PHYS 798C Fall 2025
Lecture 9 Summary

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I. THE BCS VARIATIONAL CALCULATION

A. Expectation values

We first evaluated the expectation value $\langle\Psi_{BCS}| H - \mu N_{op} |\Psi_{BCS}\rangle$ for the kinetic energy and the potential energy using the properties of the creation and annihilation operators. The result is
$\langle\Psi_{BCS}| H - \mu N_{op} |\Psi_{BCS}\rangle = 2\sum_k \xi_k |v_k|^2 + \sum_{k,l} V_{k,l} u_k v_k^* u_l^* v_l$.
The kinetic energy is the sum over all k-states of the single-particle energies times the probability that the Cooper pair at that momentum state is occupied, times 2 for the two electrons that make up the Cooper pair. The potential energy is constrained by matrix elements. Initially the Cooper pair at $(l, -l)$ must be occupied while that at $(k, -k)$ must be empty. In the final state the pair at $(k, -k)$ must be filled while that at $(l, -l)$ is left empty. This brings in the four factors of u's and v's. A more detailed derivation is given in Annett, problem 6.2 (solutions in the back of the book).

B. The Variational Calculation

The actual calculation is quite simple and elegant. Assume for now that the u's and v's are real. This is OK because it assumes for the moment that the macroscopic phase of the coherent state Cooper pair WF is fixed at zero. Given the constraint that $|u_k|^2 + |v_k|^2 = 1$, one has just a single parameter, namely the angle θ_k to keep track of, such that $u_k = \sin(\theta_k)$ and $v_k = \cos(\theta_k)$.
The terms in the expectation value can now be written using double angle formulas as $v_k^2 = \cos^2(\theta_k) = \frac{1}{2}(1 + \cos(2\theta_k))$, and $u_k v_k u_l v_l = \frac{1}{2}\sin(2\theta_k)\frac{1}{2}\sin(2\theta_l)$.
The expectation value is now

$$\langle\Psi_{BCS}| H - \mu N_{op} |\Psi_{BCS}\rangle = \sum_{k=k_1}^{k_M} \xi_k(1 + \cos(2\theta_k)) + \frac{1}{4}\sum_{k,l}^{k_M,l_M} V_{k,l}\sin(2\theta_k)\sin(2\theta_l) \tag{1}$$

Taking the derivative with respect to $\theta_{k'}$ (i.e. $\frac{\partial}{\partial\theta_{k'}}\langle\Psi_{BCS}| H - \mu N_{op} |\Psi_{BCS}\rangle$) yields the following result, $\tan(2\theta_k) = \frac{1}{2\xi_k}\sum_l V_{k,l}\sin(2\theta_l)$.

C. Definition of the Energy Gap and Quasiparticle Energy

Make the following two definitions:
$\Delta_k \equiv -\sum_l V_{k,l} u_l v_l = -\frac{1}{2}\sum_l V_{k,l}\sin(2\theta_l)$, which defines the "energy gap" of the superconductor. This will turn out to be the gap in the single-particle excitation spectrum out of the BCS ground state. It can also serve informally as a rough "order parameter" of the superconducting state, although this is not a rigorous definition of a superconducting order parameter. Where does this entity come from? Basically it is the expectation value of the Cooper pair destruction operator, $\Delta \sim \sum_k \langle c_{-k,\downarrow} c_{k,\uparrow}\rangle$. Recall from the coherent state of a harmonic oscillator that $|\alpha\rangle$ is the eigenfunction of the lowering operator: $a_- |\alpha\rangle = \alpha |\alpha\rangle$. The Cooper pair destruction operator P_k plays a similar role here, with the BCS ground state acting as a coherent state of Cooper pairs. The energy gap is some measure of how many Cooper pairs there are in the coherent state.
$E_k \equiv \sqrt{\Delta_k^2 + \xi_k^2}$ is the quasiparticle energy. Note that the minimum energy of a quasiparticle excitation (discussed later) is the energy gap, $E_k \geq \Delta$.
With these definitions, the variational equation can now be written as,
$\tan(2\theta_k) = -\frac{\Delta_k}{\xi_k}$.

With some further trigonometric gamesmanship, one can write the u's and v's in terms of these newly defined quantities:
$\sin(2\theta_k) = 2u_k v_k = +\frac{\Delta_k}{E_k}$

and, $\cos(2\theta_k) = v_k^2 - u_k^2 = -\frac{\xi_k}{E_k}$

D. Self-Consistent Gap Equation

Now use the above expression for the product of $u_k v_k$ back in the definition of the energy gap to obtain the celebrated **self-consistent gap equation**:
$\Delta_k = -\frac{1}{2}\sum_l \frac{\Delta_l}{\sqrt{\Delta_l^2+\xi_l^2}} V_{k,l}$.
In general this can be challenging to solve, but we will consider two simple cases here.

1. Self-Consistent Gap Equation for the Normal State

First look at the trivial solution $\Delta_k = 0$ for all k. Going back to the u's and v's, this means that $\sin(2\theta_k) = 2u_k v_k = 0$ for all k and,
$\cos(2\theta_k) = v_k^2 - u_k^2 = -\frac{\xi_k}{E_k} = \begin{cases} -1 & \xi_k > 0 \\ +1 & \xi_k < 0 \end{cases}$
This is a peculiar situation in which all Cooper states are occupied below $\xi = 0$ and all Cooper pair states are un-occupied above $\xi = 0$. In other words: $u_k = 1$ and $v_k = 0$ for $\xi_k > 0$, and $u_k = 0$ and $v_k = 1$ for $\xi_k < 0$. Roughly speaking this is like the state $|F\rangle$ that we introduced earlier, but it involves all electrons being bound in Cooper pairs with properly anti-symmetrized WFs inside the Fermi sphere, and all states outside un-occupied.
However, consider the potential energy term $\sum_{k,l} V_{k,l} u_k v_k u_l v_l$. This term is identically zero as it has zero contributions from all k because of the result that $2u_k v_k = 0$. Hence this "normal state" does not take advantage of the pairing interaction and is not a superconductor!
Next we will find a non-trivial solution to the self-consistent gap equation.

2. Self-Consistent Gap Equation for the Superconducting State

Take another look at the celebrated self-consistent gap equation:
$\Delta_k = -\frac{1}{2}\sum_l \frac{\Delta_l}{\sqrt{\Delta_l^2+\xi_l^2}} V_{k,l}$.
Now look for a non-trivial solution.
Put in the Cooper pairing potential approximation as,
$V_{k,l} = \begin{cases} -V & |\xi_k|, |\xi_l| \leqslant \hbar\omega_c \\ 0 & |\xi_k| \text{ and/or } |\xi_l| > \hbar\omega_c \end{cases}$
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.
Note that this choice of $V_{k,l}$ dictates that the energy gap will only exist over a limite energy range,
$\Delta_k = \begin{cases} \Delta & |\xi_k| < \hbar\omega_c \\ 0 & |\xi_k| > \hbar\omega_c \end{cases}$

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 and spherical Fermi surface. 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 from $-\hbar\omega_c$ to $+\hbar\omega_c$ 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 the binding energy of the Cooper pair. In fact it will turn out that BCS predicts a universal value for the ratio $\Delta/k_B T_c$ in the weak coupling approximation.

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 Cooper pairs from states inside the filled Fermi sea to un-occupied Cooper pair states outside specifically to "activate" the pairing interaction. This in turn creates an overall *decrease* of the energy of the superconductor relative to the normal metal state.