Cooper Problem

As discussed earlier, the order parameter in a SC is of the form $\langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \rangle$, where $|\vec{k}| \simeq k_F$, i.e. it involves a bound state between two e^-'s close to the Fermi surface. One can get a hint of this incipient instability of the Fermi surface by considering the quantum mechanical problem of just two e^-s outside the Fermi surface that are forced to live outside the Fermi surface due to Pauli exclusion (all states inside the Fermi surface are occupied). In the center of mass frame, the schrodinger's eqn. is

$$\left[\frac{p^2}{2\mu} + V_{eff}(r)\right]\psi(r) = E\,\psi(r)$$

where $\mu = \frac{m}{2}$ is the reduced mass in the center of mass frame and V_{eff} is the inter-particle potential. Fourier transforming,

$$2\varepsilon_p\,\psi(p) + \sum_{k'} V_{eff}(k-k')\,\psi(k') = E\,\psi(k).$$

We choose $V_{eff}(k-k') = -V_0$ if $k_F < k, k' < k_F + \delta k$ where $\delta k \ll k_F$ and $V_{eff}(k-k') = 0$ otherwise.

Corresponding to the cutoff δk, one may define an energy scale ω_D

$$\frac{(k_F+\delta k)^2}{2m} - \frac{k_F^2}{2m} = \omega_D.$$

The schrodinger's eqn becomes,

$$-V_0 \underbrace{\sum_p{}' \psi(p)}_{= \chi} = (E - 2\varepsilon_p)\psi(p)$$

$$\Rightarrow \sum_p -\left(\frac{V_0}{E - 2\varepsilon_p}\right)\chi = \chi$$

$$\Rightarrow -V_0 \int_{E_F}^{E_F + \omega_D} \frac{d\varepsilon\, N(\varepsilon)}{E - 2\varepsilon} = 1$$

where, as mentioned above, $\omega_D \ll E_F$.

$$\Rightarrow +\frac{V_0 N(E_F)}{2} \log\left[\frac{E - 2(E_F + \omega_D)}{E - 2E_F}\right] = 1$$

$$\Rightarrow E = 2E_F - 2\omega_D e^{-2/V_0 N(E_F)}$$

Binding energy of cooper pair.

Compare with $|\Delta| = \frac{t}{|U|} e^{-1/N(E_F)|U|}$ for attractive-U Hubbard model mean-field.

BCS Theory

BCS mean-field theory is quite similar to the mean-field theory for the attractive U Hubbard model we earlier studied.

Our starting point is the following interacting Hamiltonian:

$$H = \sum_k \underbrace{(\varepsilon_k - \mu)}_{\tilde{\varepsilon}_k} c^\dagger_{k\sigma} c_{k\sigma} - V_0 \sum_{kk'}{}' c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow}$$

where the prime (') on the sum in the interaction term indicates that we are restricting the interaction to momenta close to the Fermi energy, with $|\varepsilon_k| - E_F \leq \omega_D$.

Next we solve this problem using mean-field approximation:

$$c^\dagger_{k\uparrow}\, c^\dagger_{-k\downarrow}\, c_{-k'\downarrow}\, c_{k'\uparrow}$$

$$\simeq \phi^*_k\, c_{-k'\downarrow}\, c_{k'\uparrow} + \phi_{k'}\, c^\dagger_{k\uparrow}\, c^\dagger_{-k\downarrow} - \phi_{k'}\, \phi^*_k$$

where $\phi^*_k = \langle c^\dagger_{k\uparrow}\, c^\dagger_{-k\downarrow} \rangle$.

lets define $V_0 \sum_k \phi^*_k = \Delta^*$.

$$\Rightarrow H_{MF} = \sum_k \tilde{\varepsilon}_k\, c^\dagger_k c_k - \sum_k \left[\Delta^*\, c^\dagger_{k\uparrow}\, c^\dagger_{-k\downarrow} + \text{h.c.}\right] + 2\frac{|\Delta|^2}{V_0} N$$

where N is the total system size. Upto simple re-definition of variables, this is identical to the mean-field for the attractive U Hubbard model. ($U\Delta \to \Delta$).

Therefore the mean-field solv. is

$$|\Delta| = 2\omega_D \, e^{-2/N(E_F)V_0}$$

It's instructive to understand the ground state wave-fn, within the mean-field.

Claim: the mean-field ground state is given by:

$$|\psi\rangle_{MF} = \prod_k \left[\cos\left(\frac{\theta_k}{2}\right) + \sin\left(\frac{\theta_k}{2}\right) c^+_{k\uparrow} c^+_{-k\downarrow}\right]|0\rangle$$

where $\tan(\theta_k) = -\frac{\Delta}{\tilde{\varepsilon}_k}$ where Δ is defined above, and is to be determined by minimizing the ground state energy.

Let's derive this result.

$$H_{MF} = \sum_k \tilde{\varepsilon}_k c^\dagger_k c_k - \sum_k [\Delta^* c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + h.c.] + 2\frac{|\Delta|^2}{V_0} N$$

Let's choose the phase of Δ so that it is real

$$\Rightarrow H_{MF} = \sum_k \underbrace{[c^\dagger_{k\uparrow} \quad c_{-k\downarrow}]}_{\psi^\dagger_k} \underbrace{\begin{bmatrix} \tilde{\varepsilon}_k & -\Delta \\ -\Delta & -\tilde{\varepsilon}_k \end{bmatrix}}_{h_k} \underbrace{\begin{bmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{bmatrix}}_{\psi_k} + \text{const.}$$

$$= \sum_k \psi^\dagger_k h_k \psi_k + \text{const.}$$

One may now diagonalize the 2×2 matrix h_k using a unitary transformation

$$U^\dagger_k h_k U_k = D_k = \text{diagonal matrix}.$$

so that

$$H_{MF} = \sum_k \underbrace{\varphi^\dagger_k U_k}_{\eta^\dagger_k} \underbrace{U_k^\dagger h_k U_k}_{D_k} \underbrace{U_k^\dagger \varphi_k}_{\eta_k}$$

$$= \sum_k \eta^\dagger_k D_k \eta_k$$

The explicit form of U_k and D_k may be obtained by writing,

$h_k = E_k \vec{\tau} \cdot \hat{n}$ where $E_k = \sqrt{\Delta^2 + \tilde{\varepsilon}_k^2}$

$\hat{n} = -\frac{\Delta}{E_k}\hat{x} + \hat{z}\frac{\tilde{\varepsilon}_k}{E_k}$ is a unit vector

and $\vec{\tau} = (\tau^x, \tau^y, \tau^z)$ are Pauli matrices that act on the Hilbert space spanned by the vectors $\vec{\varphi}_k$. Therefore,

$$h_k = E_k \begin{bmatrix} \cos(\theta_k) & -\sin(\theta_k) \\ -\sin(\theta_k) & -\cos(\theta_k) \end{bmatrix}$$

where $\sin(\theta_k) = \frac{\Delta}{E_k}$, $\cos(\theta_k) = \frac{\tilde{\varepsilon}_k}{E_k}$.

One can check that the following unitary diagonalizes h_k,

$$U_k = \begin{bmatrix} \sin(\theta_{k/2}) & \cos(\theta_{k/2}) \\ \cos(\theta_{k/2}) & -\sin(\theta_{k/2}) \end{bmatrix}$$

and the eigenvalues are

$$D_k = \begin{bmatrix} -E_k & \\ & E_k \end{bmatrix}.$$

while the eigenvectors are

$$\eta_k = U_k \psi_k$$

$$= \begin{bmatrix} \sin\left(\frac{\theta_k}{2}\right) & \cos\left(\frac{\theta_k}{2}\right) \\ \cos\left(\frac{\theta_k}{2}\right) & -\sin\left(\frac{\theta_k}{2}\right) \end{bmatrix} \begin{bmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{bmatrix}$$

$$= \begin{bmatrix} \sin\left(\frac{\theta_k}{2}\right) c_{k\uparrow} + \cos\left(\frac{\theta_k}{2}\right) c^\dagger_{-k\downarrow} \\ \cos\left(\frac{\theta_k}{2}\right) c_{k\uparrow} - \sin\left(\frac{\theta_k}{2}\right) c^\dagger_{-k\downarrow} \end{bmatrix} \equiv \begin{bmatrix} \chi^\dagger_{-k\downarrow} \\ \chi_{k\uparrow} \end{bmatrix}$$

In terms of new fermion operators γ_k.

$$H_{MF} = \begin{bmatrix} \gamma_{-k\downarrow} & \gamma^\dagger_{k\uparrow} \end{bmatrix} \begin{bmatrix} -\epsilon_k & \\ & \epsilon_k \end{bmatrix} \begin{bmatrix} \gamma^\dagger_{-k\downarrow} \\ \gamma_{k\uparrow} \end{bmatrix}$$

$$= \sum_k \epsilon_k \left[\gamma^\dagger_{k\uparrow} \gamma_{k\uparrow} + \gamma^\dagger_{k\downarrow} \gamma_{k\downarrow} \right].$$

Note that $\epsilon_k = \sqrt{\xi_k^2 + \Delta^2} > 0$,

so that creating an excitation of the γ operators always costs energy.

Therefore, the ground state wfn must satisfy,

$$\gamma_{k\uparrow} |BCS\rangle = 0$$

$$\gamma_{k\downarrow} |BCS\rangle = 0.$$

One may verify that the following state satisfies this condition:

$$|BCS\rangle = \prod_k \left[\cos\left(\frac{\theta_k}{2}\right) + \sin\left(\frac{\theta_k}{2}\right) c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right]|0\rangle$$

This state is automatically normalized, $\langle BCS | BCS\rangle = 1$. It is customary to denote $\cos\left(\frac{\theta_k}{2}\right) = u_k$, $\sin\left(\frac{\theta_k}{2}\right) = v_k$.

Explicitly, $u_k = \cos(\theta_k/2) = \sqrt{\frac{\epsilon_k + \hat{\xi}_k}{2\epsilon_k}}$,

$$v_k = \sin(\theta_k/2) = \sqrt{\frac{\epsilon_k - \hat{\xi}_k}{2\epsilon_k}} \qquad \left(\epsilon_k = \sqrt{\hat{\xi}_k^2 + \Delta^2}\right)$$

Self-consistency:

We still need to find Δ self-consistently

$$V_0 \sum_k \langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\rangle = \Delta(T)$$

Using the relation between c and χ, this becomes,

$$V_0 \sum_k u_k v_k \left[1 - \sum_\sigma \langle \gamma^\dagger_{k\sigma} \gamma_{k\sigma} \rangle\right]$$

$$= V_0 \sum_k u_k v_k \left[1 - 2 n_F(E_k)\right]$$

$$= \Delta(T)$$

where n_F is the Fermi-Dirac fn.

Substituting the expression for u_k, v_k,

$$V_0 \int \frac{d\varepsilon \; N(\varepsilon) \left[1 - 2 n_F(E)\right]}{2 \sqrt{\Delta^2(T) + \varepsilon^2}} = 1$$

This is the famous BCS gap eqn.

Note that $E = \sqrt{\varepsilon^2 + \Delta^2}$, and

$$1 - 2 n_F(E) = 1 - \frac{1}{1 + e^{\beta E}}$$

$$= \tanh\left(\frac{\beta E}{2}\right).$$

Let's consider various limits of the gap Eqn.

$T = 0$:

$$\frac{V_0}{2} \int \frac{N(\varepsilon)\, d\varepsilon}{\sqrt{\Delta^2 + \varepsilon^2}} = 1$$

$$\Rightarrow \frac{V_0}{2} N(E_F) \int_{-\omega_D}^{\omega_D} \frac{d\varepsilon}{\sqrt{\Delta^2 + \varepsilon^2}} \approx 1$$

$$\Rightarrow \frac{V_0}{2} \times 2\, N(E_F) \int_{\Delta}^{\omega_D} \frac{d\varepsilon}{\varepsilon} \approx 1$$

$$\Rightarrow \Delta(T=0) \approx \omega_D\, e^{-1/V_0 N(E_F)}$$

[One may do the integral exactly as well.

$$\int_0^{\omega_D} \frac{d\varepsilon}{\sqrt{\Delta^2 + \varepsilon^2}} = \int_0^{\omega_D/\Delta} \frac{dx}{\sqrt{1 + x^2}} = \sinh^{-1}\left[\frac{\omega_D}{\Delta}\right]$$

$$\Rightarrow \Delta(T=0) = \frac{\omega_D}{\sinh\left[1/V_0 N(E_F)\right]}$$

Assuming $V_0 N(E_F) \ll 1$, $\sinh\left[\frac{1}{V_0 N(E_F)}\right] \approx \frac{e^{\frac{1}{V_0 N(E_F)}}}{2}$

$$\Rightarrow \quad \Delta(T=0) \approx 2\omega_D \, e^{-1/V_0 N(E_F)} \; \Big]$$

$T = T_c$:

At T_c, $\Delta = 0$ $\Rightarrow$

$$\frac{V_0}{2} N(E_F) \int_{-\omega_D}^{\omega_D} \frac{\tanh\left(\frac{\beta_c \varepsilon}{2}\right)}{\varepsilon} \, d\varepsilon = 1$$

Again, this integral can be done approximately.

$$\int_0^{\omega_D} \frac{\tanh(\beta_c \varepsilon/2)}{\varepsilon} \, d\varepsilon = \int_0^{\beta_c \omega_D} \frac{\tanh(x/2)}{x} \, dx$$

$$\approx \log\left[\frac{\omega_D}{T_c}\right]$$

$$\Rightarrow \quad T_c \approx \omega_D \, e^{-1/V_0 N(E_F)} .$$

A more accurate treatment of the integral yields.

$$T_c \approx 1.14\, \omega_D\, e^{-1/V_0 N(E_F)}$$

Comparing the expressions for $\Delta(T=0)$ and T_c,

$$\frac{2\Delta(T=0)}{T_c} = \frac{4}{1.14} \approx 3.52.$$

This ratio serves as a signature of the validity of the BCS mean-field, and therefore, if violated, indicates that fluctuations beyond mean-field may be important.

BCS Wave-fn in Real Space

Recall,

$$|BCS\rangle = \prod_k \left[u_k + v_k \, c^\dagger_{k\uparrow} \, c^\dagger_{-k\downarrow} \right] |0\rangle$$

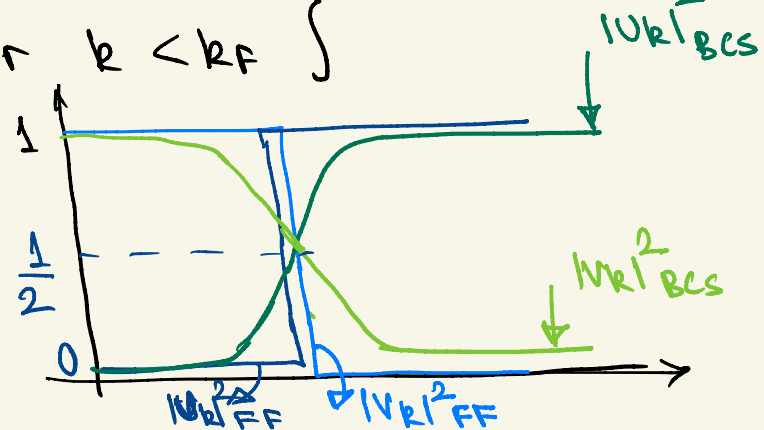
where $u_k = \sqrt{\dfrac{E_k + \tilde{\varepsilon}_k}{2E_k}}$,

$$v_k = \sqrt{\frac{E_k - \tilde{\varepsilon}_k}{2E_k}}, \quad E_k = +\sqrt{\tilde{\varepsilon}_k^2 + \Delta^2}$$

In a fermi gas ($\Delta = 0$), so that,

$u_k = 0$ for $k < k_F$,
$= 1$ for $k > k_F$

$v_k = 0$ for $k > k_F$
$= 1$ for $k < k_F$



Upto normalization,

$$|BCS\rangle = \prod_k \left[1 + \frac{v_k}{u_k} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \right] |0\rangle$$

$$= e^{\sum_k \left[\frac{v_k}{u_k} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \right]} |0\rangle$$

[since $(c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow})^2 = 0$].

One may now consider $|BCS\rangle$ in 'canonical ensemble' where the no. of particles is fixed. Denoting the wfn. with N particles as $P_N |BCS\rangle$ where P_N denotes the projection onto the Hilbert space corresponding to N particles, $P_N |BCS\rangle =$

$$\left[\sum_k \frac{v_k}{u_k} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \right]^{N/2} |0\rangle$$

$$= \left[\sum_{rr'} g(r-r') \, c^{\dagger}_{r\uparrow} c^{\dagger}_{r'\downarrow} \right]^{N/2} |0\rangle$$

where $g(r) = \int \frac{v_k}{u_k} e^{ik \cdot r}$

One may interpret the expression for $P_N|BCS\rangle$ as a condensate of cooper pairs where the wavefn. profile for a pair is given by $g(r)$.

One may now approximately evaluate $g(r)$ using $\frac{v_k}{u_k} = \frac{|\Delta|}{E_k + \tilde{\xi}_k} \approx \frac{|\Delta|}{2E_k}$

$$\Rightarrow g(r) \approx |\Delta| \int \frac{e^{i\vec{k} \cdot \vec{r}}}{\sqrt{\tilde{\xi}_k^2 + \Delta^2}}$$

$$\tilde{\xi}_k = \frac{k^2 - k_F^2}{2m} = \frac{(k-k_F)(k+k_F)}{2m}$$

$$\simeq v_F (k - k_F), \text{ where } k = |\vec{k}|$$

$$g(r) \approx |\Delta| \int \frac{e^{i\vec{k}\cdot\vec{r}}\, d^d k}{\sqrt{v_F^2 (k - k_F)^2 + \Delta^2}}$$

$$\sim \frac{e^{-r/\xi}}{r^{d-1}}$$

where $\xi = \frac{v_F}{\Delta}$ is the "coherence length",

which denotes the length scale over which cooper pairs are entangled.