# 561 Fall 2005 Lecture 9

## Phonons and Electron-Phonon Interactions in Metals

See Phillips 10.1-10.3; Pines, ch. 5; Nozieres and Pines, vol. 1, p 237 ff); Mahan, Ch. 1.3, 2.7-8, 6.4

### 1. The Electron-Nucleus System, beyond the adiabatic approximation

As we derived in Lectures 2-4, the hamiltonian for the system of electrons and nuclei can be written:

$$H = H_e + H_{ph} + H_{e-ph} \tag{1}$$

where $H_e$ is the hamiltonian for the electrons moving in the presence of fixed nuclei, and $H_{ph}$ is the hamiltonian for nuclei moving with effective interactions determined by the electrons assuming they evolve in their instantaneous (adiabatic) ground state as a function of the nuclear positions. The final term $H_{e-ph}$ is the interaction term in which the motion of the nuclei causes transitions among the electronic states.

In the abiabatic approximation (ignoring $H_{e-ph}$) the problem is separable. The states of the electrons are the eigenstates of $H_e$ that describes interacting electrons in the presence of fixed nuclei. We have described the electron problem in terms of a perturbation expansion in the interaction expanded in a basis of non-interacting states. The most important point from our work so far is that even in the presence of large electron-electron interactions, *it is reasonable to describe the states in a metal near the Fermi energy as quasiparticles, which are modified particles with the same quantum numbers are independent particles.*

The nuclear vibration problem described by $H_{ph}$ can be solved exactly within the harmonic approximation, by the transformation to normal modes. These states form the independent particle basis for many-body anharmonic effects. Below we first review the description of harmonic phonons in terms of Green's functions.

Then we consider the effect of $H_{e-ph}$ upon the electronic states, and conversely the effect of the electronic states upon the phonons.

### 2. Transformation to normal modes and Green's functions for Phonons

From lecture 4: Within the harmonic approximation, the normal modes for a crystal are phonons. The quantum system can be treated by solving the classical equations of motion for the classical oscillator eigenmodes and quantizing the oscillators. From the Bloch theorem the eigenmodes can be classified by the **q**, e.g., for one atom per cell, (with a normalization volume of N cells)

$$u_I = \frac{1}{\sqrt{N}} \sum_q u_q e^{iqR_I^0} \; ; \; p_I = M \frac{du_I}{dt} = \frac{1}{\sqrt{N}} \sum_q p_q e^{iqR_I^0}, \tag{2}$$

The classical hamiltonian becomes

$$H = \sum_q \left[ \frac{1}{2M} p_q^* p_q + \frac{M}{2} \omega_q^2 u_q^* u_q \right]. \tag{3}$$

where

$$M\omega_q^2 \equiv \sum_J D_{IJ} e^{iq(R_I^0 - R_J^0)}. \tag{4}$$

Defining new operators

$$Q_q = \left(\frac{M\omega_q}{2\hbar}\right)^{1/2} u_q, \quad P_q = \left(\frac{1}{2\hbar M\omega_q}\right)^{1/2} u_q, \tag{5}$$

the hamiltonian becomes

$$H = \sum_q \hbar\omega_q \left[P_q^* P_q + Q_q^* Q_q\right]. \tag{6}$$

Quantizing the independent oscillators, the creation and annihilation operators are

$$a_q^\dagger = (Q_q^* - iP_q), \quad a_q = (Q_q + iP_q^*), \tag{7}$$

and the quantum hamiltonian operator becomes

$$\hat{H} = \frac{1}{2}\sum_q \hbar\omega_q \left[a_q^\dagger a_q + a_q a_q^\dagger\right] = \sum_q \hbar\omega_q \left[a_q^\dagger a_q + \frac{1}{2}\right]. \tag{8}$$

where the $a_q^\dagger$ and $a_q$ are the creation and annihilation operators, with the normalized displacements given by

$$Q_q = (a_q + a_{-q}^\dagger). \tag{9}$$

**Phonon Green's functions**

We will label the phonon Green's function as $D_q$ following the notation of Mahan. The desired Green's function follow immediately from our previous analysis of a single oscillator and analysis closely related to that for electron Green's functions (see Lectures 6 and 6a). The time-ordered form is given by:

Define the Green's function by

$$D_q(t) = -i\langle T[\widehat{Q}_q((t)\widehat{Q}_{-q}(0)]\rangle, \tag{10}$$

This is the form needed in perturbation theory in terms of the interactions. The general form at finite T is given below. First we consider T=0 where Green's function for the harmonic lattice is given by inserting the expression for $Q$ in terms of $a_q$ and $a_{-q}^\dagger$, and noting that the only non-zero terms are for the ordering $\langle a_q a_q^\dagger\rangle$. It is easy to show that the time-ordered form is

$$D_q^t(t) = -i\left[\Theta(t)e^{-i\omega_q t} + \Theta(-t)e^{i\omega_q t}\right], \tag{11}$$

which has the Fourier transform

$$D_q^t(\omega) = \frac{1}{\omega - \omega_q + i\eta} - \frac{1}{\omega + \omega_q - i\eta} = \frac{1}{\omega^2 - \omega_q^2 + 2i\omega_q\eta}, \quad \eta > 0. \tag{12}$$

Note that this is the time-ordered form which has poles in the lower part of the complex plane ($Im\omega < 0$ for $\omega > 0$ and in the upper part of the complex plane ($Im\omega > 0$ for $\omega < 0$. The poles are shown in the figure and one can note the similarity to the time-ordered electron Green's function. The retarded form has poles only in the lower plane. It is easily

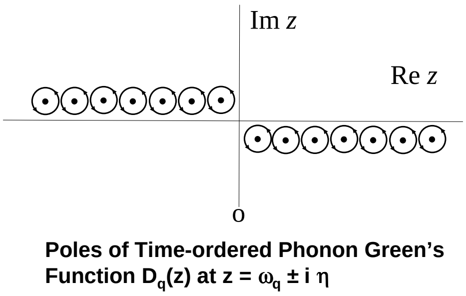

Figure 1: Poles for the time-ordered phonon Green's function.

found by replacing $-i\eta$ with $+i\eta$ in the second term of the middle expression in Eq. 13, which leads to the same expression as that given in lecture 4,

$$D_q^{ret}(\omega) = \frac{1}{\omega - \omega_q + i\eta} - \frac{1}{\omega + \omega_q + i\eta} = \frac{1}{\omega^2 - \omega_q^2 + 2i\omega\eta}, \quad \eta > 0. \tag{13}$$

The phonon Green's functions have the same analytic structures as the dielectric function and polarizability (retarded response functions) given in Lecture 5b, and the RPA form of the polarizability given in Lecture 8 (where we gave the time-ordered form needed for the RPA calculations of the self-energies).

The phonon Green's functions can also be written explicitly for finite temperature in the harmonic approximation. Using the phonon occupation number $N_q = \langle a_q^\dagger a_q \rangle = \frac{1}{e^{\beta\omega_q}+1}$, the expressions become (see Mahan 2.9):

$$\begin{aligned} D_q^t(t) &= -i\left[(N_q + \Theta(t))e^{-i\omega_q t} + (N_q + \Theta(-t))e^{i\omega_q t}\right], & (14)\\ D_q^{ret}(t) &= -i\Theta(t)\left[e^{-i\omega_q t} + e^{i\omega_q t}\right] = -2\Theta(t) sin(\omega_q t) & (15) \end{aligned}$$

and

$$\begin{aligned} D_q^t(\omega) &= \frac{N_q + 1}{\omega^2 - \omega_q^2 + 2i\omega_q\eta}, & (16)\\ D_q^{ret}(\omega) &= \frac{1}{\omega^2 - \omega_q^2 + 2i\omega\eta}, \quad \eta > 0 & (17) \end{aligned}$$

The change from T=0 is the occupation number in the time ordered form.

### 3. The Electron-Phonon Interaction

The Electron-Phonon Interaction represents the fact that the nuclear motions can cause transitions between the electronic states. In second quantized form the el-ph interaction term is (see Phillips Sec. 10.3, Mahan Sec. 1.3):

$$H_{e-ph} = \sum_{q,p,\sigma} M_{q,p} c^{+}_{p+q,\sigma} c_{p,\sigma}((a_q + a^\dagger_{-q})), \tag{18}$$

where $M$ denotes an electron-phonon matrix element denoted by the vertex in Fig. 2. In general there is a sum over the different phonons at each $q$, which we have omitted for

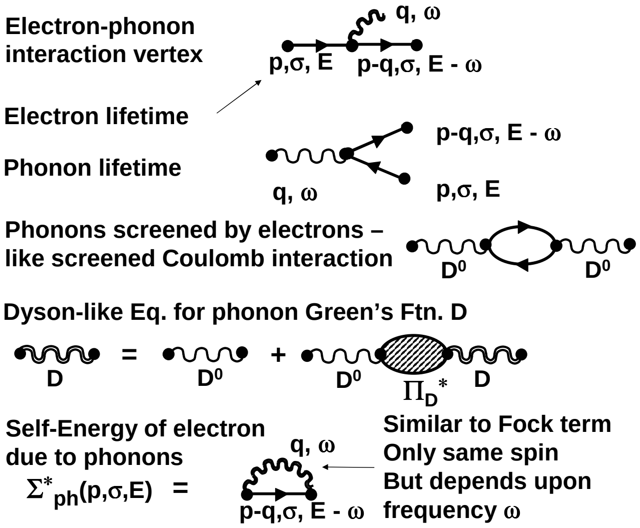

Figure 2: Various aspects of the electron-phonon interaction as discussed in the text

simplicity. From the definition of the coupling term it follows that the matrix element for nuclear displacements in the $x$ direction is given by

$$M_q = -\frac{1}{(NM)^{1/2}} \int d^3r \phi_p^*(r) \left[ \sum_I \frac{dV(r - R_I)}{dx} e^{iqR_I^0} \right] \phi_{p-q}(r) \tag{19}$$

where the minus sign comes from changing the derivative from $R$ to $r$. (In general there is a sum over the different phonons at each $q$, which we have omitted for simplicity.) The matrix element is independent of $p$ if the wavefunctions are plane waves, which we will assume for simplicity.

Key Point: phonons create potentials that are screened just like the Coulomb interaction by the electrons, with the difference that the characteristic frequencies are low $\approx$ phonon frequencies instead of $\approx$ plasmon frequencies

## 3. Comments on the Electron-Phonon Interaction

- Renormalized phonons (frequencies for nuclei screened by electrons)

  We can derive again the basic idea that the electrons screen the motion of the nuclei, which is the basic idea of the adiabatic approximation. If we start from completely decoupled nuclei and electrons, then the zero-order hamiltonian for nuclear motion is bare nuclei with a rigid background of electrons. Then the Coulomb interactions between the nuclei would lead to plasmons with frequency $\Omega_q$ for $q \to 0$. Putting in screening is exactly the same as for the Coulomb interaction discussed before; the result is the frequencies are renormalized to

$$\omega_q^2 = \Omega_q^2 - \frac{q^2}{4\pi e^2} |V_q|^2 (1 - \epsilon^{-1}(q, \omega \approx 0)) \tag{20}$$

The structure of the dielectric function leads to Kohn anomalies, etc. (Log terms in the Lindhard dielectric function). For $q \rightarrow 0$ this leads to accoustic modes with velocity of sound s given by $s = v_F(\Omega_p^2/3\omega_p^2) = v_F(Z/3)(m/M)$, where $v_F$ is the Fermi velocity, $\Omega_p$ is the ion plasma frequency and $\omega_p$ is the electron plasma frequency.

- Meaning of the electron-phonon interaction matrix element

  For the same reasons as given above the potential created by the phon is screened, so that in the expression for the matrix $M$, the potential is screened by the electrons. *Thus the electron-phonon interaction matrix element in all the following should be taken as a screened matrix element, screened by the electron dielectric function.*

- Electron-Phonon Interactions within the RPA

  The RPA provides a feasible way to calculate and include the screening. In the homogeneous gas the screening is described by the Lindhard function, which captures many key features.

### 4. Consequences of the Electron-Phonon Interaction

- Phonon Lifetime - acoustic attenuation in a metal due to excitation of the electrons by phonons - See Phillips 10.4

- Electron lifetime - scattering of electrons by phonons - a dominant cause of resistivity - see Phillips - we will consider (notes presented in class) the scattering rate; in terms of the rate the conductivity can be calculated from the Boltzman Eq., as described by Ashcroft and Mermin and many other texts.

  Note: This is an example of the imaginary part of the self energy denoting energy loss.

- Renormalized electron (enhanced mass) Demonstration that if the electrons have an imaginary self energy (damping) then they *must* also cause a frequency dependent real self-energy (change of mass) Notes provided in class.

- Induced electron-electron interactions

  Leads to attractive interaction and is the mechanism for superconductivity in ordinary ("low temperature") superconductors. We will consider the attractions later which have the form

$$H_{eff} = \sum_{q,p,p'} \frac{|V_q|^2}{\omega^2 - \omega_q^2 + i\eta} c^+_{p+q} c^+_{p'-q} c_p c_{p'} . \tag{21}$$

(This is described in Nozieres and Pines, vol. 1, p 243 ff.)