Lecture 5 Summary

PHYS798S Spring 2016

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The Cooper pairing problem

0.1 Review of Free Electron Fermi Gas Model of a Metal

Metals are made up of positively charged ions and the "free" electrons (meaning that they are not localized to the ions, but can go anywhere in the metal)
The electrons are assumed to not interact with each other or with the ions, except through the Pauli exclusion principle
We solved the single-particle Schrodinger equation for a free particle in a box of size $L \times L \times L$ obeying perioidic boundary conditions: $\psi(x+L, y, z) = \psi(x, y, z)$
The solutions are plane (running) waves: $\psi \sim \frac{1}{\sqrt{V}} e^{i \vec{k} \cdot \vec{r}}$, with $\vec{k} = \{k_x, k_y, k_z\}$
$V = L^3$ is the volume of the metal box
The eigen-energies are $E = \hbar^2 k^2 / 2m$
The solutions are also eigenfunctions of the linear momentum operator, with eigenvalue $\hbar \vec{k}$
The periodic boundary conditions force the momenta to be discrete and labeled by three integers which can be positive, negative, or zero
No two identical electrons with overlapping wavefunctions can occupy the same exact quantum state (i.e. the same exact list of eigenvalues)
All states are filled starting at $E = 0$, and then up to the last occupied state at the Fermi energy $E_F = \hbar^2 k_F^2 / 2m$. The collection of filled states is called the Fermi sea. In this simple free-electron model the surface of filled states is a sphere in momentum space (aka reciprocal space or k-space).
Typical Fermi energies for metals are on the scale of 1 to 10 eV
The density of electronic states for free electrons in a 3D metal $D(E) \sim E^{1/2}$
The density of electronic states can be determined from measurements of the electronic specific heat at low temperatures $C_{el} = \gamma T$, where $\gamma = \frac{\pi^2}{3} D(E_F) k_B^2$
In Al the density of states at the Fermi energy is about 0.57 states/atom/eV

0.2 Cooper's Calculation

Consider a metal at zero temperature with all of the electrons in the ground state occupying all states within the Fermi sphere, and no states occupied outside.

Now add two electrons to states outside the Fermi sphere. They do not interact with the electrons in the Fermi sea except through the Pauli exclusion principle - they cannot occupy any states inside the sphere in momentum space. The two electrons can interact with each other.
The objective now is to write down an ansatz for the two-electron wavefunction, put it in to the Schrodinger equation, and solve for the eigen-energy. If the ground state energy is less than $2E_F$ then a bound state of the two electrons is formed, and we are a step closer to a microscopic understanding of superconductivity.

We take the two-particle wavefunction to be of the form $\Psi(1,2) \sim \psi(\overrightarrow{r}_1 - \overrightarrow{r}_2)\, e^{i\overrightarrow{Q}\cdot\overrightarrow{R}} \chi(\sigma_1, \sigma_2)$, where ψ is the relative coordinate ($\overrightarrow{r} = \overrightarrow{r_1} - \overrightarrow{r_2}$) wavefunction, $\overrightarrow{R}$ and $\overrightarrow{Q}$ are the center of mass position and momentum, respectively and χ is the two-electron spinor wavefunction.

In the ground state we expect the center of mass momentum to be zero $\overrightarrow{Q} = 0$. This means that the two electrons have equal and opposite momenta $\hbar\overrightarrow{k}$ and $-\hbar\overrightarrow{k}$. The two-particle wavefunction Ψ must be anti-symmetric upon exchange of all the labels of the two particles. One way to accomplish this is to have a symmetric relative wavefunction $\psi \sim \cos(\overrightarrow{k}\cdot\overrightarrow{r})$ where $\overrightarrow{r} = \overrightarrow{r}_1 - \overrightarrow{r}_2$ is the relative coordinate, times an anti-symmetric spinor, namely the spin-singlet $|00\rangle$. The other option is to have an anti-symmetric relative wavefunction $\psi \sim \sin(\overrightarrow{k}\cdot\overrightarrow{r})$ times a symmetric spinor, namely the spin-triplet set of states $|11\rangle$, $|10\rangle$ and $|1-1\rangle$. Because we anticipate there will be an attractive interaction, we choose the symmetric space wavefunction since this brings the two particles closer together. Finally, the general ansatz is a sum over all possible states $(\overrightarrow{k}, -\overrightarrow{k})$ outside the filled Fermi sphere, weighted by a $\overrightarrow{k}$-dependent factor $g_{\overrightarrow{k}}$: $\Psi(1,2) = \sum_{k>k_F} g_{\overrightarrow{k}} \cos\left(\overrightarrow{k}\cdot\overrightarrow{r}\right)|00\rangle$.

0.3 Two-particle Schodinger Equation

Substituting the anstaz wavefunction in to the 2-electron Schrodinger equation, multiplying through by $e^{-i\overrightarrow{k'}\cdot\overrightarrow{r}}$ and integrating over all space yields the following result.
$(E - 2\varepsilon_k)\, g_{\overrightarrow{k}} = \sum_{\overrightarrow{k}'} g_{\overrightarrow{k}'} V_{\overrightarrow{k},\overrightarrow{k}'}$
where $\varepsilon_k \equiv \hbar^2 k^2/2m$ and we have defined the Fourier transform of the pairing interaction,
$V_{\overrightarrow{k},\overrightarrow{k}'} = \int_{Volume} d^3r V(\overrightarrow{r}) e^{i\left(\overrightarrow{k}-\overrightarrow{k}'\right)\cdot\overrightarrow{r}}$.
$V_{\overrightarrow{k},\overrightarrow{k}'}$ characterizes the strength of the potential for scattering a pair of electrons with momentum $(\overrightarrow{k}, -\overrightarrow{k})$ to momentum $(\overrightarrow{k'}, -\overrightarrow{k'})$. If we can find a set of g_k with $E < 2E_F$ then a bound pair exists.
Cooper introduced a simplified potential,

$V_{\vec{k},\vec{k'}} = \begin{cases} -V & E < \hbar\omega_c \\ 0 & E > \hbar\omega_c \end{cases}$
where energy is measured relative to the Fermi energy, $V > 0$, and $\hbar\omega_c$ is the energy scale of the pairing interaction. We shall see that for "conventional" superconductors the ion lattice vibrations will set this energy scale, and it is about 10 meV in a metal like Pb. This pairing interaction will be studied in detail in the next lecture. Using this potential, the Schrodinger equation now becomes,
$g_{\vec{k}} = \frac{V \sum_{\vec{k_F} < \vec{k}\,' < \vec{k_c}} g_{\vec{k}}}{2\varepsilon_k - E}$. Note the restricted sum on k'.
Summing both sides on k, cancelling the sums on k' of $g_{k'}$, one arrives at,
$\frac{1}{V} = \sum_{\vec{k_F} < \vec{k}\,' < \vec{k_c}} \frac{1}{2\varepsilon_k - E}$
We can replace the sum on k by an integral on energy through use of the density of states, $D(\varepsilon)$ with $\varepsilon = \hbar^2 k^2/2m$,
$\frac{1}{V} = \int_{E_F}^{E_F + \hbar\omega_c} \frac{D(\varepsilon)d\varepsilon}{2\varepsilon - E}$.
Since $\hbar\omega_c << E_F$ we can take the density of states to be constant and equal to that at the Fermi energy, $D(E_F)$. The integral is now straightforward and one finds (excercise for the reader!) that the energy eignevalue is,
$E = 2E_F + \frac{2\hbar\omega_c}{1 - e^{2/D(E_F)V}}$.
At first glance it appears that $E > 2E_F$, but examine the exponential with the dimensionless quantity $D(E_F)V$ more closely. If we take the "weak coupling approximation" and assume that $D(E_F)V << 1$, then the eigenenergy can be written to good approximation as,
$E \simeq 2E_F - 2\hbar\omega_c e^{-2/D(E_F)V}$, which is less than $2E_F$, showing that a bound state, a Cooper pair, is formed.
Note that the binding energy is non-analytic in the small parameter, meaning that this result cannot be derived by ordinary perturbation theory, accounting for the many failures to produce a theory of superconductivity before BCS.

0.4 Binding Energy Systematics

The binding energy depends on the energy scale of the ion vibrations $\hbar\omega_c$ as well as the strength of the pairing interaction V and the density of states (DOS) at the Fermi energy $D(E_F)$. Let's examine these dependencies, assuming that the superconducting transition temperature scales with the binding energy of the Cooper pair, i.e. $k_B T_c \sim 2\hbar\omega_c e^{-2/D(E_F)V}$.