

# PHYS 798C Spring 2024

## Lecture 6 Summary

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### I. MICROSCOPIC ORIGIN OF THE PAIRING INTERACTION

#### A. Electron-Phonon Pairing Interaction

What is  $V_{\vec{k},\vec{k}'}$ ? Where does it come from and how can we control or modify it? How can the electron-phonon mechanism be generalized to other types of pairing mechanisms?

The key physics is the retarded interaction between two electrons mediated by the relatively slowly moving ion lattice. We will build up a calculation of  $V_{\vec{k},\vec{k}'}$  in steps, starting with the static screening case and then taking on the dynamic screening of both electrons and ions in a solid.

#### B. Electron in Free Space

In free space electrons interact by means of the bare Coulomb interaction:  $V(r) = e^2/4\pi\epsilon_0 r$ . We will work in momentum space, so look at the Coulomb interaction there. The Fourier transform is proportional to  $V(q) = e^2/\epsilon_0 q^2$ , where  $\vec{q} = \vec{k} - \vec{k}'$  is the momentum transfer in scattering an electron from momentum  $\vec{k}$  to momentum  $\vec{k}'$ . This  $V(q)$  is a purely repulsive interaction, as expected.

#### C. Two-Electron Static Interaction in a Solid

The Cooper electrons are actually in a solid, which is a highly polarizable medium. For the moment we shall consider just the polarization properties of the electron gas. Consider a metal in electrostatic equilibrium ( $\vec{E} = 0$  inside). Now add a single impurity charge and calculate its potential everywhere in the solid. In other words, we will add an external charge density  $\rho_{ext}$  and calculate how the medium responds. The electrons are very light and mobile compared to the ions, so we shall focus on just their response.

The calculation of static screening in an electron gas is done in Kittel *Introduction to Solid State Physics* Chapter 10, or in Ashcroft and Mermin *Solid State Physics* Chapters 17 and 26.

The constitutive equation for a linear dielectric is  $\vec{D} = \epsilon_0 \epsilon \vec{E} = \epsilon_0 \vec{E} + \vec{P}$ , where  $\epsilon$  is the dielectric function and  $\vec{P}$  is the polarization. From Maxwell's equations we have  $\nabla \cdot \vec{D} = \rho_{ext}$ , whereas  $\nabla \cdot \vec{E} = \rho_{total}/\epsilon_0 = (\rho_{ext} + \rho_{bound})/\epsilon_0$ , where the charges are distinguished by being either externally imposed or bound. The bound charge arises from the screening response of the electrons and ions in the solid. Note that one can calculate the dielectric function  $\epsilon$  as  $\epsilon = \frac{|\vec{D}|}{\epsilon_0 |\vec{E}|} = \frac{\rho_{ext}}{\rho_{Total}}$ .

Consider a solid made up of positive ions and a gas of free electrons. One can create an externally imposed positive charge distribution by mechanically deforming the lattice, for example, thus creating an externally induced sinusoidal charge density of wavenumber  $q$  as  $\rho_{ext} \sim \rho_0 \sin(qx)$ . It can be shown (Kittel, Ashcroft+Mermin cited above) that one can write the resulting potential associated with this disturbance as,

$V(q) = \frac{e^2}{\epsilon_0 \epsilon(q) q^2}$ , with  $\epsilon(q) = 1 + \frac{k_{TF}^2}{q^2}$ . Here  $k_{TF}$  is the Thomas-Fermi screening wavenumber and is defined as  $k_{TF}^2 \equiv \frac{3}{2} \frac{n_0 e^2}{\epsilon_0 E_F}$ , where  $n_0$  is the electron density.

Thus the static screened Coulomb interaction is given by,

$$V(q) = \frac{e^2/\epsilon_0}{q^2 + k_{TF}^2}.$$

Fourier transforming back to real space gives the screened Coulomb potential:

$$V(r) = \frac{e^2}{4\pi\epsilon_0 r} e^{-k_{TF} r} \text{ (also known as the Yukawa potential in nuclear physics).}$$

The interaction is still  $1/r$  at small distances, but is exponentially suppressed on the scale of  $1/k_{TF}$  and beyond. This is the result of "screening", the metal re-distributes charge in such a way as to "hide" the externally-imposed charge, as best as possible.

For the case of Al, one can plug in the numbers and find that  $\lambda_{TF} = 1/k_{TF} = 0.5$  Angstroms, about the Bohr radius of the Hydrogen atom! This very short length scale is of atomic dimensions, calling in to question whether the calculation is valid in this limit. Nevertheless it shows that the electronic screening length in metals is quite short.

Calculations by Mott using this potential are able to account for the residual resistivity of Cu (valence 1) alloyed with impurities of Zn (valence 2), Ga (valence 3), Ge (valence 4), and As (valence 5). Note that even with static screening the interaction of two electrons is still entirely repulsive.

#### D. Dynamic Screening in a Solid

The key physics is that the electrons move quickly ( $v_F = 2 \times 10^6$  m/s) and the ions move slowly (sound speed is  $10^3$  to  $10^4$  m/s). Thus the electrons are able to screen out externally imposed charge on the time scale of the inverse electron plasma frequency  $1/\omega_{p,e} \sim 10^{-16}$  s, whereas the lattice responds on much longer time scales. Here the electron plasma frequency is defined as  $\omega_{p,e}^2 \equiv \frac{n_0 z^2 e^2}{\epsilon_0 m_e}$ , where  $n_0$  is the atom number density,  $z$  is the valence of the atoms, and  $m_e$  is the electron mass. The plasma frequency is the maximum "sloshing frequency" of the electron gas in the metal. Likewise one can treat the ions as a charged fluid and define an ion plasma frequency as  $\omega_{p,i}^2 \equiv \frac{n_0 z^2 e^2}{\epsilon_0 M}$ , where  $M$  is the ion mass. This turns out to be a much lower frequency scale, typically  $f_{pi} = \frac{\omega_{p,i}}{2\pi} \sim 10^{13}$  Hz.

We will transform the Maxwell constitutive relations into momentum space:  $qE(q) = \frac{\rho_{Total}(q)}{\epsilon_0}$ , and  $qD(q) = \rho_{ext}(q)$ , so that  $\epsilon(q, \omega) = \frac{D(q)}{\epsilon_0 E(q)} = \frac{\rho_{ext}(q)}{\rho_{Total}(q)} = \frac{\rho_{ext}(q)}{\rho_i(q) + \rho_e(q) + \rho_{ext}(q)}$ .

Thus the dynamically screened Coulomb interaction is assumed to be given by,

$$V(q, \omega) = \frac{e^2/\epsilon_0}{\epsilon(q, \omega)q^2}.$$

Once again imagine imposing an external charge that is modulated in both time and space ( $\rho_{ext} \sim \rho_0 e^{i(\vec{q}\cdot\vec{r} - \omega t)}$ ). Treating the ion lattice as a fluid (the 'Jellium model') that responds to this external perturbation (see Kittel, Ashcroft and Mermin, or deGennes) yields

$$\epsilon(q, \omega) = 1 - \frac{\omega_{p,i}^2}{\omega^2} + \frac{k_{TF}^2}{q^2}.$$

Note that this expression only works in a limited range of frequency and is incorrect in the  $\omega \rightarrow 0$  limit (where it ignores the ion-ion repulsion), and the  $\omega \rightarrow \infty$  limit where it ignores the electron screening.

The dielectric function can also be written over a common denominator as

$$\epsilon(q, \omega) = \frac{\omega^2 q^2 - \omega_{p,i}^2 q^2 + k_{TF}^2 \omega^2}{\omega^2 q^2}.$$

The dynamically screened Coulomb interaction for a dynamic perturbation at  $(q, \omega)$  is,

$$V(q, \omega) = \frac{e^2/\epsilon_0}{q^2 + k_{TF}^2 - \frac{\omega_{p,i}^2}{\omega^2} q^2}$$

In a solid there is a naturally occurring (spontaneous) charge perturbation at a specific frequency and wavenumber. This collective excitation of the ions and electrons corresponds to a situation where no external charge is imposed ( $\rho_{ext} = 0$ ), and corresponds to the zero of the dielectric function written above (recall that  $\epsilon(q, \omega) = \frac{\rho_{ext}(q)}{\rho_{Total}(q)}$ ). Using the expression for  $\epsilon(q, \omega)$  in the previous paragraph, this leads to a collective mode dispersion relation of  $\omega_q = \omega_{p,i} \frac{q}{\sqrt{q^2 + k_{TF}^2}}$ , where  $\omega_q$  is the frequency of this longitudinal acoustic phonon mode. This expression shows that the phonon has a linear dispersion  $\omega_q \sim \omega_{p,i} \frac{q}{k_{TF}}$  at small  $q$  on the scale of the Brillouin zone edge and below (since  $k_{TF} \gg k_{BZ}$  typically). The pre-factor of  $q$  can be compared to the speed of sound in the metal. For Al this predicts a sound speed of 9000 m/s, whereas it is measured to be about 6400 m/s at room temperature.

Using the phonon mode frequency in place the ion plasma frequency (i.e. substituting  $\omega_{p,i}^2 = \frac{\omega_q^2}{q^2} (q^2 + k_{TF}^2)$ ), the electron-phonon pairing interaction can now be written as,

$$V(q, \omega) = \frac{e^2/\epsilon_0}{q^2 + k_{TF}^2} \left[ 1 + \frac{\omega_q^2}{\omega^2 - \omega_q^2} \right] = V_{TF, Coulomb}(q) + V_{el-ph}(q, \omega)$$

Note that the first term is purely repulsive, while the second term can be attractive, and both are on the same order of magnitude. Clearly for  $\omega < \omega_q$  this interaction is attractive, and resembles to some extent the simple attractive interaction introduced by Cooper. (Also note that  $\omega_q < \omega_{p,i}$ .)

Now we re-interpret this  $V(q, \omega)$  as the pairing interaction in the context of the Cooper pairing scenario (see Ashcroft and Mermin, *Solid State Physics*, pages 518-519). First we recall that  $\vec{q} = \vec{k} - \vec{k}'$ , the momentum transfer when a pair scatters from states labeled by  $(\vec{k}, -\vec{k})$  to states labeled by  $(\vec{k}', -\vec{k}')$ . In general, these two single-particle states  $\vec{k}$  and  $\vec{k}'$  can have different energy. We can interpret  $\hbar\omega$  as the energy difference between the two states:  $\omega = \frac{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}}{\hbar}$ . Some comments. First, since the phonon energy is limited by the **Debye frequency**  $\Omega_D$ , hence the two sets of states involved in the scattering process must have an energy difference less than this to enjoy the attractive interaction. The second comment is that the large negative interaction energy arises from '**overscreening**' of the electron-electron interaction, as mediated by the ions/phonons. Thus literally means that the combined ion and electron screening overdoes it, and actually enhances the effective size of the externally imposed charge! Keep in mind that this is a dynamical (finite frequency) effect, not a static effect.