PHYS 798C Spring 2024
Lecture 10 Summary

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I. THE BCS GROUND STATE

A. 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,
$\langle\Psi_{BCS}| H - \mu N_{op} |\Psi_{BCS}\rangle = 2\sum_k \xi_k v_k^2 + \sum_{k,l} V_{k,l} u_k v_k u_l v_l$.
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 out" the Cooper pair distribution (at $T = 0$!) and move Cooper pairs 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: $\frac{\mu_0}{2}H_c^2(0) = \frac{1}{2}N(E_F)\Delta^2(0)$. Here we are using $N(E_F)$ to represent the density of states per unit energy and per unit volume. This result for the critical field will be generalized to non-zero temperature later.

B. 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 inside the Fermi sea, and leave all states outside empty, 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, $\Delta = 0$, and no Δ^2/V contributions to the energy.

II. 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 will 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 operations on 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 taken with the superconducting wavefunction that will ultimately result from this calculation. 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. The expectation value in b_k will be zero in the normal state because of the incoherent nature of the wavefunction. (Recall from the harmonic oscillator case that the coherent state wavefunction is the eigenfunction of the lowering operator.) This definition of b_k is in the spirit of mean field theory, in which the expectation value $\langle c_{-k,\downarrow} c_{k,\uparrow} \rangle$, and the energy gap, will be determined self consistently.
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,
$c_{-l,\downarrow} c_{l,\uparrow} = b_l + (c_{-l,\downarrow} c_{l,\uparrow} - b_l)$.
This separation into "mean" and "fluctuating" parts is again in the spirit of mean field theory.
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 once we find the wavefunction.
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 $\gamma_{k0} = u_k c_{k,\uparrow} - v_k c_{-k,\downarrow}^+$ 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. (Note that these operators involve creating particles and holes in different linear combinations.) 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.

A. 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) $\left[2\xi_k u_k v_k + \Delta_k^* v_k^2 - \Delta_k u_k^2\right]$.
We can eliminate all of the ugly terms in the transformed Hamiltonian by making a second constraint on the u's and v's, namely to make the bracket term [...] in the model Hamiltonian equal to zero. That leads to a quadratic equation for the quantity $\Delta_k^* v_k/u_k$ whose solution yields $\Delta_k^* v_k/u_k = E_k - \xi_k$, which is real. Here again we have $E_k = \sqrt{\Delta_k^2 + \xi_k^2}$. If we take the convention that u_k is real (as in the previous calculation), then it must be that v_k and Δ have the same phase. This phase factor is the same for all k and endows the energy gap with the macroscopic quantum phase factor in the superconducting state. With the two constraints on the u's and v's, we can now solve for them in terms of known quantities, and the result is
$v_k^2 = \frac{1}{2}\left[1 - \frac{\epsilon_k - \mu}{\sqrt{\Delta^2 + (\epsilon_k - \mu)^2}}\right]$, and
$u_k^2 = 1 - v_k^2 = \frac{1}{2}\left[1 + \frac{\epsilon_k - \mu}{\sqrt{\Delta^2 + (\epsilon_k - \mu)^2}}\right]$,
exactly as before in the zero-temperature variational calculation!

The resulting diagonalized Hamiltonian is,
$H_M - \mu N_{op} = \sum_k (\xi_k - E_k + \Delta_k b_k^*) + \sum_k E_k \left(\gamma_{k0}^+ \gamma_{k0} + \gamma_{k1}^+ \gamma_{k1}\right)$.
The first sum reproduces the ground state BCS energy. The second sum represents excitations out of the ground state. It counts excitations of energy E_k through the $\gamma^+\gamma$ number operators.
These excitations are gapped by Δ, and as such are very rarely created at low temperatures when $k_B T << \Delta$. Note that there is a gap in the *energy* spectrum of these excitations, but no gap in the *momentum*. The excitations are called **Bogoliubons** or **quasi-particles**.