

Lecture 7 Summary

PHYS798S Spring 2016

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Microscopic Origin of the Pairing Interaction

0.1 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.

0.2 Two-Electron Interaction in Free Space

Two electrons interact by means of the bare Coulomb interaction: $V(r) = k_e e^2 / r$ where $k_e = 1/4\pi\epsilon_0$. 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, which is a purely repulsive interaction, as expected.

0.3 Two-Electron Static Interaction in a Solid

The 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 electron and calculate its potential everywhere in the solid.

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 ϵ 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.

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,

$$V(q) = \frac{e^2}{\epsilon_0 \epsilon(q) q^2}, \text{ with } \epsilon(q) = 1 + \frac{k_{TF}^2}{q^2}. \text{ Here } k_{TF} \text{ is the Thomas-Fermi screening}$$

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:

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

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.

0.4 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 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 10^{13} Hz.

Thus the dynamic 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. Treating the ion lattice as a fluid 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 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, ω) 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 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, and corresponds to the zero of the dielectric function written above. This leads to a collective mode dispersion relation of $\omega_q = \omega_{p,i} \frac{q}{\sqrt{q^2 + k_{TF}^2}}$, where ω_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, 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.

Taking the Fourier transform of this interaction in to the time domain yields,

$$V(q, t) \propto \frac{e^2/\epsilon_0}{q^2 + k_{TF}^2} \{ \delta(t) - \pi \sin(\omega_q t) \}.$$

This reveals that the two electrons will encounter a strong repulsive interaction if they come to the same location at the same time, but they will enjoy an attractive interaction if one arrives after the other, on the scale of the phonon vibration period. The picture is that the first electron travels through the lattice and leaves behind a time-delayed polarization of the slowly-moving ion lattice. The second electron comes along later, moving in the opposite direction, and enjoys an attractive interaction to the ion concentration. This retarded interaction is the key to avoiding the strong bare electron-electron repulsion.

0.5 Pairing Interaction in Cuprates

The cuprate pairing interaction is electronic in nature, involving only the electron system. Antiferromagnetic spin fluctuations lead to an entirely repulsive interaction. However when it is Fourier transformed into real space, there are attractive pieces at finite separation of the two electrons, leading to a finite

angular momentum "d-wave" pairing state.

0.6 Consequences of the electron-phonon pairing interaction

Going back to the Cooper pairing calculation, we proposed that the T_c of the superconductor is proportional to the binding energy of the Cooper pair: $k_B T_c \sim 2\hbar\omega_c e^{-2/D(E_F)V}$. We now see that Cooper's cutoff energy is in fact the phonon energy $\hbar\omega_q$. The phonon frequency in turn is related to the vibrational frequency of the ions, which scales as $\omega_q \sim \sqrt{k/M}$, where k is some measure of the restoring force and M is the average ion mass. Hence there is an expectation that as the isotope ratio of a superconducting metal changes, one should have $T_c M^\alpha = \text{constant}$, where the simplest expectation is that the "isotope effect exponent" $\alpha = 0.5$. Many experiments have been done to measure the "isotope effect" on T_c in "conventional" elemental superconductors, and they are generally consistent with this dependence. This is considered one piece of "smoking gun evidence" in support of the electron-phonon pairing mechanism (we will see even more compelling evidence later). s-p-bonded metals such as Pb and Hg have $\alpha = 0.5$ to good approximation. d-electron metals generally show smaller values of α , all the way down to zero. Those metals are thought to have strong Coulomb repulsion, which appears at frequency scales above the phonon frequency. A model that incorporates this effect successfully predicts a decrease in α , as shown on the Supplementary Materials part of the class web site.

Finally, the absence of the superconductivity in Cu, Ag, and Au is presumably due to their small values of electron-phonon coupling.