Lecture 9 Summary

PHYS798S Spring 2016

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Writing down the BCS Ground State Wavefunction

0.1 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 2 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 $(10^{40})^{10^{22}}$, a number too big to contemplate.
Given this situation we will resort to a statistical treatment of the ground state WF.

0.2 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. 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.
We reviewed the properties of coherent states in the 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). 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:
$|\alpha\rangle = e^{-|\alpha^2|/2}e^{\alpha a^+}\psi_0(x)$
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.
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 $< n >= |\alpha|^2$.
The coherent state has a well-defined phase but maximally uncertain number of particles. The number-phase uncertainty relation is $\Delta n \Delta\theta > 1/2$.

0.3 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.
A proposed BCS ground state Cooper pair WF ansatz is therefore:
$|\Psi_{BCS}\rangle =$ const $e^{\sum_k \alpha_k P_k^+}|0\rangle$, where $|0\rangle$ is the vacuum state.
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,
$|\Psi_{BCS}\rangle =$ 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 set.
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.

0.4 BCS Pairing Hamiltonian

The bare minimum Hamiltonian has just kinetic energy of the electrons and the Cooper pairing potential,
$H = \sum_{k,\sigma} \epsilon_k n_{k,\sigma} + \sum_{k,l} V_{k,l} c^+_{k,\uparrow} c^+_{-k,\downarrow} c_{-l,\downarrow} c_{l,\uparrow}$
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.

0.5 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 $L = U - \mu N$. We will do a variational calculation to extremalize the expectation value of the Landau potential, $\delta \langle \Psi_{BCS} | H - \mu N_{op} | \Psi_{BCS} \rangle = 0$.