Lecture 11 Summary

PHYS798S Spring 2016

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The BCS Ground State

0.1 Self-Consistent Gap Equation - Continued

Last time we derived the celebrated self-consistent gap equation:
$\Delta_k = -\frac{1}{2}\sum_l \frac{\Delta_l}{\sqrt{\Delta_l^2+\xi_l^2}} V_{k,l}$,
and we examined the solution with $\Delta = 0$. Now look for a non-trivial solution.

Put in the Cooper pairing potential as,
$V_{k,l} = \begin{cases} -V & |\xi_k|, |\xi_l| \leqslant \hbar\omega_c \\ 0 & |\xi_k|, |\xi_l| > \hbar\omega_c \end{cases}$
with V a positive number. This creates an attractive pairing interaction within a "skin" of thickness $\hbar\omega_c$ around the Fermi energy. It is a bit more democratic now, not just pertaining to a chosen pair of electrons, but acting on all electrons near the chemical potential.

With this, the self-consistent gap equation becomes,
$\Delta_k = +\frac{V}{2}\sum_l^{Restricted} \frac{\Delta_l}{\sqrt{\Delta_l^2+\xi_l^2}}$, where the sum is now restricted to those values of k and l that give non-zero pairing interaction.
Since the right-hand side is independent of k, it must be that $\Delta_k = \Delta_l = \Delta$, independent of k. This is a consequence of the simple proposed pairing interaction. Hence we have
$1 = +\frac{V}{2}\sum_l^{Restricted} \frac{1}{\sqrt{\Delta_l^2+\xi_l^2}}$

Converting from a sum on l to an integral on energy brings in the density of states $D(E)$ and allows us to solve for Δ in closed form:
$\Delta = \frac{\hbar\omega_c}{\sinh(1/D(E_F)V)}$
Once again, if we take the "weak coupling" approximation $D(E_F)V << 1$, this yields, $\Delta \approx 2\hbar\omega_c e^{-1/D(E_F)V}$, a result very similar to the Cooper result for T_c. In fact it will turn out that BCS predicts a universal value for the ratio $\Delta/k_B T_c$.

Going back to the u's and v's, we now have two equations and expressions for everything inside them: $v_k^2 - u_k^2 = -\frac{\xi_k}{E_k}$, and $u_k^2 + v_k^2 = 1$.
These can be solved uniquely for u_k^2 and v_k^2:

$v_k^2 = \frac{1}{2}\left[1 - \frac{\epsilon_k - \mu}{\sqrt{\Delta^2 + (\epsilon_k - \mu)^2}}\right]$, and
$u_k^2 = 1 - v_k^2 = \frac{1}{2}\left[1 + \frac{\epsilon_k - \mu}{\sqrt{\Delta^2 + (\epsilon_k - \mu)^2}}\right]$.
These expressions give us the occupation probability for the Cooper pairs as a function of k, or energy. See the plot on the Supplementary Information part of the class web site. The Cooper pair occupation probability is very close to the smeared Fermi function for single particle state occupation probability at T_c, which is a surprising result, given that we are calculating a zero-temperature property of the superconductor! In fact the superconductor makes an interesting gambit: it promotes many electrons from states inside the filled Fermi sea to un-occupied states outside specifically to "activate" the pairing interaction and create an overall decrease of the energy of the superconductor relative to the normal metal state.

0.2 Energetics of the Superconducting Ground State

Now that we have explicit expressions for the u's and v's, we can evaluate the ground state expectation value of the Landau potential,
$\langle\Psi_{BCS}| H - \mu N_{op} |\Psi_{BCS}\rangle = 2\sum_l \xi_k v_k^2 + \sum_{k,l} V_{k,l} u_k v_k u_l v_l$.
Also recall the definition of the energy gap, now in terms of the u's and v's: $\Delta_k = -\sum_l V_{k,l} u_l v_l$.
Putting in the expressions for the u's and v's yields,
$\langle\Psi_{BCS}| H - \mu N_{op} |\Psi_{BCS}\rangle_S = \sum_k \left(\xi_k - \frac{\xi_k^2}{E_k}\right) - \Delta^2/V$, for the superconducting state, and
$\langle\Psi_{BCS}| H - \mu N_{op} |\Psi_{BCS}\rangle_N = \sum_{k<k_F} 2\xi_k$ for the normal state at T = 0.

Taking the difference in expectation values and converting from sums to integrals on energy yields,
$\langle\Psi_{BCS}| H - \mu N_{op} |\Psi_{BCS}\rangle_S - \langle\Psi_{BCS}| H - \mu N_{op} |\Psi_{BCS}\rangle_N = \left(\frac{\Delta^2}{V} - \frac{1}{2}D(0)\Delta^2\right) - \frac{\Delta^2}{V}$. The term in (...) is the increase in kinetic energy, while the second term is the change in potential energy. The superconductor pays a large energy cost to "smear" the electron distribution (at T = 0!) and move electrons from states inside the Fermi sea to un-occupied states outside. This allows the product $u_k v_k$ to become non-zero around the chemical potential (as shown in the slide in the Supplementary material) and create a negative pairing interaction and a non-zero "energy gap" Δ.

The Condensation Energy of the superconducting state is thus:
$U_S(T=0) - U_N(T=0) = -\frac{1}{2}D(E_F)\Delta^2(0)$.
Note that in the BCS weak coupling approximation this energy gain is much smaller than the kinetic energy investment, on the order of 10 %.

We can represent the condensation energy in terms of a thermodynamic critical field H_c as: $\frac{\mu_0}{2}H_c^2(0) = \frac{1}{2}D(E_F)\Delta^2(0)$. This will be generalized to non-zero temperature later.

0.3 Superconductivity as a Coherent State of Cooper Pairs

The pairing interaction is always present. In particular it is present above T_c. Why does it not make a contribution to the energy of a metal in the normal state?
1) At $T = 0$ we saw that the ground state of a "normal metal" is to fill all states in the Fermi sea such that the product $u_k v_k = 0$ for all k. This leads to zero energy gap and no contribution to the energy from $V_{k,l}$.

2) At $T > 0$ there is a smeared Fermi distribution, creating non-zero values for $u_k v_k$ around the Fermi energy. However, the complex nature of the u's and v's plays a role. Write the energy gap as $\Delta_k = -\sum_l V_{k,l} u_l |v_l| e^{i\phi_l}$. In the superconducting state the wavefunction is a coherent state in which each term in this sum has the same phase $\phi_l = \phi$, allowing the terms to add coherently and produce a non-zero Δ. This phase ϕ is in fact the phase of the macroscopic quantum wavefunction that describes the superconductor. In the normal state these phases are random, leading to an incoherent sum and no Δ^2/V contributions to the energy.

0.4 Finite Temperature BCS

We now explore the properties of BCS theory at finite temperature. This will lead to quasi-particle excitations out of the ground state. This calculation also serves as an independent way to determine the ground state properties of the BCS Hamiltonian, so you soon see some "old friends" from the previous calculation!
Start with the BCS pairing Hamiltonian:
$H - \mu N_{op} = \sum_{k,\sigma} \xi_k c^+_{k,\sigma} c_{k,\sigma} + \sum_{k,l} V_{k,l} c^+_{k,\uparrow} c^+_{-k,\downarrow} c_{-l,\downarrow} c_{l,\uparrow}$.
The kinetic energy term is nice - it is diagonal. The potential energy term is quartic and involves 4 different states - it is not diagonal. We will now go through a 2-step process to diagonalize this Hamiltonian, and in the process create operators that destroy Cooper pairs (more precisely they prevent the occupation of a particular Cooper pair) and create quasi-particle excitations. These are the most elementary excitations out of the BCS ground state, and will play a major role in the perturbation theory of the BCS Hamiltonian.

In the first step, break the quartic term into a product of two new operators. Define $b_k = \langle c_{-k,\downarrow} c_{k,\uparrow} \rangle$, where the expectation value is with the superconducting wavefunction. Because the BCS wavefunction is a coherent superposition of systems with all possible numbers of Cooper pairs, this expectation value for the Cooper pair destruction operator will be non-zero in general.
Likewise define the adjoint operator as $b^+_k = \left\langle c^+_{k,\uparrow} c^+_{-k,\downarrow} \right\rangle$.

Now write the bare destruction operators from the quartic term as a "mean" part (namely b_k) and a "fluctuating" part, namely everything else, as,
$c_{-l,\downarrow}c_{l,\uparrow} = b_l + (c_{-l,\downarrow}c_{l,\uparrow} - b_l)$.
Substitute this and the adjoint version in to the Hamiltonian and ignore second order "fluctuating" terms to arrive at the "BCS Model Hamiltonian":
$H_M - \mu N_{op} = \sum_{k,\sigma} \xi_k c^+_{k,\sigma} c_{k,\sigma} + \sum_{k,l} V_{k,l} \left[c^+_{k,\uparrow} c^+_{-k,\downarrow} b_l + b^+_k c_{-l,\downarrow} c_{l,\uparrow} - b^+_k b_l \right]$, where the b_k will be determined self-consistently.
Now define a new quantity (remember that this is an independent calculation) that will soon be interpreted as an "energy gap":
$\Delta_k \equiv -\sum_l V_{k,l} b_l$.
With this definition, the model Hamiltonian can be written as ,
$H_M - \mu N_{op} = \sum_{k,\sigma} \xi_k c^+_{k,\sigma} c_{k,\sigma} - \sum_k \left(c^+_{k,\uparrow} c^+_{-k,\downarrow} \Delta_k + \Delta^*_k c_{-k,\downarrow} c_{k,\uparrow} - b^+_k \Delta_k \right)$.
Now the Hamiltonian is bi-linear in the c's, so we can take the next step to diagonalize the Hamiltonian.

In the second step we shall carry out the Bogoliubov-Valatin transformation to a new set of operators that will create quasi-particle excitations. This transformation will diagonalize the model Hamiltonian.
$c_{k,\uparrow} = u^*_k \gamma_{k0} + v_k \gamma^+_{k1}$
$c^+_{-k,\downarrow} = -v^*_k \gamma_{k0} + u_k \gamma^+_{k1}$
where the u's and v's are just parameters of this transformation (for the moment) with the constraint $|u_k|^2 + |v_k|^2 = 1$ to make the transformation unitary.

The inverse transformation is;
$\gamma^+_{k0} = u^*_k c^+_{k,\uparrow} - v^*_k c_{-k,\downarrow}$ and,
$\gamma^+_{k1} = u^*_k c^+_{-k,\downarrow} + v^*_k c_{k,\uparrow}$.
One can see that the γ^+_{k0} operator decreases momentum by k and spin by $\hbar/2$ with probability $|u_k|^2 + |v_k|^2 = 1$, using what we anticipate will be the interpretation of $|u_k|^2$ and $|v_k|^2$. Likewise, the operator γ^+_{k1} increases momentum by k and spin by $\hbar/2$ with probability 1. As such, these operators create Fermionic excitations which will come to be known as Bogoliubons or Quasi-Particles. In fact, one can show,
$\gamma_{k0} |\Psi_{BCS}\rangle = 0$, and $\gamma_{k1} |\Psi_{BCS}\rangle = 0$, showing that the BCS ground state wavefunction is the vacuum state for quasi-particles.

0.5 Meanwhile, Back at the Hamiltonian

With the substitution of the transformed operators, the model Hamiltonian becomes,
$H_M - \mu N_{op} = \sum_k$ (nice terms involving diagonal operators) + (undesired cross terms)$\left(2\xi_k u_k v_k + \Delta^*_k v^2_k - \Delta_k u^2_k\right)$.