BCS Theory of Superconductivity

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What is BCS Theory?

The Nobel Prize in Physics 1972

"for their jointly developed theory of superconductivity, usually called the BCS-theory"

What is BCS Theory?

- First “working” microscopic theory for superconductors.
- It’s a mean-field theory.
- In it’s original form only applied for conventional superconductors.
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Outline

1. Cooper-Pairs
   - Formation of Pairs
   - Origin of Attractive Interaction

2. BCS Theory
   - The model Hamiltonian
   - Bogoliubov-Valatin-Transformation
   - Calculation of the condensation energy

3. Finite Temperatures
   - Excitation Energies and the Energy Gap
   - Determination of $T_c$
   - Temperature dependence of the energy gap
   - Thermodynamic quantities
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Let's assume the following things:

- Consider a material with a filled Fermi sea at $T = 0$.
- Add two more electrons that
  - interact attractively with each other but
  - don’t interact with the other electrons except via Pauli-principle.
Formation of Pairs

Look for the groundstate wavefunction for the two added electrons, which has zero momentum:

$$\psi_0(r_1, r_2) = \sum_k \left( g_k e^{i k \cdot r_1} e^{-i k \cdot r_2} \right) \left( |\uparrow \downarrow\rangle - |\downarrow \uparrow\rangle \right)$$

The total wavefunction has to be antisymmetric with respect to exchange of the two electrons. The spin part is antisymmetric and therefore the spacial part has to be symmetric.

$$\Rightarrow g_k = g_{-k}.$$
Formation of Pairs

Inserting this into the Schrödinger equation of the problem leads to the following equation for the determination of the coefficients $g_k$ and the energy eigenvalue $E$:

$$ (E - 2\epsilon_k) g_k = \sum_{k > k_F} V_{kk'} g_{k'} , $$

where

$$ V_{kk'} = \frac{1}{\Omega} \int V(\mathbf{r}) e^{i(k' - k) \cdot \mathbf{r}} d\mathbf{r} $$

($\mathbf{r}$: distance between the two electrons, $\Omega$: normalization volume, $\epsilon_k$: unperturbed plane-wave energies).
Formation of Pairs

Since it is hard to analyze the situation for general $V_{kk'}$, assume:

$$V_{kk'} = \begin{cases} 
-\nu, & E_F < \epsilon_k < E_F + \hbar \omega_c \\
0, & \text{otherwise}
\end{cases}$$

with $\hbar \omega_c$ a cutoff energy away from $E_F$. 
Formation of Pairs

With this approximation we get:

\[
\frac{1}{V} = \sum_{k > k_F} \frac{1}{2\epsilon_k - E} = N(0) \int_{E_F}^{E_F + \hbar \omega_c} \frac{d\epsilon}{2\epsilon - E}
\]

\[
= \frac{1}{2} N(0) \ln \left( \frac{2E_F - E + 2\hbar \omega_c}{2E_F - E} \right).
\]

If \( N(0)V \ll 1 \), we can solve approximatively for the energy \( E \)

\[
E \approx 2E_F - 2\hbar \omega_c e^{-\frac{2}{N(0)V}} < 2E_F.
\]
Origin of Attractive Interaction

Negative terms come in when one takes the motion of the ion cores into account, e.g. considering electron-phonon interactions. The physical idea is that

- the first electron polarizes the medium by attracting positive ions;
- these excess positive ions in turn attract the second electron, giving an effective attractive interaction between the electrons.
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Having seen that the Fermi sea is unstable against the formation of a bound Cooper pair when the net interaction is attractive, we must then expect pairs to condense until an equilibrium point is reached. We need a smart way to write down antisymmetric wavefunctions for many electrons. This will be done in the language of second quantization.
BCS Theory

Introduce the creation operator $c_{k\sigma}^\dagger$, which creates an electron of momentum $k$ and spin $\sigma$, and the corresponding annihilation operator $c_{k\sigma}$. These operators obey the standard anticommutation relations for fermions:

$$\{ c_{k\sigma}, c_{k'\sigma'}^\dagger \} \equiv c_{k\sigma} c_{k'\sigma'}^\dagger + c_{k'\sigma'}^\dagger c_{k\sigma} = \delta_{kk'} \delta_{\sigma\sigma'}$$

$$\{ c_{k\sigma}, c_{k'\sigma'} \} = 0 = \{ c_{k\sigma}^\dagger, c_{k'\sigma'}^\dagger \}.$$

Additionally, the particle number operator $n_{k\sigma}$ is defined by

$$n_{k\sigma} \equiv c_{k\sigma}^\dagger c_{k\sigma}.$$
We start with the so-called

**pairing-hamiltonian**

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

presuming that it includes the terms that are decisive for superconductivity, although it omits many other terms which involve electrons not paired as \((\mathbf{k} \uparrow, -\mathbf{k} \downarrow)\).
The model Hamiltonian

We then add a term $-\mu N$, where $\mu$ is the chemical potential, leading to

$$\mathcal{H} - \mu N = \sum_{k\sigma} \xi_k n_{k\sigma} + \sum_{kl} V_{kl} c_{k\uparrow}^\dagger c_{l\downarrow}^\dagger c_{-k\downarrow} c_{l\uparrow}^\dagger.$$ 

The inclusion of this factor is mathematically equivalent to taking the zero of kinetic energy to be at $\mu$ (or $E_F$).
Bogoliubov-Valatin-Transformation

Define:

\[ b_k \equiv \langle c_{-k}\downarrow c_k\uparrow \rangle \]

Because of the large number of particles involved, the fluctuations of \( c_{-k}\downarrow c_k\uparrow \) about these expectations values \( b_k \) should be small. Therefore express such products of operators formally as

\[ c_{-k}\downarrow c_k\uparrow = b_k + (c_{-k}\downarrow c_k\uparrow - b_k) \]

and neglect quantities which are bilinear in the presumably small fluctuation term in parentheses.
Bogoliubov-Valatin-Transformation

Inserting this in our pairing Hamiltonian we obtain the so-called model-hamiltonian

\[ \mathcal{H}_M - \mu N = \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{kl} V_{kl} \left( c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger b_l + b_k^* c_{-l\downarrow} c_{l\uparrow} - b_k^* b_l \right) \]

where the \( b_k \) are to be determined self-consistently.
Bogoliubov-Valatin-Transformation

Defining further

\[ \Delta_k = - \sum_l V_{kl} b_l = - \sum_l V_{kl} \langle c_{-k\downarrow} c_{k\uparrow} \rangle \]

leads to the following form of the model-hamiltonian

\[ \mathcal{H}_M - \mu \mathcal{N} = \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} - \sum_k (\Delta_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + \Delta_k^* c_{-k\downarrow} c_{k\uparrow} - \Delta_k b_k^*) \]
Bogoliubov-Valatin-Transformation

This Hamiltonian can be diagonalized by a suitable linear transformation to define new Fermi operators $\gamma_k$:

\[
\begin{align*}
  c_{k\uparrow} &= u_k^* \gamma_{k\uparrow} + v_k \gamma_{-k\downarrow} \\
  c_{-k\downarrow}^\dagger &= -v_k^* \gamma_{k\uparrow} + u_k \gamma_{-k\downarrow}^\dagger
\end{align*}
\]

with $|u_k|^2 + |v_k|^2 = 1$. Our "job" is now to determine the values of $v_k$ and $u_k$. 
The model Hamiltonian

\[ \mathcal{H}_M - \mu \mathcal{N} = \sum_k \xi_k \left( (|u_k|^2 - |v_k|^2)(\gamma_{k\uparrow} \gamma_{k\uparrow} + \gamma_{-k\downarrow} \gamma_{-k\downarrow}) \right. \]

\[ + 2|v_k|^2 + 2u_k^* v_k^* \gamma_{-k\downarrow} \gamma_{k\uparrow} + 2u_k v_k \gamma_{k\uparrow}^\dagger \gamma_{-k\downarrow}^\dagger \right) \]

\[ + \sum_k \left( (\Delta_k u_k v_k^* + \Delta_k^* u_k^* v_k)(\gamma_{k\uparrow}^\dagger \gamma_{k\uparrow} + \gamma_{-k\downarrow}^\dagger \gamma_{-k\downarrow} - 1) \right. \]

\[ + (\Delta_k v_k^*^2 - \Delta_k^* u_k^*^2) \gamma_{-k\downarrow} \gamma_{k\uparrow} \]

\[ + (\Delta_k^* v_k^2 - \Delta_k u_k^2) \gamma_{k\uparrow}^\dagger \gamma_{-k\downarrow}^\dagger + \Delta_k b_k^* \right). \]
Choose $u_k$ and $v_k$ so that the coefficients of $\gamma_{-k\downarrow}\gamma_{k\uparrow}$ and $\gamma_{k\uparrow}^\dagger\gamma_{-k\downarrow}^\dagger$ vanish.

\[
\Rightarrow 2\xi_k u_k v_k + \Delta_k^* v_k^2 - \Delta_k u_k^2 = 0
\]

\[
\Rightarrow \left( \frac{\Delta_k^* v_k}{u_k} \right)^2 + 2\xi_k \left( \frac{\Delta_k^* v_k}{u_k} \right) - |\Delta_k|^2 = 0
\]

\[
\Rightarrow \frac{\Delta_k^* v_k}{u_k} = \sqrt{\xi_k^2 + |\Delta_k|^2 - \xi_k} \equiv E_k - \xi_k
\]
Bogoliubov-Valatin-Transformation

This gives us an equation for the $v_k$ and $u_k$ as

$$|v_k|^2 = 1 - |u_k|^2 = \frac{1}{2} \left( 1 - \frac{\xi_k}{E_k} \right).$$
The BCS ground state

BCS took as their form for the ground state

$$|\psi_G\rangle = \prod_k (u_k + v_k c_k^{\dagger} c_{-k\downarrow}^{\dagger}) |0\rangle$$

where $|u_k|^2 + |v_k|^2 = 1$. This form implies that the probability of the pair $(k \uparrow, -k \downarrow)$ being occupied is $|v_k|^2$, whereas the probability that it is unoccupied is $|u_k|^2 = 1 - |v_k|^2$.

Note: $|\psi_G\rangle$ is the vacuum state for the $\gamma$ operators, e.g.

$$\gamma_{k\uparrow} |\psi_G\rangle = 0 = \gamma_{-k\downarrow} |\psi_G\rangle$$
Calculation of the condensation energy

We can now calculate the groundstate energy to be

\[
\langle \Psi_G | \mathcal{H} - \mu N | \Psi_G \rangle = 2 \sum_k \xi_k v_k^2 + \sum_{kl} V_{kl} u_k v_k u_l v_l
\]

\[
= \sum_k \left( \xi_k - \frac{\xi_k^2}{E_k} \right) - \frac{\Delta^2}{V}
\]

The energy of the normal state at \( T = 0 \) corresponds to the BCS state with \( \Delta = 0 \) and \( E_k = |\xi_k| \). Thus

\[
\langle \Psi_n | \mathcal{H} - \mu N | \Psi_n \rangle = \sum_{|k| < k_F} 2 \xi_k
\]
Calculation of the condensation energy

Thus, the condensation energy is given by

$$\langle E \rangle_s - \langle E \rangle_n = \sum_{|k| > k_F} \left( \xi_k - \frac{\xi_k^2}{E_k} \right) + \sum_{|k| < k_F} \left( -\xi_k - \frac{\xi_k^2}{E_k} \right) - \frac{\Delta^2}{V}$$

$$= 2 \sum_{|k| > k_F} \left( \xi_k - \frac{\xi_k^2}{E_k} \right) - \frac{\Delta^2}{V}$$

$$= \left( \frac{\Delta^2}{V} - \frac{1}{2} N(0) \Delta^2 \right) - \frac{\Delta^2}{V} = -\frac{1}{2} N(0) \Delta^2$$
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Excitation Energies and the Energy Gap

With the above choice of the $u_k$ and $v_k$, the model-hamiltonian becomes

$$H_M - \mu N = \sum_k (\xi_k - E_k + \Delta_k b_k^*) + \sum_k E_k (\gamma_{k\uparrow} \gamma_{k\uparrow} + \gamma_{-k\downarrow} \gamma_{-k\downarrow}).$$

$$E_k = \sqrt{\Delta_k^2 + \xi_k^2}$$
Excitation Energies and the Energy Gap

Figure: Energies of elementary excitations in the normal and superconducting states as functions of $\xi_k$. 
Inserting the $\gamma$ operators in the definition of $\Delta_k$ gives

$$\Delta_k = - \sum_l V_{kl} \langle c_{-l\downarrow} c_{l\uparrow} \rangle$$

$$= - \sum_l V_{kl} u_l^* v_l \langle 1 - \gamma_{l\uparrow}^\dagger \gamma_{l\uparrow} - \gamma_{-l\downarrow}^\dagger \gamma_{-l\downarrow} \rangle$$

$$= - \sum_l V_{kl} u_l^* v_l (1 - 2f(E_l))$$

$$= - \sum_l V_{kl} \frac{\Delta_l}{2E_l} \tanh \frac{\beta E_l}{2}$$
Using again the approximated potential $V_{kl} = -V$, we have $\Delta_k = \Delta_l = \Delta$ and therefore

$$\frac{1}{V} = \frac{1}{2} \sum_k \frac{\tanh(\beta E_k/2)}{E_k}.$$ 

This formula determines the critical temperature $T_c$!
Determination of $T_c$

The critical temperature $T_c$ is the temperature at which $\Delta_k \to 0$ and thus $E_k \to \xi_k$. By inserting this in the above formula, rewriting the sum as an integral and changing to a dimensionless variable we find

$$\frac{1}{N(0)V} = \int_0^{\beta_c \hbar \omega_c / 2} \frac{\tanh x}{x} dx = \ln \left( \frac{2e^\gamma}{\pi} \beta_c \hbar \omega_c \right)$$

($\gamma \approx 0.577...$: the Euler constant)
Determination of $T_c$

Critical temperature $T_c$

$$kT_c = \beta_c^{-1} \approx 1.13\hbar\omega_c e^{-1/N(0)V}$$
Determination of $T_c$

For small temperatures we find

\[
\frac{1}{N(0)V} = \int_0^{\hbar \omega_c} \frac{d\xi}{(\xi^2 + \Delta^2)^{1/2}}
\]

\[\Rightarrow \Delta = \frac{\hbar \omega_c}{\sinh(1/N(0)V)} \approx 2\hbar \omega_c e^{-1/N(0)V},\]

which shows that $T_c$ and $\Delta(0)$ are not independent from each other

\[
\frac{\Delta(0)}{kT_c} \approx \frac{2}{1.13} \approx 1.764
\]
Temperature dependence of the energy gap

Rewriting again

\[ \frac{1}{V} = \frac{1}{2} \sum_{k} \frac{\tanh(\beta E_k/2)}{E_k}. \]

in an integral form and inserting \( E_k \) gives

\[ \frac{1}{N(0)V} = \int_{0}^{\hbar \omega_c} \frac{\tanh \left( \frac{\hbar \omega_c}{2} \beta (\xi^2 + \Delta^2)^{1/2} \right)}{(\xi^2 + \Delta^2)^{1/2}} d\xi, \]

which can be evaluated numerically.
Temperature dependence of the energy gap

**Figure:** Temperature dependence of the energy gap with some experimental data (Phys. Rev. 122, 1101 (1961))
Temperature dependence of the energy gap

Near $T_c$ we get

\[
\frac{\Delta(T)}{\Delta(0)} \approx 1.74 \left(1 - \frac{T}{T_c}\right)^{1/2}, \quad T \approx T_c,
\]

which shows the typical square root dependence of the order parameter for a mean-field theory.
Thermodynamic quantities

With $\Delta(T)$ determined, we know the fermion excitation energies $E_k = \sqrt{\xi_k^2 + \Delta(T)^2}$. Then the quasi-particle occupation numbers will follow the Fermi-function $f_k = (1 + e^{\beta E_k})^{-1}$, which determine the electronic entropy for a fermion gas

$$S_{es} = -2k \sum_k ((1 - f_k) \ln(1 - f_k) + f_k \ln f_k).$$
Thermodynamic quantities

Figure: Electronic entropy in the superconducting and normal state.
Given $S_{es}(T)$, we find the specific heat

$$C_{es} = -\beta \frac{dS_{es}}{d\beta} = 2\beta k \sum_k -\frac{\partial f_k}{\partial E_k} \left( E_k^2 + \frac{1}{2\beta} \frac{d\Delta^2}{d\beta} \right)$$

In the normal state we have

$$C_{en} = \frac{2\pi^2}{3} N(0) k^2 T.$$
We expect a jump in the specific heat from the superconducting to the normal state:

\[
\Delta C = (C_{es} - C_{en})|_{T_c} = N(0) \left( \frac{-d\Delta^2}{dT} \right)|_{T_c} \approx 9.4N(0)k^2T_c
\]
Thermodynamic quantities

**Figure**: Experimental data for the specific heat in the superconducting and normal state (Phys. Rev. **114**, 676 (1959))
Type I superconductors

Figure: Phase diagram of a Type I superconductor
Vortex-State

The Nobel Prize in Physics 2003

"for pioneering contributions to the theory of superconductors and superfluids"

Type I and Type II superconductors

By applying Ginzburg-Landau theory for superconductors one finds two characteristic lengths:

1. The Landau penetration depth for external magnetic fields $\lambda$ and
2. the Ginzburg-Landau coherence length $\xi$, which characterizes the distance over which $\psi$ can vary without undue energy increase.
Type I and Type II superconductors

Define

\[ \kappa \equiv \frac{\lambda}{\xi} \]

By linearizing the GL equations near \( T_c \) one can find:

\[ \kappa < \frac{1}{\sqrt{2}} : \text{Type I superconductor} \]

\[ \kappa > \frac{1}{\sqrt{2}} : \text{Type II superconductor} \]
Type II superconductors

Figure: Phase diagram of a Type II superconductor
As a solution of the GL equation, one could find the following form of the orderparameter:

$$\psi(x, y) = \frac{1}{N} \sum_{n=-\infty}^{\infty} \exp \left( \frac{\pi (ixy - y^2)}{\omega_1 \Im \omega_2} + i\pi n \right)$$

$$+ \frac{i\pi (2n + 1)}{\omega_1} (x + iy) + i\pi \frac{\omega_2}{\omega_1} n(n + 1)$$

$$N = \left( \frac{\omega_1}{2 \Im \omega_2} \exp \left( \frac{\Im \omega_2}{\omega_1} \right) \right)^{1/4}$$
Vortex-State

**Figure:** Square and triangle symmetric state of the vortex lattice in a density plot of $|\Psi|^2$. 
Vortex-State

Figure: Square and triangle symmetric state of the vortex lattice in a 3D plot.
Summary

- An attractive interaction between electrons will result in forming bound Cooper pairs.
- The model-hamiltonian can be diagonalized using a Bogoliubov-Valatin-Transformation.
- The order parameter in a superconductor is the energy-gap $\Delta$.
- BCS-Theory gives a prediction of the critical temperature $T_c$ and the energy gap $\Delta(T)$.
- Vortices will be observed in Type II superconductors.
Thank you for your attention!

Are there any questions?