Writing down the BCS Ground State Wavefunction

0.1 How NOT to do it

We need to put \( N \) electrons into \( M \gg N \) 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 \( \left( \frac{M}{N/2} \right)^N \sim M^N \). 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,

\[ |\alpha\rangle = e^{-|\alpha|^2/2} \left( \psi_0(x) + \frac{\alpha}{\sqrt{4!}} \psi_1(x) + \frac{\alpha^2}{\sqrt{2!}} \psi_2(x) + \cdots \right), \]

where \( \alpha \) 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 $\alpha$.

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: $\Delta n = \sqrt{< n^2 >} - < n >^2 = |\alpha|^2$. This means that $\Delta n/n = 1/\sqrt{n}$.

Finally, the number of excitations in the coherent state is Poisson distributed: $P_n = \frac{|\alpha|^n}{n!} e^{-|\alpha|^2}$, 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:

$|\Psi_{BCS}\rangle = \text{const} \ e^{\sum_k \alpha_k P_k^+} |0\rangle$, where $|0\rangle$ is the vacuum state.

The $\alpha_k$ 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,

$|\Psi_{BCS}\rangle = \text{const} \ \prod_{k=k_1}^{k_M} (1 + \alpha_k P_k^+) |0\rangle$, where $|0\rangle$ 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!):

$|\Psi_{BCS}\rangle = \prod_{k=k_1}^{k_M} (u_k + v_k c_{k,\uparrow}^+ c_{-k,\downarrow}^-) |0\rangle$,

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,

$|\Psi_{BCS}\rangle = \prod_{k=k_1}^{k_M} (u_k |\phi_k(0)\rangle + v_k |\phi_k(1)\rangle)$, 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
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,

\[
H = \sum_{k,\sigma} \epsilon_k n_{k,\sigma} + \sum_{k,l} V_{k,l} c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger c_{-l,\downarrow} c_{l,\uparrow}
\]

The kinetic energy is just the bare single-particle energy \(\epsilon_k = \frac{\hbar^2 k^2}{2m}\) 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 \(\mu\). 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,

\[
\delta \langle \Psi_{\text{BCS}} | H - \mu N_{\text{op}} | \Psi_{\text{BCS}} \rangle = 0.
\]