbf{R})$ in the jellium gives a charge density fluctuation[4] $-nZe\nabla \cdot \mathbf{u}$. This interacts with the electron gas through the Coulomb interaction, leading to the interaction

$$H_{int}^{jellium} = Ze^2 \sum_{\sigma} \int d^3r d^3r' \; \psi_{\sigma}^{\dagger}(\mathbf{r})\psi_{\sigma}(\mathbf{r}) \frac{1}{|\mathbf{r} - \mathbf{r}'|} \nabla \cdot \mathbf{u}(\mathbf{r}'), \tag{18}$$

[3]... justified by the large masses and correspondingly long timescales for ionic motion (Born-Oppenheimer)

[4]Recall from E& M the polarization charge density is $\rho_P = -\nabla \cdot \mathbf{P}$, where $\mathbf{P}$ is the polarization, and the polarization due to a density n of dipole moments $\mathbf{p} = Ze\mathbf{u}$ is therefore $nZe\mathbf{u}$.

and then quantizing the ionic displacements $u_i = R_i - R_i^0$ as in Eq.(13), one finds

$$H_{int}^{jellium} = \sum_{\mathbf{k}\mathbf{k}'\sigma} c_{\mathbf{k}'\sigma}^\dagger c_{\mathbf{k}\sigma} \left(a_\lambda(\mathbf{q}) + a_\lambda^\dagger(\mathbf{q}) \right) \frac{4\pi i \mathbf{q}\cdot\mathbf{e}_\lambda(\mathbf{q})}{M^{1/2}} \frac{Ze^2 n}{q^2} \quad (19)$$

Comparing with Eq. (15), we see that the effective e-ph coupling constant in an isotropic system is

$$\boxed{g(q) = \frac{4\pi i Z e^2 n^{1/2}}{q M^{\frac{1}{2}}}}. \quad (20)$$

4.1.3 Screening.

The first point I would like to review is the renormalization of the electron-phonon coupling which leads to screening and the recovery of the acoustic spectrum. The main point is to realize that the singular behavior is due to the long-range Coulomb interaction, which will be screened. Any time a phonon of momentum q is excited, it creates charge density fluctuations because the ions are positively charged. These then interact with the electron gas. The bare potential created by the charge fluctuation is proportional to the electron-phonon coupling constant, so screening the ionic charge amounts to replacing the bare coupling g with a screened coupling

$$\bar{g}(q, \omega_n) = g(q)/\epsilon(q, \omega_n), \quad (21)$$

where $q = k' - k$ and $\epsilon(q, \omega_n) = 1 - V(q)\chi(q, \omega_n)$ is the RPA dielectric constant. The frequency dependence of the dielectric constant will become important for us on scales of the Debye frequency ω_D or smaller, and this is normally a very small scale by

electronic standards! So for most purposes we keep a frequency-independent screened coupling $\bar{g}(q) \simeq g(q)/\epsilon(q,0)$.

We would like to see that this screening recovers acoustic modes as observed and expected. The *bare* interaction Hamiltonian may be written in the Jellium model as (see Eq. (15)

$$H_{int} = \sum_q g(q) n_{-q} Q_q \tag{22}$$

with $n_q = \Sigma_{\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}}$. Consider now the entire Hamiltonian for the phonon coordinates, including the coupling to the electron gas (recall derivation of normal modes for linear chain in Section 1):

$$H_{ph} + H_{int} = \frac{1}{2} \sum_{\mathbf{q}} \left(\frac{1}{M} P_{\mathbf{q}} P_{-\mathbf{q}} + M \omega_{pl}^{ion\,2} Q_{\mathbf{q}} Q_{-\mathbf{q}} + 2 g_{\mathbf{q}} Q_{\mathbf{q}} n_{-\mathbf{q}} \right) \tag{23}$$

The Heisenberg equation of motion for the operator $Q_{\mathbf{q}}$ becomes (check!)

$$\ddot{Q}_{\mathbf{q}} + \omega_{pl}^{ion\,2} Q_{\mathbf{q}} + g_{-\mathbf{q}} n_{\mathbf{q}} = 0 \tag{24}$$

We noted above that the ionic charge density fluctuation *induced* by an ionic displacement $\mathbf{u}$ was $en^{ion} = -nZe\nabla \cdot \mathbf{u}$; in Fourier space with Eq. (13) this reads

$$n^{ion}_{\mathbf{q}} = -iZ\sqrt{\frac{n}{M}} q Q_{\mathbf{q}} \tag{25}$$

Also recall the definition of the dielectric constant

$$\epsilon = \frac{\text{“external charge”}}{\text{total charge}}. \tag{26}$$

Now the total charge fluctuation is just electronic + ionic $n_{\mathbf{q}} + n^{ion}_{\mathbf{q}}$, so

$$n_{\mathbf{q}} \;=\; n^{ion}_{\mathbf{q}}(1 - 1/\epsilon) = -iZ\sqrt{\frac{n}{M}} q Q_{\mathbf{q}} (1 - 1/\epsilon) \tag{27}$$

$$= iZ\sqrt{\frac{n}{M}}qQ_{\mathbf{q}}\left(\frac{k_{TF}^2}{q^2+k_{TF}^2}\right), \tag{28}$$

where in the last step we have used the Thomas-Fermi approximation for the dielectric function, $\epsilon = 1 + k_{TF}^2/q^2$.

$$\omega_{phonon}^2 = \omega_{pl}^{ion\,2}\left[1 - \frac{k_{TF}^2}{q^2+k_{TF}^2}\right]. \tag{29}$$

Equation of motion becomes

$$\begin{aligned} 0 &= \ddot{Q}_{\mathbf{q}} + \omega_{pl}^{ion\,2}Q_{\mathbf{q}} + \underbrace{\left(\frac{4\pi i Z e^2 n^{1/2}}{qM^{\frac{1}{2}}}\right)} iZ\sqrt{\frac{n}{M}}qQ_{\mathbf{q}}\left(\frac{k_{TF}^2}{q^2+k_{TF}^2}\right) \\ &= \ddot{Q}_{\mathbf{q}} + \omega_{pl}^{ion\,2}\left[1 - \left(\frac{k_{TF}^2}{q^2+k_{TF}^2}\right)\right]Q_{\mathbf{q}}. \end{aligned} \tag{30}$$

So the phonon oscillation frequencies are

$$\omega_{phonon}^2 = \omega_{pl}^{ion\,2}\left(\frac{q^2}{q^2+k_{TF}^2}\right) \tag{31}$$

Since $k_{TF}^2 = 6\pi n e^2/E_F$, we do in fact recover *acoustic* phonons $i\omega_n = cq$ as $q \to 0$, with speed

$$c = (m/3M)^{1/2}v_F. \tag{32}$$

So we have proven that sound propagates in a metal, which you already knew, but it is important to remember that screening makes it happen!

4.2 Polarons

4.3 Bloch resistivity

4.4 Effective $e^- - e^-$ interaction

For superconductivity it will be important to understand why one electron attracts each other effectively by polarizing the lattice. We now have at our disposal the effective screened electron-phonon interaction with coupling constant $g_{\mathbf{k}\mathbf{k}'}$ and renormalized phonon frequencies $\omega_\lambda(\mathbf{q})$. An interaction between electrons must involve the 1st electron polarizing the lattice, and the second interacting with this polarization, i.e. it must be a 2nd-order process in the coupling constant g. We can represent these processes in terms of Feynman-type pictures: The amplitude of the first pro-

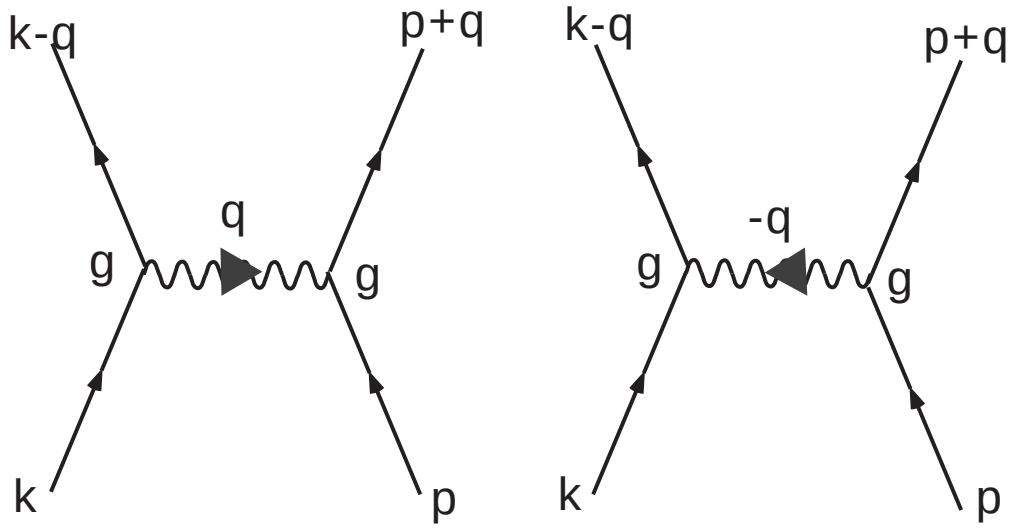

Figure 1: Electron-electron interaction due to phonon exchange. Straight lines are electrons, wiggly are phonons, vertices are e-ph coupling constants g.

cess, according to 2nd-order perturbation theory, where the 1st

electron emits a phonon, is

$$V_q^1 = \frac{|g_q|^2}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}} - \omega_{\mathbf{q}}} \tag{33}$$

whereas for the process where it absorbs a phonon we get

$$V_q^2 = \frac{|g_q|^2}{\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{p}+\mathbf{q}} - \omega_{\mathbf{q}}}. \tag{34}$$

Note as usual we have energy conservation at every scattering event depicted in these processes, i.e.

$$\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{p}} = \epsilon_{\mathbf{k}-\mathbf{q}} + \epsilon_{\mathbf{p}+\mathbf{q}} \tag{35}$$

and I've assumed $\omega_{\mathbf{q}} = \omega_{-\mathbf{q}}$. According to quantum mechanics the two amplitudes contribute additively:

$$V_q = V_q^1 + V_q^2 == \frac{|g_q|^2 \omega_{\mathbf{q}}}{(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}})^2 - \omega_{\mathbf{q}}^2}. \tag{36}$$

Let's analyze this expression for the "effective electron-electron interaction" qualitatively. We will primarily be interested in $\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}} \ll \omega_{\mathbf{q}}$, since this situation corresponds to electrons with their momenta both quite close to the Fermi surface, well within a shell of width ω_D, a typical phonon energy.

- attractive
- ind. of $\mathbf{k} \Rightarrow$ isotropic
- rapidly decreases when $\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}} \sim \omega_D$.
- energy space: interaction spread over $\omega_D \Rightarrow$ in time space it's *retarded*
- comparable when spread over time to Coulomb interactions: some metals superconducting, some not.