PHYS 798C Spring 2024
Lecture 8 Summary

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I. WRITING DOWN THE BCS GROUND STATE WAVEFUNCTION

A. How NOT to do it

We need to put N electrons into $M >> N$ available single-particle states in a way that incorporates Cooper pairing. All electrons have to be treated on an equal footing - no two can be treated differently from all the rest. There is an enormous number of ways to arrange the electrons into $N/2$ Cooper pairs in M states, of order $\binom{M}{N/2} \sim M^N$. Roughly, this number of possibilities is of order $10^{(10^{20})}$, a number too big to contemplate (see Tinkham, p.50).
Given this situation we will resort to a *statistical treatment* of the ground state WF.

B. Coherent States of the QM Harmonic Oscillator

It turns out that Schrieffer's ansatz for the BCS ground state WF is a Coherent State of Cooper pairs, although the explicit concept of such a state did not exist at the time!
The fact that the MQWF description of a superconductor (predicting fluxoid quantization and the Josephson effect) is so successful, motivates the search for a ground state WF with a well-defined macroscopic quantum phase. Quantum mechanical coherent states have this property.
Coherent states are also minimum uncertainty states, for the harmonic oscillator they have minimum uncertainty in the position-momentum phase space. The n^{th} harmonic oscillator state has $\langle \Delta x \rangle \langle \Delta p \rangle \sim n\hbar$, but a coherent state of n excitations has $\langle \Delta x \rangle \langle \Delta p \rangle \sim 1\hbar$.
We reviewed the properties of coherent states in the one-dimensional quantum mechanical harmonic oscillator. A coherent state $|\alpha\rangle$ can be written as,
$|\alpha\rangle = e^{-|\alpha|^2/2} \left(\psi_0(x) + \frac{\alpha}{\sqrt{1!}} \psi_1(x) + \frac{\alpha^2}{\sqrt{2!}} \psi_2(x) + \cdots \right)$, where α is an arbitrary complex number (for the moment), and the $\psi_n(x)$ are the harmonic oscillator eigenstates. This state is a superposition of all possible states with different numbers of excitations in the harmonic oscillator.
This WF can be more compactly written as an exponential of the raising operator acting on the ground state eigenfunction:
$|\alpha\rangle = e^{-|\alpha|^2/2} e^{\alpha a^+} \psi_0(x)$

A coherent state WF has the following properties:
It is an eigenfunction of the lowering operator: $a\,|\alpha\rangle = \alpha\,|\alpha\rangle$, with eigenvalue α. Note that since the lowering operator is a non-Hermitian operator, it's eigenvalue is in general complex. We write it as $\alpha = |\alpha| e^{i\theta}$. Hence each term in the coherent state wavefunction written above is based on the same phase θ, as opposed to the case where the phase in each term is randomly fluctuating. This is the difference between a coherent and incoherent state.
The expectation value of the number operator is $\langle\alpha|\, a^+ a \,|\alpha\rangle =< n >= |\alpha|^2$.
The uncertainty in the number of excitations in the coherent state is large: $\Delta n = \sqrt{< n^2 > - < n >^2} = |\alpha|$. This means that $\Delta n/n = 1/\sqrt{n}$.
Finally, the number of excitations in the coherent state is Poisson distributed: $P_n = \frac{|\alpha|^{2n}}{n!} e^{-|\alpha|^2}$, where once again the mean number of excitations is $< n >= |\alpha|^2$.
If we define $\alpha = |\alpha| e^{i\theta}$, then one can show that the number operator is equivalent to the θ derivative: $\hat{n} = \frac{1}{i} \frac{\partial}{\partial \theta}$. Hence the number operator and phase operator are conjugate quantum mechanical operators, and therefore have a non-zero commutator.
The coherent state has a well-defined phase but maximally uncertain number of particles. The number-phase uncertainty relation is $\Delta n \Delta \theta > 1/2$.

A side note on coherent states of the QM harmonic oscillator: "The coherent states are oscillating [once you add the $e^{-iE_n t/\hbar}$ time dependence to each term] Gaussian wave packets with constant width in a harmonic oscillator potential, i.e., the wave packet of the coherent state is not spreading (because all terms in the expansion are in phase). It is a wave packet with minimal uncertainty. These properties make the coherent states the closest quantum mechanical analogue to the free classical single mode field". This statement is from a review of coherent state properties. Here is in animation of a coherent state with $\alpha = 3$.

C. The BCS GS WF as a Coherent State of Cooper Pairs

Electrons are Fermions and therefore very different from the excitations of a quantum harmonic oscillator. However, Cooper pairs are "Bosonic" entities that have some of the characteristics of Bosons, so let's try making a coherent state with them.

Define the operator $P_k^+ = c_{k,\uparrow}^+ c_{-k,\downarrow}^+$ as a Cooper pair creation operator at momentum k. (Note that P_k has some Bosonic character, giving it simpler commutation properties, which will be advantageous later.)
A proposed BCS ground state Cooper pair WF ansatz is therefore:
$|\Psi_{BCS}\rangle = \text{const}\ e^{\sum_k \alpha_k P_k^+} |0\rangle$, where $|0\rangle$ is the vacuum state (empty k-space).
The α_k are complex and will be adjusted to minimize the ground state energy of the system.
The P_k^+ operators have the remarkable property that all powers from 2 and beyond are zero because when acting on a WF they try to multiply occupy a given Cooper pair state. Hence the expansion of the exponentials is terminated after 2 terms and the WF can be written as a product state as,
$|\Psi_{BCS}\rangle = \text{const} \prod_{k=k_1}^{k_M} \left(1 + \alpha_k P_k^+\right) |\phi_k(0)\rangle$, where $|\phi_k(0)\rangle$ represents the empty Cooper pair state involving k and $-k$, and we assume that $|0\rangle = \prod_{k=k_1}^{k_M} |\phi_k(0)\rangle$, and that the $|\phi_k(0)\rangle, |\phi_k(1)\rangle$ are a complete and orthonormal basis for each Cooper pair.
Normalizing this WF term by term, yields the following expression for the BCS GS WF (and Schrieffer's starting point!):
$|\Psi_{BCS}\rangle = \prod_{k=k_1}^{k_M} \left(u_k + v_k c_{k,\uparrow}^+ c_{-k,\downarrow}^+\right) |0\rangle$,
where $u_k = 1/\sqrt{1 + |\alpha_k|^2}$ and $v_k = \alpha_k/\sqrt{1 + |\alpha_k|^2}$ are complex (actually v_k has a fixed complex phase factor relative to u_k).

Expanding the vacuum state as above, we can write the BCS ground state WF ansatz as follows,
$|\Psi_{BCS}\rangle = \prod_{k=k_1}^{k_M} \left(u_k |\phi_k(0)\rangle + v_k |\phi_k(1)\rangle\right)$, showing that u_k is the amplitude for the Cooper pair $(k, -k)$ to be *empty* and v_k is the amplitude for the Cooper pair to be *occupied*.
By checking the normalization of this WF one finds that term by term it must be that $|u_k|^2 + |v_k|^2 = 1$. This suggests that $|u_k|^2$ is the probability that the Cooper pair is un-occupied and $|v_k|^2$ is the probability that it is occupied. This probabilistic interpretation will be used in the variational calculation of the ground state energy.
The next step is to find the set of (u_k, v_k) that minimize the ground state energy.

D. BCS Pairing Hamiltonian

The bare minimum Hamiltonian has just kinetic energy of the electrons and the Cooper pairing potential (sometimes called the BCS pairing Hamiltonian),
$H = \sum_{k,\sigma} \epsilon_k n_{k,\sigma} + \sum_{k,l} V_{k,l} c_{k,\uparrow}^+ c_{-k,\downarrow}^+ c_{-l,\downarrow} c_{l,\uparrow}$
The kinetic energy is just the bare single-particle energy $\epsilon_k = \hbar^2 k^2/2m$ weighted by the number operator. The potential energy destroys one pair and creates another with an amplitude $V_{k,l}$. This potential clearly preserves Cooper pairing. We will once again use Cooper's approximation to the phonon-mediated Frohlich potential $V(\vec{q}, \omega)$. One interesting feature of the potential energy is that it requires the pair at $(-l, \downarrow), (l, \uparrow)$ to be occupied, while that at $(-k, \downarrow), (k, \uparrow)$ to be *un*occupied (otherwise there will be an attempt to doubly occupy a Cooper pair state). This will require some non-trivial gymnastics of the Cooper pair occupations at zero temperature.

E. Thermodynamics

Because the BCS ground state WF is a coherent state, it represents a system with no fixed number of particles N. Hence we must use the grand canonical ensemble to treat the superconductor as a system that exchanges both energy and particles with a reservoir at temperature T and chemical potential μ.

As such we must minimize the Landau potential $\mathcal{L} = U - \mu N$. We will next do a variational calculation to extremalize the expectation value of the quantum Landau potential,
$\delta \langle\Psi_{BCS}| H - \mu N_{op} |\Psi_{BCS}\rangle = 0$.
In other words, we will be performing a variational of this quantity:
$\delta \langle\Psi_{BCS}| \sum_{k,\sigma}(\epsilon_k - \mu)n_{k,\sigma} + \sum_{k,l} V_{k,l}c^+_{k,\uparrow}c^+_{-k,\downarrow}c_{-l,\downarrow}c_{l,\uparrow} |\Psi_{BCS}\rangle = 0$.
We shall define $\xi_k \equiv \epsilon_k - \mu$, which is the energy of the single particle states relative to the chemical potential.
A simple example of a variational calculation in quantum mechanics is posted on the class website.