BCS Theory of impure superconductors

The main result we want to discuss is that in the presence of impurities that do not break time-reversal symmetry, the gap eqn. within the BCS mean-field is essentially unchanged (after making reasonable assumptions), and therefore, non-magnetic impurities have a minimal effect on the T_c and Δ for an s-wave superconductor.

Rough picture: In the absence of any impurities, the cooper pairs are made of time-reversed single-particle states: $|\vec{k}\uparrow\rangle$ and $|-\vec{k}\downarrow\rangle$. In the presence of impurities that respect the time-reversal symmetry, i.e. $[\hat{T}, \hat{H}] = 0$ where $\hat{H}$ is the Hamiltonian and $\hat{T}$ is the anti-unitary operator corresponding to time-reversal, one can again form cooper pairs between time-reversed pairs of single-particle states. Specifically, if $|E_\alpha\rangle$ is a single-particle eigenstate of H, then so is $\hat{T}|E_\alpha\rangle \equiv |E_{\tilde{\alpha}}\rangle$, with the same single-particle energy.

Thus, the BCS mean-field H takes the form:

$$H = \sum_\alpha \left[\varepsilon_\alpha (c^+_\alpha c_\alpha + c^+_{\tilde{\alpha}} c_{\tilde{\alpha}}) + \Delta (c^+_\alpha c^+_{\tilde{\alpha}} + h.c.) \right]$$

which can be diagonized in the same way as the translationally invariant version, leading to

$$|BCS\rangle = \prod_\alpha \left[u_\alpha + v_\alpha c^+_\alpha c^+_{\tilde{\alpha}} \right] |0\rangle$$

One can do a little bit better than the above mean-field.

lets do an actual calculation for an s-wave SC in the presence of time-reversal symmetric disorder.

$$H = \sum_{r\sigma} c^{+}_{\sigma}(r) \left[-\frac{\nabla^2}{2m} - E_F + \mu(r) \right] c_{\sigma}(r)$$

$$+ \sum_{r} \left[\Delta(r)\, c^{+}_{\uparrow}(r)\, c^{+}_{\downarrow}(r) + h.c. \right].$$

This Hamiltonian is time-reversal symmetric,
$c_{\uparrow}(r) \to c_{\downarrow}(r)$, $c_{\downarrow}(r) \to -c_{\uparrow}(r)$,
$i \to -i$ (i.e. $\Delta \to \Delta^*$) leaves H invariant

To diagonalize H, one considers the following unitary transformation:

$$c_\uparrow(r) = \sum_n \left[u_n(r)\, \gamma_{n\uparrow} - v^*_n(r)\, \gamma^\dagger_{n\downarrow} \right]$$

$$c_\downarrow(r) = \sum_n \left[u_n(r)\, \gamma_{n\downarrow} + v^*_n(r)\, \gamma^\dagger_{n\uparrow} \right]$$

where $\gamma_{n\sigma}$ are independent of $\vec{r}$ and the diagonalized H takes the form $H = \sum_n E_n\, \gamma^\dagger_{n\sigma} \gamma_{n\sigma}$,

which implies,

$$[H, \gamma_{n\uparrow}] = -E_n\, \gamma_{n\uparrow}$$

and $[H, \gamma^\dagger_{n\downarrow}] = E_n\, \gamma^\dagger_{n\downarrow}$.

To find equations for $u_n(r)$ and $v_n(r)$, let's calculate $[H, c_\uparrow(r)]$

$$= -\left[-\frac{\nabla^2}{2m} - E_F + \mu(r) \right] c_\uparrow(r)$$

$$- \Delta(r)\, c^\dagger_\downarrow(r)$$

$$= -\left[-\frac{\nabla^2}{2m} - E_F + \mu(r)\right] \sum_n \left[u_n(r)\, \gamma_{n\uparrow} - v_n^*(r)\, \gamma^\dagger_{n\downarrow}\right]$$

$$- \Delta(r) \sum_n \left[u^*_n(r)\, \gamma^\dagger_{n\downarrow} + v_n(r)\, \gamma_{n\uparrow}\right]$$

Using the relation between c and γ, this must also equal

$$[H, c_\uparrow(r)]$$

$$= \sum_n u_n(r)\, [H, \gamma_{n\uparrow}] - v^*_n(r)\, [H, \gamma^\dagger_{n\downarrow}]$$

$$= \sum_n \left[-u_n(r) E_n\, \gamma_{n\uparrow} - v^*_n(r)\, \gamma^\dagger_{n\downarrow}\right]$$

Now, one can match the coefficients of $\gamma_{n\uparrow}$ and $\gamma^\dagger_{n\downarrow}$ to obtain equations for $u_n(r)$ and $v_n(r)$:

$$\left[\frac{-\nabla^2}{2m} + \mu(r) - E_F\right] u_n(r) + \Delta(r)\, v_n(r)$$

$$= E_n\, u_n(r)$$

$$-\left[-\frac{\nabla^2}{2m}+\mu(r)-E_F\right]v^*_n(r)+\Delta(r)u^*_n(r)$$

$$= E_n v^*_n(r)$$

which may succintly be written as,

$$\begin{bmatrix} -\frac{\nabla^2}{2m}+\mu(r)-E_F & \Delta(r) \\ \Delta^*(r) & -\left[-\frac{\nabla^2}{2m}+\mu(r)-E_F\right] \end{bmatrix}\begin{bmatrix} u_n(r) \\ v_n(r) \end{bmatrix}$$

$$= E_n \begin{bmatrix} u_n(r) \\ v_n(r) \end{bmatrix}$$

To simplify <u>these</u> equations, let's assume that $\overline{\Delta(r)} \approx \Delta_0$ (= independent of $\vec{r}$) and solve an auxiliary eigenvalue problem,

$$\left[-\frac{\nabla^2}{2m}+\mu(r)-E_F\right]w_n(r) = \xi_n w_n(r).$$

Let's write $u_n(r) = \tilde{u}_n \, w_n(r)$

$$v_n(r) = \tilde{v}_n \, w_n(r)$$

where $\tilde{u}_n$ and $\tilde{v}_n$ are independent of r. Under such an approximation, the eigenvalue problem becomes,

$$\begin{bmatrix} \xi_n & \Delta \\ \Delta^* & -\xi_n \end{bmatrix} \begin{bmatrix} \tilde{u}_n \\ \tilde{v}_n \end{bmatrix} = E_n \begin{bmatrix} \tilde{u}_n \\ \tilde{v}_n \end{bmatrix}$$

which is identical to the BCS mean-field equations without any impurities. Note that the r-dependence has completely dropped out.

Therefore, $E_n = \pm \sqrt{\Delta^2 + \xi_n^2}$.

and $\Delta(r) = V_0 \sum_n u_n(r)\, v_n(r)$
$[1 - 2f(E_n)]$

$= V_0 \sum_n |w_n(r)|^2 \, \tilde{u}_n \tilde{v}_n [1 - 2f(E_n)]$

$= V_0 \dfrac{\Delta}{2} \sum_n \dfrac{|w_n(r)|^2 [1 - 2f(E_n)]}{\sqrt{\Delta^2 + \xi_n^2}}$

Since $w_n(r)$ is the eigenfn for the schrodingers eqn. in the absence of pairing, $\overline{|w_n(r)|^2} \sim N_F(0)$
= density of states at fermi level.

$\Rightarrow \quad \overline{\Delta} \sim e^{-1/V_0 N_F(0)}$

and $T_c \sim e^{-1/V_0 N_F(0)}$.