BCS Theory

- Many-electron version of Cooper problem:

\[ \hat{H} = H_k + \text{Hint} \] Always work with grand canonical Hamiltonian

\[ H_k = \sum_{k, \sigma} \left( \varepsilon(k) - \mu \right) \Psi_k^\dagger(k) \Psi_k(k) \]

\[ \text{Hint} = -\frac{U_0}{V} \sum_{k, k', \sigma, \sigma'} \Psi_{k, \sigma}^\dagger(k - \frac{q}{2}) \Psi_{k', -\sigma}^\dagger(k' + \frac{q}{2}) \Psi_{k', -\sigma'}(k') \Psi_{k, \sigma}(k) \]

("in shell") \[ \Rightarrow \text{Recall this means} \]
\[ \varepsilon(k), \varepsilon(k + q), \text{etc} \]
\[ \text{satisfy: } \varepsilon_k - \mu > \varepsilon(k), \varepsilon_{k+q} \]

- Simplify interaction further. Based on insight from Cooper problem, we guess that the most important part of interaction is that which scatters a pair \( \Psi_k^\dagger(k) \Psi_{-k}(-k) \) into another such pair...
Therefore, consider BCS model:

\[ H_{\text{BCS}} = H_k + H_{\text{int}} \]

\[ H_{\text{int}} = -\frac{U_0}{V} \sum_{\text{all } k, k'} \psi_{k}^\dagger \psi_{-k}^\dagger \psi_{-k'} \psi_{k'} \]

- This was important part of interaction in Cooper problem.
- We'll apply a mean-field theory here, it apply it to full Hamiltonian, nothing changes... so we may as well make this simplification.

Crucial insight from Cooper problem: Cooper pairs are bound states, if are bosons \( \Rightarrow \) they should condense.

\[ \Rightarrow \text{Expect can describe this by writing } \langle \psi_{k}^\dagger \psi_{-k}^\dagger \rangle \neq 0 \]
\[
\Psi^{-}(-\mathbf{k}) \Psi^{+}(\mathbf{k}) = \tilde{\Delta}(\mathbf{k}) + \left[ \Psi^{-}(-\mathbf{k}) \Psi^{+}(\mathbf{k}) - \tilde{\Delta}(\mathbf{k}) \right] \\
\tilde{\Delta}(\mathbf{k}) = \langle \Psi^{-}(-\mathbf{k}) \Psi^{+}(\mathbf{k}) \rangle \\
\Rightarrow \tilde{\Delta}^{\dagger}(\mathbf{k}) = \langle \Psi^{+}(\mathbf{k}) \Psi^{-}(\mathbf{k}) \rangle \\
\]

Putting this in and neglecting terms quadratic in fluctuation part:

\[
H_{\text{int}}^{\text{BCS}} \propto + \frac{U_0}{V} \left[ \sum_{\mathbf{k}} \tilde{\Delta}(\mathbf{k}) \right] \left[ \sum_{\mathbf{k}'} \tilde{\Delta}(\mathbf{k}') \right] \\
- \frac{U_0}{V} \left[ \sum_{\mathbf{k}} \tilde{\Delta}^{\dagger}(\mathbf{k}) \right] \left[ \sum_{\mathbf{k}'} \Psi^{-}(\mathbf{k}') \Psi^{+}(\mathbf{k}') \right] \\
- \frac{U_0}{V} \left[ \sum_{\mathbf{k}} \tilde{\Delta}(\mathbf{k}) \right] \left[ \sum_{\mathbf{k}'} \Psi^{+}(\mathbf{k}) \Psi^{-}(\mathbf{k}') \right] \\
\]

Define: \( \Delta = \frac{U_0}{V} \sum_{\mathbf{k}} \tilde{\Delta}(\mathbf{k}) \)
\[ H_{\text{BCS}} \approx \frac{V}{U_0} |A|^2 - \sum_{\ell} \sum \left\{ \Delta \psi^\dagger_\ell (k) \psi^\dagger_{-\ell} (-k) + h.c. \right\} \]

- **Note:** By rotating phase of \( \psi^\dagger_\ell (k) \), we can make \( \Delta \) to be real, positive — so we'll assume \( \psi^\dagger_\ell (k) \) from now on.

- This looks a lot like mean-field Hamiltonian for dilute Bose gas → expect we can solve it via similar means.

\[ H_{\text{MF}} = \text{const} + \sum_{\ell \in \text{in shell}} 3(k) \psi^\dagger_\ell (k) \psi^\dagger_{-\ell} (-k) \psi_\ell (k) \psi_{-\ell} (-k) \]

\[ - \sum_{\ell \in \text{in shell}} \Delta \left[ \psi^\dagger_\ell (k) \psi^\dagger_{-\ell} (-k) + \psi_\ell (k) \psi_{-\ell} (-k) \right] \]

\[ \Rightarrow \, \xi(k) = \frac{3}{k} - \mu. \]
Can write this in a clear way:

\[ H_{MF} = \frac{V}{U_0} \Delta^2 + \sum_{k \text{ in shell}} \varepsilon(k) + \sum_{k \text{ in shell}} \left( \Psi^+_k \Psi^+_{-k} \right) \begin{pmatrix} \varepsilon(k) & -\Delta \\ -\Delta & -\varepsilon(k) \end{pmatrix} \begin{pmatrix} \Psi^+_k \\ \Psi^+_{-k} \end{pmatrix} \]

Guess: Quasiparticles created/annihilated by:

\[ \Psi^+_k = U(k) \Psi^+_k - V(k) \Psi^+_{-k} \]
\[ \Psi^+_k = U(k) \Psi^+_k + V(k) \Psi^+_{-k} \]

\[ \Psi^+_k \Psi^+_k \]

Assume \( U \)'s and \( V \)'s are real, and \( U(k) = U(-k), \ V(k) = V(-k) \).

Can check that \( \Psi^+_k \) satisfies right form of anti-commutation relations provided \( U(k)^2 + V(k)^2 = 1 \), i.e.

\[ \{ \Psi^+_k, \Psi^+_l \} = \delta_{kk}, \]
\[ \{ \Psi^+_k, \Psi^+_l \} = 0 \]

\[ \Rightarrow \begin{pmatrix} \Psi^+_k \\ \Psi^+_{-k} \end{pmatrix} = \begin{pmatrix} U(k) & -V(k) \\ V(k) & U(k) \end{pmatrix} \begin{pmatrix} \Psi^+_k \\ \Psi^+_{-k} \end{pmatrix} \]

\[ \Rightarrow 2 \times 2 \text{ unitary matrix, since } U^2 + V^2 = 1. \]
We can choose the above config matrix to diagonalize the Hamiltonian ...

Eigenvalues at \( \begin{pmatrix} \epsilon(k) & -\Delta \\ -\Delta & -\varepsilon(k) \end{pmatrix} \) are

\[
\lambda_{\pm}(k) = \mp \sqrt{[\varepsilon(k)]^2 + \Delta^2}.
\]

\( \lambda_{\pm}(k) \equiv E(k) \).

Here:

\[
H_{MF} = \text{const.} + \sum_{\text{in shell}} \frac{1}{2} \left( \begin{array}{c} \frac{1}{2} \varepsilon(k) \end{array} \right) \left( \begin{array}{c} u(k) \\ v(k) \end{array} \right) \left( \begin{array}{cc} E(k) & -\Delta \\ -\Delta & -\varepsilon(k) \end{array} \right) \left( \begin{array}{c} u(k) \\ v(k) \end{array} \right).
\]

\[
\left( \begin{array}{c} \delta^+_k \\ \delta^-_{-k} \end{array} \right)
\]

Observe \( \begin{pmatrix} u(k) \\ -v(k) \end{pmatrix}, \begin{pmatrix} v(k) \\ u(k) \end{pmatrix} \) must be eigenvectors.

Solution: \[
\begin{align*}
U(k) &= \sqrt{\frac{1}{2}} \left(1 + \frac{\varepsilon(k)}{E(k)} \right) \\
V(k) &= \sqrt{\frac{1}{2}} \left(1 - \frac{\varepsilon(k)}{E(k)} \right)
\end{align*}
\]
If we plug this in, then:

\[ H_{MF} = \text{const} + \sum_{k \text{ in shell}} \begin{pmatrix} Y^+_k(k) \end{pmatrix} \begin{pmatrix} E(k) & 0 \\ 0 & -E(k) \end{pmatrix} \begin{pmatrix} Y_k(k) \\ \delta^+_k(k) \end{pmatrix} \]

\[ = \frac{V}{U_0} \Delta^2 + \sum_{k \text{ in shell}} \left[ \delta(k) - E(k) \right] + \sum_{k \text{ in shell}} E(k) Y^+_k(k) Y_k(k) \]

*Can we extend back outside shell in a simple way?

\[ \theta(k) \]

\[ \epsilon(k) \]

\[ \Delta \ll \omega_D, \text{ turns out to be reasonable assumption.} \]
\[ \psi^+_0(k) = \psi^+_0(k) \quad (\text{creates electron}) \]

\[ E(k) > E_F + W_D \]

\[ \psi(k) = E(k) - \mu > 0. \]

\[ \psi^+_0(k) \sim \psi^+_0(k) \quad (\text{creates hole}) \]

\[ E(k) < E_F - W_D \]

\[ -\tilde{\psi}(k) = \mu - E(k) > 0. \]

- This just says "particles" are the quasiparticles for large \( E > E_F + W_D \), and "holes" are good quasiparticles for \( E < E_F - W_D \). Mixing of particles & holes only occurs for \( E_F - W_D < E < E_F + W_D \).
\( \mathcal{H}_F = \text{const} + \sum_{k, \sigma} E(k) \psi_\sigma^+ (k) \psi_\sigma (k) \)

\[
E(k) = \sqrt{[\varepsilon(k)]^2 + \Delta^2}
\]

- On the Fermi surface, \( \varepsilon(k) = 0 \) \( \Rightarrow \) \( E(k_F) = \Delta \) energy gap.

- Intuition for the gap.
  - Mixing of electrons & holes.

\[ \xymatrix{
  & \text{electron} \\
  \text{hole} \ar[ru] \ar[ruu]_{\text{e-h mixing via DM\&BC}} \ar[r]_{\text{of Cooper pairs}} & \text{electron} & \text{hole} & (k, -k) \text{ Cooper pair}
} \]
Determination of $\Delta$:

- Use "self-consistency relation":

$$\Delta = \frac{U_o}{\sqrt{\text{shell}}} \sum_{k} \langle \Psi_t^+(k) \Psi_v^+(k) \rangle$$

Where:

$$\Psi_t^+(k) = \begin{pmatrix} u(k) \\ v(k) \end{pmatrix}$$
$$\Psi_v^+(k) = \begin{pmatrix} -v(k) \\ u(k) \end{pmatrix}$$

$$\langle \Psi_t^+(k) \Psi_v^+(k) \rangle = \left[ (u(k) \delta_t^+(k) + v(k) \delta_v(k)) \right] \left[ -v(k) \delta_t^+(k) + u(k) \delta_v(k) \right]$$

$$\Rightarrow \langle \Psi_t^+(k) \Psi_v^+(k) \rangle = \langle \Psi_t^+(k) \delta_v^+(k) \rangle + \langle \Psi_v^+(k) \delta_t^+(k) \rangle$$

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$$= U(k) V(k) \left[ \langle \delta_t^+(k) \delta_t(k) \rangle + \langle \delta_v^+(k) \delta_v(k) \rangle \right]$$

$$= U(k) V(k) \left[ 1 - \frac{2}{e^{E(k)/kT} + 1} \right]$$

$$= \frac{\Delta}{2E(k)} \left[ 1 - \frac{2}{e^{E(k)/kT} + 1} \right]$$
\[ \Delta = U_0 \int_{\varepsilon_F - W_0}^{\varepsilon_F + w_0} d\varepsilon \, D(\varepsilon) \left[ \frac{\Delta}{Z E(\varepsilon)} \right] \left[ 1 - \frac{Z}{e^{E(\varepsilon)/k_B T} + 1} \right] \]

- Always a solution \( \Delta = 0 \) (No superconductivity)
- Suppose \( \Delta \neq 0 \) and also suppose \( D(\varepsilon) \) varies only slowly within the shell, so \( D(\varepsilon) \rightarrow D(\varepsilon_F) \)

\[
\frac{1}{U_0 D(\varepsilon_F)} = \frac{1}{Z} \int_{\varepsilon_F - W_0}^{\varepsilon_F + w_0} d\varepsilon \frac{1}{E(\varepsilon)} \left[ 1 - \frac{Z}{e^{E(\varepsilon)/k_B T} + 1} \right]
\]

\[
= \int_{\varepsilon_F - w_0}^{\varepsilon_F + w_0} d\varepsilon \frac{1}{E(\varepsilon)} \left[ 1 - \frac{Z}{e^{E(\varepsilon)/k_B T} + 1} \right]
\]

\[
= \int_{\varepsilon_F}^{\varepsilon_F + w_0} d\varepsilon \frac{1}{E(\varepsilon)} \tanh \left( \frac{E(\varepsilon)}{Z k_B T} \right)
\]
Write:

\[ \frac{1}{U_0 D(\xi_F)} = \int_0^{\xi_D} \frac{d\xi}{\sqrt{\xi^2 + \Delta^2}} \tan \left( \frac{I}{2} \sqrt{\xi^2 + \Delta^2} \right) \]

This equation determines \( \Delta(T) \). If there is no solution, then presumably \( \Delta = 0 \) and there is no superconductivity.

Solve at \( T = 0 \)

\[ T = 0 \Rightarrow \beta \to \infty \Rightarrow \frac{1}{U_0 D(\xi_F)} = \int_0^{\xi_D} \frac{d\xi}{\sqrt{\xi^2 + \Delta^2}} \]

\[ \text{This always has a solution, no matter the value of } U_0 D(\xi_F) \]

\[ = \ln \left| \frac{\omega_D}{\Delta} + \frac{\sqrt{\omega^2 + \Delta^2}}{\Delta} \right| \]

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\[ = \ln \left| \frac{1}{U_0 D(\xi_F)} \right| \]

Note similarities to Cooper problem.

\[ \Delta(0) \approx 2\omega_D \xi_F \]

( Typically, \( \Delta \approx 10K \) in simple superconductors, so good approximation.)
Note from this result that as long as

\[ U_0 D(\varepsilon_F) \approx 1, \quad \Delta \ll \omega_D. \]

\[ \downarrow \]

doesn't need to be much less, since dependence on \( U_0 D(\varepsilon_F) \) is exponential.

What is \( \Delta(T) \)?

Expect something like:

\[ \Delta(T) \]

\[ \Delta(T\to0) \]

\[ T \to T_c \]

- Full curve not so easy to calculate... but would be good if can calculate \( T_c \).

- \( \Delta(T_c) = 0 \implies \frac{1}{U_0 D(\varepsilon_F)} = \int_0^{\frac{\frac{\Delta(T_c)}{2}}{\omega_D}} \frac{d\varepsilon}{\varepsilon} \tanh\left[ \frac{\varepsilon}{2k_B T_c} \right] \)

\[ \beta_c = \frac{1}{k_B T_c} \]
Integral can't be done analytically, but expect \( R_{\omega_0} \gg 1 \). Integral diverges at large \( \omega \),

\[
\text{Expect: } f(a) = \int_0^a \frac{\tanh(u)}{u} \sim \ln a + C + (\text{terms that vanish as } a \to \infty)
\]

\( C = \ln(2A) \), obtained by numerical integration.

If plot \( f(a) \) and \( \ln(2Aa) \), get:

\[
\begin{align*}
&0.5 & 1.0 & 1.5 & 2.0 \\
\text{fla} & \ln(2Aa), \text{ with } A = 1.13
\end{align*}
\]
As long as $\frac{\beta \nu_0}{2} \gg 1$, then the good approximation...

$$\frac{1}{U_0(\varepsilon_F)} = \int_0^{\frac{\beta \nu_0}{2}} \frac{du}{u^{\tan} u} \approx \ln (1.13 \beta \nu_0)$$

$$\Rightarrow k_B T_c \propto 1.13 \nu_0 e^{-\frac{1}{U_0(\varepsilon_F)}}$$

Ratio

$$\frac{A(T = 0)}{k_B T_c} \approx \frac{2}{1.13} = 1.764$$

Works pretty well in practice... not perfect, but remember our model is pretty crude.

Isotope Effect:

Since $T_c \sim \nu_0$, reasonable to guess $T_c \sim \frac{1}{M}$, as (roughly) observed.

Note that $U_0$ might have some dependence on $M$... so this should be taken with a grain of salt.
BCS Wavefunction:

Write down: \[ | \Psi_{BCS} > = N \prod_k \left( u(k) + v(k) e^{i\phi} \psi^\dagger(k) \psi^\dagger(-k) \right) | 0 > \]

Cooper pair creation operator.

Roughly looks like "BEC" of Cooper pairs... many different particle numbers, and definite phase relationship between states with different numbers.

To get a state with definite number of particles:

\[ | \Psi_{BCS}(N) > = \int_0^{2\pi} d\phi \ e^{-iN\phi} | \Psi_{BCS}(\phi) > . \]

N cooper pairs, 2N electrons

Illustrates number-phase uncertainty.
How do we know this is the right state...

Should show: \[ \langle \hat{\Phi}(k) | \Psi_{ics} \rangle = 0 \]

For example: \[ \hat{\Phi}(k) = U(k) \psi_\parallel(k) - v(k) \psi_\perp(-k) \]

\[ \langle \hat{\Phi}(k) | \Psi_{ics} \rangle = U \prod_{q \neq k} \left( U(q) + v(q) \psi_\parallel(q) \psi_\perp(q) \right) \]

\[ \times \left[ \psi_\parallel(k) - v(k) \psi_\perp(-k) \right] \left[ U(k) + v(k) \psi_\parallel(k) \psi_\perp(k) \right] \]

\[ = \left[ U(k) v(k) \psi_\parallel(-k) - U(k) v(k) \psi_\parallel(k) \right] |0\rangle = 0 \]
Another interesting property of BCS wavefunction:

- Occupation number distribution:

\[ n(k) = \langle \hat{n}_\uparrow(k) \rangle = \langle \psi_\uparrow^+(k) \psi_\uparrow(k) \rangle \]

- Noninteracting electrons, \( T=0 \Rightarrow n(k) = \Theta(k_F - |k|) \)

\[ n(k) = \langle \psi_\uparrow^+(k) \psi_\uparrow(k) \rangle \]
\[ = \langle [u(k) \gamma_\uparrow^+(k) + v(k) \gamma_\downarrow(-k)] [u(k) \gamma_\uparrow(k) + v(k) \gamma_\downarrow(k)] \rangle \]
\[ = v^2(k) \langle \gamma_\downarrow(-k) \gamma_\uparrow^+(k) \rangle = v^2(k) \]

\[ \Rightarrow n(k) = \frac{1}{2} \left( 1 - \frac{\epsilon(k)}{E(k)} \right) \]

No step function discontinuity in superconductivity stable.