Chapter 4

Microscopic Theory
Superconductivity and Low Temperature Physics I

Lecture No. 7

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Chapter 4

4. Microscopic Theory

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4. BCS Theory

- after discovery of superconductivity, initially many phenomenological theories have been developed
  - London theory (1935)
  - macroscopic quantum model of superconductivity (1948)
  - Ginzburg-Landau-Abrikosov-Gorkov theory (early 1950s)

- problem:
  - phenomenological theories do not provide insight into the microscopic processes responsible for superconductivity
  - impossible to engineer materials to increase $T_c$, if mechanisms are not known

- superconductivity originates from interactions among conduction electrons
  - theoretical models for the description of interacting electrons are required
    - very complicated: kinetic energy of conduction electrons $\sim 5$ eV, while interaction energy $\sim$ meV
      - find attractive interaction which causes ordering in electron system despite high kinetic energy
    - go beyond single electron (quasiparticle) models
    - not available at the time of discovery of superconductivity
4. BCS Theory

- development of **BCS theory by J. Bardeen, L.N. Cooper and J.R. Schrieffer** in 1957
  - key element is **attractive interaction** among conduction electrons
  - 1956: Cooper shows that attractive interaction results in **pair formation** and in turn in an instability of the Fermi sea of a free electron gas
  - 1957: Bardeen, Cooper and Schrieffer develop self-consistent formulation of the superconducting state: **condensation of pairs in coherent ground state**
  - paired electrons are denoted as **Cooper pairs**

- general description of interactions by exchange bosons
  - Bardeen, Cooper and Schrieffer identify **phonons** as the relevant exchange bosons
  - suggested by experimental observation
    \[ T_c \propto \frac{1}{\sqrt{M}} \propto \omega_{ph} \]  
    **isotope effect**
  - in general, detailed nature of exchange boson does not play any role in BCS theory
  - many possible exchange bosons:
    - **magnons, polarons, plasmons, polaritons, spin fluctuations**, ....
4. BCS Theory

Isotop effect yields hint on type of exchange boson:

Data from:
E. Maxwell, Phys. Rev. 86, 235 (1952)
B. Serin, C.A. Reynolds, C. Lohman, Phys. Rev. 86, 162 (1952)

\[
T_c \propto \frac{1}{\sqrt{M}}
\]

In general: \( T_c \propto \frac{1}{M^{\beta^*}} \)

<table>
<thead>
<tr>
<th>Element</th>
<th>Hg</th>
<th>Sn</th>
<th>Pb</th>
<th>Cd</th>
<th>Tl</th>
<th>Mo</th>
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<td>0,33</td>
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</table>
4.1 Attractive Electron–Electron Interaction

- **intuitive assumption:**
  superconductivity results from *ordering phenomenon of conduction electrons*

- **problem:**
  - conduction electrons have *large (Fermi) velocity* due to Pauli exclusion principle: $\approx 10^6 \text{ m/s} \approx 0.01 \text{ c}$
  - corresponding (Fermi) temperature is above 10 000 K
  - in contrast: transition to superconductivity occurs at $\approx 1 - 10 \text{ K} (\approx \text{ meV})$

- **task:**
  - find *interaction mechanism* that results in ordering of conduction electrons despite their high kinetic energy
  - initial attempts fail:
    - Coulomb interaction (Heisenberg, 1947)
    - magnetic interaction (Welker, 1929)
    - .....
4.1.1 Phonon Mediated Interaction

- known fact since 1950:
  - $T_c$ depends on isotope mass

- conclusion:
  - lattice plays an important role for superconductivity
  - initial proposals for phonon mediated e-e interaction (1950):
    
    H. Fröhlich, J. Bardeen

- static model of lattice mediated e-e interaction:
  - one electron causes elastic distortion of lattice:
    - attractive interaction with positive ions results in positive charge accumulation
  - second electron is attracted by this positive charge accumulation:
    - effective binding energy

  intuitive picture, but has to be taken with care

  wrong suggestion:
  - Cooper pairs are stable in time such as hydrogen molecule
  - pairing in real space

http://www.max-wissen.de/
4.1.1 Phonon Mediated Interaction

- **dynamic model of lattice mediated e-e interaction:**
  - moving electrons distort lattice, causing temporary positive charge accumulation along their path
    - track of positive charge cloud
    - positive charge cloud can attract second electron
  - important: positive charge cloud rapidly relaxes again → *dynamic model*

![Diagram of electron interaction](image)

- important question: How fast relaxes positive charge cloud when electron moves through the lattice?
- characteristic time scale $\tau$:
  - frequency $\omega_q$ of lattice vibrations (phonons): $\tau = 1/\omega_q$
  - $\omega_q \approx 10^{12} - 10^{13}$ 1/s (maximum frequency: Debye frequency $\omega_D$)
4.1.1 Phonon Mediated Interaction

- resulting range of interaction (order of magnitude estimate)
  - how far can a second electron be, to be attracted by the positive space charge before it relaxes
  - characteristic velocity of conduction electrons: \( v_F \approx \text{few } 10^6 \text{ m/s} \)

  \[ \text{interaction range: } v_F \cdot \tau \approx 10^6 \frac{\text{m}}{\text{s}} \cdot 10^{-13} \text{ s} \approx 0.1 \text{ \(\mu\)m} \] (is related to GL coherence length)

- important fact:
  - retarded reaction of slow ions results in large interaction range
    \( \Rightarrow \) retardation of interaction
  - retarded interaction is essential for achieving attractive interaction
    \( \Rightarrow \) without any retardation:
    - short interaction range
    - Coulomb repulsion between electrons dominates

- retarded interaction has been addressed during discussion of screening of phonons in metals

  \( \Rightarrow \) retardation interaction potential:

  \[
  V(q, \omega) = \frac{e^2}{\varepsilon(q, \omega) \varepsilon_0 q^2} = \left( \frac{e^2}{\epsilon_0 (q^2 + k_s^2)} \right) \left( 1 + \frac{\tilde{\Omega}_p^2(q)}{\omega^2 - \tilde{\Omega}_p^2(q)} \right)
  \]

  screened Coulomb potential
  \[ \frac{1}{k_s} = \text{Thomas-Fermi screening length} \]

  q-dependent plasma frequency of the screened ions

  \[ \tilde{\Omega}_p^2(q) = \Omega_p^2(q) \left( 1 + \frac{k_s^2}{q^2} \right) \]

  correction term is negative for \( \omega < \tilde{\Omega}_p(q) \) \( \Rightarrow \) overscreening
4.1.1 Phonon Mediated Interaction

\[ V(q, \omega) = \frac{e^2}{\epsilon(q, \omega) \epsilon_0 q^2} \]

\[ = \left( \frac{e^2}{\epsilon_0 (q^2 + k_s^2)} \right) \left( 1 + \frac{\tilde{\Omega}_p^2(q)}{\omega^2 - \tilde{\Omega}_p^2(q)} \right) \]

**Effective e-ph interaction potential**
4.1.2 Cooper-Pairs

- **Question**: How can we formally describe the pairing interaction?

- **starting point**: free electron gas at $T = 0$ (all states occupied up to $E_F = \frac{\hbar^2 k_F^2}{2m}$)

- **Gedanken experiment**:
  - add two further electrons, which can interact via the lattice
  - describe the interaction by exchange of *virtual phonon*
    virtual phonon: is generated and reabsorbed again within time $\Delta t \lesssim 1/\omega_q$

- wave vectors of electrons after exchange of virtual phonon with wave vector $q$:
  - electron 1: $k'_1 = k_1 + q$
  - electron 2: $k'_2 = k_2 - q$

- total momentum is conserved: $K = k_1 + k_2 = k'_1 + k'_2 = K'$

- note: - since at $T = 0$ all states are occupied below $E_F$, additional states have to be at $E > E_F$
  - maximum phonon energy: $\hbar \omega_q = \hbar \omega_D$ (Debye energy)
    - accessible energy interval: $[E_F, E_F + \hbar \omega_D]$
    - interaction takes place in a spherical shell with radius $k_F$ and thickness $\Delta k \approx \frac{m \omega_D}{\hbar k_F}$
    - for given $K$ only specific wave vectors $k_1, k_2$ are allowed for interaction process
4.1.2 Cooper-Pairs

\[ K = k_1 + k_2 > 0 \]

\[ K = k_1 + k_2 = 0 \]

**possible phase space for interaction**

**possible phase space is complete spherical shell**

- **important conclusion**: available phase space for interaction is maximum for \( K = 0 \) or equivalently \( k_1 = -k_2 \)

**Cooper pairs with zero total momentum**: \((k, -k)\)

\[
\frac{\hbar^2 k_F^2}{2m} + \hbar \omega_D \approx \frac{\hbar^2 (k + \Delta k)^2}{2m} = \frac{\hbar^2 k_F^2}{2m} + \frac{\hbar^2 k_F \Delta k}{m}
\]

\[ \Delta k = \frac{m \omega_D}{\hbar k_F} \]
4.1.2 Cooper-Pairs

wave function of Cooper pairs and corresponding energy eigenvalues:

- two-particle wave function is chosen as product of two plane waves
  \[ \psi(r_1, r_2) = a \exp(\imath k_1 \cdot r_1) \exp(\imath k_2 \cdot r_2) = a \exp(\imath k \cdot r) \quad \text{with } k = k_1 = -k_2, \quad r = r_1 - r_2 \]

- since pair-correlated electrons are permanently scattered into new states in interval \([k_F, k_F + \Delta k]\)
  \n  \[ \rightarrow \text{pair wave function} = \text{superposition of product wave functions} \]

\[
\psi(r_1, r_2) = \sum_{k = k_F}^{k_F + \Delta k} a_k \exp(\imath k \cdot r)
\]

- note:
  \- electron with \(k < k_F\) cannot participate in interaction since all states are occupied
  \- we will see later that superconductor overcomes this problem by rounding-off \(f(E)\) even at \(T = 0\)
    \- superconductor first has to pay (kinetic) energy for rounding-off \(f(E)\)
    \- energy is obtained back by pairing interaction (potential energy)
    \- net energy gain
4.1.2 Cooper-Pairs

wave function of Cooper pairs and corresponding energy eigenvalues:

- we assume that pairing interaction only depends on relative coordinate \( \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \)

- Schrödinger equation:

\[
-\frac{\hbar^2}{2m} \left( \nabla_1^2 + \nabla_2^2 \right) \psi(\mathbf{r}_1, \mathbf{r}_2) + V(\mathbf{r}) \psi(\mathbf{r}_1, \mathbf{r}_2) = E \psi(\mathbf{r}_1, \mathbf{r}_2)
\]

- insert \( \psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{k=k_F}^{k_F+\Delta k} a_k e^{i\mathbf{k} \cdot \mathbf{r}} \), multiply by \( e^{-i\mathbf{k}' \cdot \mathbf{r}} \) and integrate over sample volume \( \Omega \)

\[
\int_\Omega \frac{\hbar^2 k^2}{m} \sum_{k=k_F}^{k_F+\Delta k} a_k \exp(i\mathbf{k} \cdot \mathbf{r}) \exp[-i(\mathbf{k}' \cdot \mathbf{r})] \, dV + \int_\Omega V(\mathbf{r}) \sum_{k=k_F}^{k_F+\Delta k} a_k \exp(i\mathbf{k} \cdot \mathbf{r}) \exp[-i(\mathbf{k}' \cdot \mathbf{r})] \, dV = \int_\Omega E \sum_{k=k_F}^{k_F+\Delta k} a_k \exp(i\mathbf{k} \cdot \mathbf{r}) \exp[-i(\mathbf{k}' \cdot \mathbf{r})] \, dV
\]

- integration over sample volume \( \Omega \):

\[
\int_\Omega \exp[i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}] \, dV = \begin{cases} 
0 & \text{for } \mathbf{k} \neq \mathbf{k}' \\
\Omega & \text{for } \mathbf{k} = \mathbf{k}' 
\end{cases}
\]

\[
\int_\Omega \frac{\hbar^2 k^2}{m} \sum_{k=k_F}^{k_F+\Delta k} a_k \exp(i\mathbf{k} \cdot \mathbf{r}) \exp[-i(\mathbf{k}' \cdot \mathbf{r})] \, dV + \int_\Omega V(\mathbf{r}) \sum_{k=k_F}^{k_F+\Delta k} a_k \exp(i\mathbf{k} \cdot \mathbf{r}) \exp[-i(\mathbf{k}' \cdot \mathbf{r})] \, dV = \int_\Omega E \sum_{k=k_F}^{k_F+\Delta k} a_k \exp(i\mathbf{k} \cdot \mathbf{r}) \exp[-i(\mathbf{k}' \cdot \mathbf{r})] \, dV
\]

 scattering integral

\[
\frac{\hbar^2 k^2}{m} a_k \Omega
\]

\[
E a_k \Omega
\]
4.1.2 Cooper-Pairs

- we use abbreviation

\[ V_{k,k'} = V_{k_1,k_2,q} = V(k-k') = V(q) = \frac{1}{\Omega} \int V(r) \, e^{i(k-k') \cdot r} \, dV = \frac{1}{\Omega} \int V(r) \, e^{i q \cdot r} \, dV \]

with \( k_1 = k, k_2 = -k, q = k - k' \)

- result

\[ (E - \frac{\hbar^2 k^2}{m}) a_k = \sum_{k' = k_F}^{k_F + \Delta k} a_{k'} V_{k,k'} \]

**problem:**
we have to know all matrix elements \( V_{k,k'} \)!!!

- simplifying assumption to solve the problem:

\[ V_{k,k'} = \begin{cases} -V_0 & \text{for } k' > k_F, k < k_F + \Delta k \\ 0 & \text{else} \end{cases} \]

with \( \Delta k = \frac{m \omega_D}{\hbar k_F} \)

\[ (E - \frac{\hbar^2 k^2}{m}) a_k = \sum_{k' = k_F}^{k_F + \Delta k} a_{k'} V_{k,k'} \]  

\[ a_k = \frac{-V_0}{E - \left( \frac{\hbar^2 k^2}{m} \right)} \sum_{k' = k_F}^{k_F + \Delta k} a_{k'} \]
4.1.2 Cooper-Pairs

- summing up over all \( k \) using \( \sum_k a_k = \sum_{k'} a_{k'} \) yields:

\[
\sum_{k=k_F}^{k_F+\Delta k} a_k = V_0 \sum_{k=k_F}^{k_F+\Delta k} \frac{1}{\left(\frac{\hbar^2 k^2}{m} - E\right)} \sum_{k'=k_F}^{k_F+\Delta k} a_{k'}
\]

\[
1 = V_0 \sum_{k=k_F}^{k_F+\Delta k} \frac{1}{\left(\frac{\hbar^2 k^2}{m} - E\right)}
\]

- we introduce pair density of states \( \tilde{D}(E) = D(E)/2 \): sum \( \Rightarrow \) integral

\[
1 = V_0 \int_{E_F}^{E_F+\hbar \omega_D} \frac{d\epsilon}{2\epsilon - E} \quad \text{with} \quad \epsilon = \frac{\hbar^2 k^2}{2m}
\]
4.1.2 Cooper-Pairs

- integration and resolving for $E$ results in

$$1 = V_0 \frac{D(E_F)}{2} \int_{E_F}^{E_F + \hbar \omega_D} \frac{d\varepsilon}{(2\varepsilon - E)} = V_0 \frac{D(E_F)}{2} \cdot \frac{1}{2} \ln|2\varepsilon - E|$$

$$E = 2E_F - 2\hbar \omega_D \frac{\exp\left(-\frac{4}{V_0 D(E_F)}\right)}{1 - \exp\left(-\frac{4}{V_0 D(E_F)}\right)}$$

$$\exp\left(-\frac{4}{V_0 D(E_F)}\right) = \frac{|2E_F - E|}{|2E_F + 2\hbar \omega_D - E|}$$

$$\Rightarrow \frac{4}{V_0 D(E_F)} = \ln|2E_F - E| - \ln|2E_F - E|$$

$$\Rightarrow [2E_F + 2\hbar \omega_D - E] \exp\left(-\frac{4}{V_0 D(E_F)}\right) = |2E_F - E|$$

$$\Rightarrow [2E_F - E] \left[1 - \exp\left(-\frac{1}{V_0 D(E_F)}\right)\right] = 2\hbar \omega_D \exp\left(-\frac{1}{V_0 D(E_F)}\right)$$

- for weak interaction $V_0 D(E_F) \ll 1$ we obtain:

$$E \approx 2E_F - 2\hbar \omega_D \exp\left(-\frac{4}{V_0 D(E_F)}\right)$$

- binding energy of Cooper pairs is $\propto \hbar \omega_D$ (isotope effect as $\omega_D \propto M^{-1/2}$)

- as $\hbar \omega_D \ll E_F$ and $\exp\left(-\frac{4}{V_0 D(E_F)}\right) \ll 1 \Rightarrow$ binding energy is very small
4.1.2 Cooper-Pairs

- binding energy of Cooper pairs:

\[ E \approx 2E_F - 2\hbar \omega_D \exp\left( -\frac{4}{V_0 D(E_F)} \right) \]

**important result:**

- energy of interacting electron pair is smaller than \( 2E_F \)
- bound pair state (Cooper pair)
- binding energy depends on \( V_0 \) and maximum phonon energy \( \hbar \omega_D \)

**Note 1:**

- electrons with \( k < k_F \) cannot participate in interactions as all states for \( E < E_F \) are occupied (no free scattering state)
- superconductor solves this problem by smearing out Fermi distribution even at \( T = 0 \)
  - superconductor first has to pay kinetic energy to occupy state above \( E_F \)
  - increase of kinetic energy is overcompensated by pairing energy (potential energy)
  - total energy is reduced \( \Rightarrow \) **condensation energy**

**Note 2:**

- in Gedanken experiment we have considered only two additional electrons above \( E_F \)
- in real superconductor: interaction of all electrons in energy interval around \( E_F \)
- electron gas becomes instable against pairing
  - instability causes transition into new ground state: **BCS ground state**
4.1.2 Cooper-Pairs

estimate of the interaction range from the uncertainty relation

\[ \Delta k = \frac{m \omega_D}{\hbar k_F} = \frac{\omega_D}{v_F} \Rightarrow \Delta x = \frac{1}{\Delta k} = \frac{v_F}{\omega_D} \]

with \( v_F \sim 10^6 \text{ m/s} \) and \( \omega_D \sim 10^{13} \text{ s}^{-1} \) \( \Rightarrow \) interaction range \( R \sim 100 \text{ nm} \)

how many Cooper pairs do we find in volume \( \frac{4}{3} \pi R^3 \) defined by interaction range

\[ \begin{align*}
&\text{electro\text{on density in metal:} } D(E_F)/V \sim 10^{28} \text{ eV}^{-1} \text{ m}^{-3} \\
&\text{relevant energy interval: } \hbar \omega_D \sim 0.01 - 0.1 \text{ eV} \\
N &= 10^{28} \cdot \hbar \omega_D \cdot \frac{4}{3} \pi (10^{-7})^3 \sim 10^5 - 10^6
\end{align*} \]

\( \Rightarrow \) strong overlap of pairs

\( \Rightarrow \) formation of coherent many body state
4.1.2 Cooper-Pairs

Attractive interaction via exchange of virtual phonons: how does the matrix element \( V_{k,k'} = V_{k_1,k_2,q} \) look like?

- Pure Coulomb interaction
  \[
  V(q) = \frac{e^2}{\epsilon_0 q^2} = \int \left( \frac{e^2}{4\pi \epsilon_0 r} \right) e^{-i q \cdot r} \, d^3r
  \]
  Positive matrix element \( \rightarrow \) repulsive interaction

- Screened Coulomb interaction
  \[
  V(q,\omega) = \frac{e^2}{\epsilon_0 (q^2 + k_s^2)} = \int \left( \frac{e^2}{4\pi \epsilon_0 r} e^{-i k_s r} \right) e^{-i q \cdot r} \, d^3r
  \]
  Positive matrix element \( \rightarrow \) repulsive interaction
  \( k_s = \) Thomas-Fermi wave number, \( k_s \sim \pi/a \)

- Screened Coulomb interaction in metals:
  \[
  V(q,\omega) = \frac{e^2}{\epsilon(q,\omega) \epsilon_0 q^2} = \left( \frac{e^2}{\epsilon_0 (q^2 + k_s^2)} \right) \left( 1 + \frac{\Omega_p^2(q)}{\omega^2 - \tilde{\Omega}_p^2(q)} \right)
  \]
  Negative matrix element if \( \epsilon(q,\omega) < 0 \) \( \rightarrow \) attractive interaction

  \( \Omega_p^2(q) = \Omega_p^2 / \left[ 1 + \frac{k_s^2}{q^2} \right] \)

  For small energy differences \( (E_k - E_{k'})/\hbar = \omega < \tilde{\Omega}_p(q) \) of the participating electrons
  \( \rightarrow \) denominator gets negative
  \( \rightarrow \) attractive interaction
  \( \rightarrow \) cut-off frequency: \( \omega = \tilde{\Omega}_p \approx \omega_D \) (Debye-Frequenz)
4.1.3 Symmetry of Pair Wavefunction

What is the symmetry of the pair wavefunction?

- **Important**: pair consists of two fermions \( \Rightarrow \) total wavefunction must be antisymmetric: minus sign for particle exchange

\[
\Psi(r_1, \sigma_1, r_2, \sigma_2) = \frac{1}{\sqrt{V}} e^{iK_s \cdot r_s} f(k, r) \chi(\sigma_1, \sigma_2) = -\Psi(r_2, \sigma_2, r_1, \sigma_1)
\]

center of mass motion  
orbital spin  
we assume \( K_s = 0 \)  
part part  

- possible *spin wavefunctions* \( \chi(\sigma_1, \sigma_2) \) for electron pairs

\[
S = \begin{cases} 
0 & m_s = 0 \quad \chi^a = \frac{1}{\sqrt{2}} (\uparrow \downarrow - \downarrow \uparrow) \quad \Rightarrow \text{singlet pairing}, \\
1 & m_s = \begin{cases} 
-1 & \chi^s = \downarrow \downarrow \\
0 & \chi^s = \frac{1}{\sqrt{2}} (\uparrow \downarrow + \downarrow \uparrow) \\
+1 & \chi^s = \uparrow \uparrow 
\end{cases} \quad \Rightarrow \text{triplet pairing},
\end{cases}
\]

antisymmetric spin wavefunction  
symmetric orbital function:  
\( L = 0, 2, \ldots \) (s, d, ....)  

antisymmetric orbital function:  
symmetric spin wavefunction  
\( L = 1, 3, \ldots \) (p, f, ....)
4.1.3 Symmetry of Pair Wavefunction

What is the symmetry of the pair wavefunction?

<table>
<thead>
<tr>
<th>Singlet-Pairing</th>
<th>$S = 0$</th>
<th>$L = 0, 2, 4, ...$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triplet-Pairing</td>
<td>$S = 1$</td>
<td>$L = 1, 3, 5, ...$</td>
</tr>
</tbody>
</table>

- **s-wave superconductor** ($L = 0$)
- **p-wave superconductor** ($L = 1$)
- **d-wave superconductor** ($L = 2$)

- **Symmetric orbital wavefunction**
- **Antisymmetric orbital wavefunction**

- **Metallic superconductors:**
  - $S = 0, L = 0$
- **High temperature (cuprate) superconductors:**
  - $S = 0, L = 2$
- **Suprafluid $^3$He:**
  - $S = 1, L = 1$
4.1.3 Symmetry of Pair Wavefunction

- isotropic interaction: \( V_{k,k'} = -V_0 \)
  - interaction only depends on \(|k|\)
  - in agreement with angular momentum \( L = 0 \) (s-wave superconductor)

- corresponding spin wavefunction must be antisymmetric
  - spin singlet Cooper pairs \( (S = 0) \)

- resulting Cooper pair: \((k \uparrow, -k \downarrow)\)
  - spin singlet Cooper pair \((L = 0, S = 0)\)
  - \( L = 0, S = 0 \) is realized in metallic superconductors (s-wave superconductor)
  - higher orbital momentum wavefunction in cuprate superconductors (HTS):
    - \( L = 2, S = 0 \) (d-wave superconductor)

- spin triplet Cooper pairs \( (S = 1) \):
  - realized in superfluid \(^3\)He: \( L = 1, S = 1 \) (p-wave pairing)
  - evidence for \( L = 1, S = 1 \) also for some heavy Fermion superconductors (e.g. UPt\(_3\))
4.1.3 Symmetry of Pair Wavefunction

$L = 0, S = 0$

$\Delta(k) = \Delta_m$

$L = 2, S = 0$

$\Delta(k) = \frac{\Delta_m}{2} (\cos k_y a - \cos k_x a)$

Superconductivity gets an iron boost
Igor I. Mazin
4.1.3 Symmetry of Pair Wavefunction

**Example: iron-based superconductors – iron pnictides**

- **a.** $s$-wave, e.g. in aluminium
- **b.** $d$-wave, e.g. in copper oxides
- **c.** two-band $s$-wave with the same sign, e.g. in MgB$_2$
- **d.** an $s$-wave, e.g. in iron-based SC
4.1.3 Symmetry of Pair Wavefunction

Example: UPt$_3$

Phase diagram

- Normal phase
- Magnetic field (T)
- Temperature (K)

$f$-wave ($E_{2u}$) Cooper pair wavefunction in three-dimensional momentum space

Michael R. Norman, Science 332, 196-200 (2011)
Summary of Lecture No. 7 (1)

- **microscopic theory of superconductivity**
  - problem: (i) high kinetic energy of conduction electrons: $E_{\text{kin}} \sim \text{eV}$ (corresponding to $T \sim 10\,000\,\text{K}$)
    
  (ii) small interaction strength: $E_{\text{int}} \sim \text{meV}$ (corresponding to $T \sim 10\,\text{K}$)
    
  $\Rightarrow$ find interaction resulting in ordering of conduction electrons despite high $E_{\text{kin}}$
  
  - Cooper (1956): even weak attractive interaction results in instability of free electron gas
    
  $\Rightarrow$ pair formation: Cooper pairs
  
  - general description of interaction by Feynman diagram:
    
    $\Rightarrow$ which exchange boson results in attractive interaction of conduction electrons?
    
    $\Rightarrow$ many candidates: phonon, magnon, polariton, plasmon, polaron, bipolaron, ...

- **isotope effect as „smoking gun“ experiment (1951/1952)**
  
  - transition temperature of different isotopes: $T_c \propto 1/\sqrt{M}$
    
    $\Rightarrow$ as phonon frequency $\omega_{\text{ph}} \propto 1/\sqrt{M}$ $\Rightarrow T_c \propto \omega_{\text{ph}}$
    
    strong evidence for attractive interaction by exchange of virtual phonons

- **BCS-Theorie (1957)**
  
  - qualitative discussion of attractive interaction: slow reaction of positive ions
    
    $\Rightarrow$ retarded interaction
  
  - estimate of interaction range $R \approx v_F \tau \approx v_F/\omega_D$ ($\omega_D$ = Debye frequency)
    
    $v_F \approx 10^6\,\text{m/s}, \omega_D \approx 10^{13}\,\text{s}^{-1} \Rightarrow R \approx 100\,\text{nm}$
  
  - $R \gg$ interaction range of screened Coulomb interaction of conduction electrons
Summary of Lecture No. 7 (2)

• **attractive electron-electron interaction**
  
  - attractive interaction via lattice vibrations (exchange of virtual phonons: Fröhlich, Bardeen)
  
  - scattering matrix element
    
    (i) pure Coulomb interaction:  
    \[ V(q) = \frac{e^2}{\varepsilon_0 q^2} \]  
    (always positive \(\rightarrow\) repulsive interaction)
    
    (ii) screened Coulomb interaction:  
    \[ V(q, \omega) = \frac{e^2}{\varepsilon(q, \omega) \varepsilon_0 q^2} = \left( \frac{e^2}{k_S^2 + q^2} \right) \left( 1 + \frac{\Omega_p^2(q)}{\omega^2 - \Omega_p^2(q)} \right) \]

  ➢ for \(E_k - E_{k'} = \hbar \omega < \hbar \Omega_p(q)\) of involved electrons: denominator becomes negative  
    \(\rightarrow\) negative matrix element \(\rightarrow\) attractive interaction
  
  ➢ **cut-off frequency:**  
    \(\omega = \Omega_p \approx \omega_D\) (Debye frequency)

• **Cooper pairs**
  
  - „Gedanken“ experiment:
    we add 2 additional electrons to Fermi sea at \(T = 0\) and let them interact via exchange of phonons with wave number \(q\)
  
  - scattering process:
    
    electron 1:  
    \[ k_1 \rightarrow k_1' = k_1 + q \]
    
    electron 2:
    \[ k_2 \rightarrow k_2' = k_2 - q \]
    
    total momentum:
    \[ K = k_1 + k_2 = k_1' + k_2' = K' \]

  - only states with \(E > E_F\) are accessible due to full Fermi sea

  - as \(\omega_{ph} < \omega_D\), interaction takes place in energy interval \([E_F, E_F + \hbar \omega_D]\) corresponding to  
    \( k_F \leq k \leq k_F + \frac{\omega_{ph}}{\hbar k_F} = k_F + \Delta k \)

  - conservation of total momentum \(\rightarrow\) wave vectors of scattering electron must be within cut surface of two intersecting circular rings of thickness \(\Delta k\)

  ➢ maximum cut surface (phase space) is obtained for \(K = 0\) or \(k_1 = -k_2\)  
    \(\rightarrow\) **Cooper pairs** \((k, -k)\)
**Summary of Lecture No. 7 (3)**

- **Cooper pair interaction**
  - Ansatz: pair wave function = superposition of product wave functions:
    \[ \Psi(r_1, r_2) = \sum_{k=k_F} a_k \exp(i k \cdot r) \]
    \[ r = r_2 - r_1 \]
  - Schrödinger equation:
    \[ -\frac{\hbar^2}{2m} \left( \nabla_1^2 + \nabla_2^2 \right) \Psi(r_1, r_2) + V(r) \Psi(r_1, r_2) = E \Psi(r_1, r_2) \]
  - Vereinfachung:
    \[ V_{k,k'} = \begin{cases} -V_0 & \text{for } k' > k_F, k < k_F + \Delta k \\ 0 & \text{else} \end{cases} \]
    \[ \text{with } \Delta k = \frac{m\omega_D}{\hbar k_F} \]
  - total energy:
    \[ E \approx 2E_F - 2\hbar\omega_D \exp \left( -\frac{4}{V_0 D(E_F)} \right) \]
    for weak interaction: \( V_0 D(E_F) \ll 1 \)
    binding energy:
    \[ E - 2E_F \propto \hbar\omega_D \text{ (phonon energy)} \]
  - uncertainty relation:
    \[ \Delta k \Delta x \geq 1 \Rightarrow \Delta x \leq \frac{1}{\Delta k} = \frac{v_F}{\omega_D} \approx 100 \text{ nm} \]

- **symmetry of the pair wave function**
  - two fermions \( \rightarrow \) total wave function must be antisymmetric

<table>
<thead>
<tr>
<th>Singlet Pairing</th>
<th>( S = 0 )</th>
<th>( L = 0, 2, 4, ... )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triplet Pairing</td>
<td>( S = 1 )</td>
<td>( L = 1, 3, 5, ... )</td>
</tr>
</tbody>
</table>

- examples: metallic superconductors: \( S = 0, L = 0 \), high-temperature cuprate superconductors: \( S = 0, L = 2 \), superfluid \( ^3\text{He} \): \( S = 1, L = 1 \)
Chapter 4

4. Microscopic Theory
   4.1 Attractive Electron-Electron Interaction
       4.1.1 Phonon Mediated Interaction
       4.1.2 Cooper Pairs
       4.1.3 Symmetry of Pair Wavefunction
   4.2 BCS Ground State
       4.2.1 The BCS Gap Equation
       4.2.2 Ground State Energy
       4.2.3 Bogoliubov-Valatin Transformation and Quasiparticle Excitations
   4.3 Thermodynamic Quantities
   4.4 Determination of the Energy Gap
       4.4.1 Specific Heat
       4.4.2 Tunneling Spectroscopy
   4.5 Coherence Effects
4.2 The BCS Ground State

• discussed so far:
  ➢ nature of the attractive interaction
  ➢ attractive interaction of conduction electrons by exchange of virtual phonons (only two electrons added to Fermi sea)
    ➔ pair formation: Cooper pair
  ➢ symmetry of the pair wave function

• not yet discussed:
  ➢ How does the ground state of the total electron system look like?
  ➢ What is the ground state energy?

• we expect:
  ➢ pairing mechanism goes on until the Fermi sea has changed significantly
  ➢ if pairing energy goes to zero, pairing process will stop
  ➢ detailed theoretical description is complicated ➔ we discuss only basics
formalism of second quantization (occupation number representation) is used (>1927, Dirac, Fock, Jordan et al.)

- 2nd quantization formalism is useful to describe quantum many-body systems
- quantum many-body states are represented in the so-called Fock (number) state basis
  → Fock states are constructed by filling up each single-particle state with a certain number of identical particles

\[ |n_1, n_2, n_3, \ldots, n_\alpha, \ldots \rangle \quad n_\alpha \text{ particles in state } \psi_\alpha \quad n_\alpha = \begin{cases} 0,1 & \text{fermions} \\ 0,1,2,3,\ldots & \text{bosons} \end{cases} \]

- 2nd quantization formalism introduces the creation and annihilation operators to construct and handle the Fock states
- 2nd quantization formalism is also known as the canonical quantization in quantum field theory, in which the fields (wave functions of matter) are upgraded to field operators → analogous to 1st quantization, where the physical quantities are upgraded to operators

conduction electrons can be described by wave pakets

introduction of field operators (2nd quantization of a wave function)

\[ \hat{\Psi}_\sigma (\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_k \hat{c}_k \sigma \ e^{i \mathbf{k} \cdot \mathbf{r}} \quad \leftrightarrow \quad \hat{c}_\sigma (\mathbf{k}) = \hat{c}_k \sigma = \frac{1}{\sqrt{V}} \sum_k \hat{\Psi}_\sigma \ e^{-i \mathbf{k} \cdot \mathbf{r}} \]

annihilation operator
(destruits state with wave number \( \mathbf{k} \))

creation operator
(ceates state with wave number \( \mathbf{k} \))
4.2 The BCS Ground State

formalism of second quantization (occupation number representation) is used (>1927, Dirac, Fock, Jordan et al.)

basic relations (fermionic operators):

\[
\hat{c}^{\dagger}_{k\sigma} |0\rangle = |1\rangle \quad \hat{c}_{k\sigma} |0\rangle = 0 \quad \hat{c}^{\dagger}_{k\sigma} |1\rangle = 0 \quad \hat{c}_{k\sigma} |1\rangle = |0\rangle
\]

\[
\hat{c}^{\dagger}_{k\sigma} \hat{c}_{k\sigma} = n_{k\sigma} \quad \hat{c}_{k\sigma} \hat{c}^{\dagger}_{k\sigma} = 1 - n_{k\sigma} \quad \langle 0 | n_{k\sigma} | 0 \rangle = 0; \quad \langle 1 | n_{k\sigma} | 1 \rangle = 1
\]

particle number operator

Pauli exclusion principle

anti-commutation relations (for fermions):

\[
\{\hat{c}_{k\sigma}, \hat{c}^{\dagger}_{k'\sigma'}\} = \hat{c}_{k\sigma} \hat{c}^{\dagger}_{k'\sigma'} + \hat{c}^{\dagger}_{k'\sigma'} \hat{c}_{k\sigma} = \delta_{kk'} \delta_{\sigma\sigma'}
\]

\[
\{\hat{c}_{k\sigma}, \hat{c}_{k'\sigma'}\} = \{\hat{c}^{\dagger}_{k\sigma}, \hat{c}^{\dagger}_{k'\sigma'}\} = 0
\]
4.2 The BCS Ground State

Formalism of second quantization (occupation number representation) is used (>1927, Dirac, Fock, Jordan et al.)

Pair creation and annihilation operators:

\[ P_k^\dagger = \hat{c}_k^\dagger \hat{c}_{-k\downarrow} \quad \text{pair creation operator} \]

\[ P_k = \hat{c}_{-k\downarrow} \hat{c}_k^\dagger \quad \text{pair annihilation operator} \]

\[ [P_k, P_{k'}] = \hat{c}_{-k\downarrow} \hat{c}_k^\dagger \hat{c}_{-k'\downarrow} \hat{c}_{k'\uparrow} - \hat{c}_{-k'\downarrow} \hat{c}_k^\dagger \hat{c}_{-k\downarrow} \hat{c}_{k'\uparrow} = 0 \]

The last two operators of the first term on the r.h.s. can be moved to the front by an even number of permutations ➔ sign is preserved

\[ [P_k^\dagger, P_{k'}^\dagger] = \hat{c}_k^\dagger \hat{c}_{-k\downarrow} \hat{c}_{k'\uparrow} \hat{c}_{-k'\downarrow} - \hat{c}_{k'\uparrow} \hat{c}^\dagger_{-k\downarrow} \hat{c}^\dagger_k \hat{c}_{-k'\downarrow} = 0 \]

\[ [P_k, P_{k'}^\dagger] = \delta_{kk'} (1 - n_{k\uparrow} - n_{-k\downarrow}) \] (see next slide)

Powers of pair operators

\[ P_k^\dagger P_k = (P_k^\dagger)^2 = \hat{c}_k^\dagger \hat{c}_{-k\downarrow} \hat{c}_k^\dagger \hat{c}_{-k\downarrow} = \hat{c}_k^\dagger \hat{c}_{-k\downarrow} \hat{c}_k^\dagger \hat{c}_{-k\downarrow} = 0 \]

Antisymmetry of fermionic wavefunction requires that powers of the pair operators disappear

- Some of the commutator relations of the pair operators are similar to those of bosons, although the pair operators consist only of electron (fermionic) operators
- \( [P_k, P_k^\dagger] \neq 0 \) but not equal to \( \delta_{kk'} \) as expected for bosons, depends on \( k \) and \( T \)
- Pair operators do commute but are no bosonic operators

Formalism of second quantization (occupation number representation) is used (>1927, Dirac, Fock, Jordan et al.)

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Powers of pair operators

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- Pair operators do commute but are no bosonic operators
4.2 The BCS Ground State

Formalism of second quantization (occupation number representation) is used (>1927, Dirac, Fock, Jordan et al.)

Pair creation and annihilation operators:

\[
\begin{align*}
[P_{k}, P_{k}^{\dagger}] &= \hat{c}_{-k \downarrow} \hat{c}_{k \uparrow}^{\dagger} \hat{c}_{k' \downarrow}' \hat{c}_{-k' \uparrow}' - \hat{c}_{k \uparrow}' \hat{c}_{-k' \downarrow}' \hat{c}_{k \downarrow} \hat{c}_{k' \uparrow}
\end{align*}
\]

\[
= \hat{c}_{-k \downarrow} (1 - \hat{c}_{k \uparrow}' \hat{c}_{k \downarrow}) \hat{c}_{-k' \uparrow}' - \hat{c}_{k \uparrow}' \hat{c}_{-k' \downarrow}' \hat{c}_{k \downarrow} \hat{c}_{k' \uparrow}
\]

\[
= (1 - \hat{c}_{k \uparrow}' \hat{c}_{k \downarrow}) \hat{c}_{-k' \downarrow}' - \hat{c}_{k \uparrow}' \hat{c}_{-k' \downarrow}' \hat{c}_{k \downarrow} \hat{c}_{k' \uparrow}
\]

\[
= (1 - \hat{c}_{k \uparrow}' \hat{c}_{k \downarrow})(1 - \hat{c}_{-k \downarrow}' \hat{c}_{-k \uparrow}) - \hat{c}_{-k' \downarrow}' \hat{c}_{-k \downarrow} \hat{c}_{k' \uparrow} \hat{c}_{k \uparrow}
\]

\[
= \delta_{kk'} (1 - n_{k \downarrow})(1 - n_{-k \uparrow}) - n_{-k \downarrow} n_{k \uparrow}
\]

\[
[P_{k}, P_{k}^{\dagger}] = \delta_{kk'} (1 - n_{k \downarrow} - n_{-k \uparrow})
\]
4.2 The BCS Ground State

Formalism of second quantization (occupation number representation) is used (>1927, Dirac, Fock, Jordan et al.)

BCS Hamiltonian for $N$ interacting electrons

$$\mathcal{H}_{BCS} = \sum_{\sigma} \sum_{i=1}^{N} \left( -\frac{\hbar^2}{2m} \nabla_i^2 + V_{\text{ext}}(\mathbf{r}) \right) + \frac{1}{2} \sum_{\sigma} \sum_{i,j=1}^{N} V_{\text{int}}(\mathbf{r}_i - \mathbf{r}_j)$$

- Spin
- Kinetic energy
- Potential energy
- Interaction energy

Insertion of field operators and integration over volume $\Rightarrow$ FT of $\mathcal{H}_{BCS}$ into $k$-space

(see R. Gross, A. Marx, „Festkörperphysik“, 4. Auflage, appendix H.2 or exercise sheet No. 7)

$$\mathcal{H}_{BCS} = \sum_{\sigma} \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} + \frac{1}{2} \sum_{\sigma_1,\sigma_2} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}} V_{\mathbf{q}} \hat{c}_{\mathbf{k}_1+\mathbf{q},\sigma_1}^\dagger \hat{c}_{\mathbf{k}_2-\mathbf{q},\sigma_2} \hat{c}_{\mathbf{k}_2,\sigma_2} \hat{c}_{\mathbf{k}_1,\sigma_1}$$

- Energy of non-interacting free electron gas
- Interaction energy

Operator describes scattering from state $(\mathbf{k}_1, \sigma_1 ; \mathbf{k}_2, \sigma_2)$ into $(\mathbf{k}_1 + \mathbf{q}, \sigma_1 ; \mathbf{k}_2 - \mathbf{q}, \sigma_2)$ by exchange of phonon with wave vector $\mathbf{q}$
4.2 The BCS Ground State

**formalism of second quantization (occupation number representation) is used** (>1927, Dirac, Fock, Jordan et al.)

**BCS Hamiltonian for** \( N \) **interacting electrons**

simplification of interaction term for pairs with \( k_1 = k, \ k_2 = -k, \ \sigma_1 = \uparrow, \ \sigma_2 = \downarrow \) and \( V_q = V_{k,k'} \) with \( q = k - k' \)

\[
\frac{1}{2} \sum_{\sigma_1, \sigma_2} \sum_{k_1,k_2,q}^N V_q \hat{c}^\dagger_{k_1+q,\sigma_1} \hat{c}^\dagger_{k_2-q,\sigma_2} \hat{c}_{k_2,\sigma_2} \hat{c}_{k_1,\sigma_1} \Rightarrow \sum_{k,k'}^N V_{k,k'} \hat{c}^\dagger_{k_1} \hat{c}^\dagger_{-k_1} \hat{c}_{-k_1} \hat{c}_{k_1} \\
\text{summation over spin yields factor 2}
\]

\( \hat{c}^\dagger_\uparrow \hat{c}^\dagger_\downarrow \hat{c}_{-\downarrow} \hat{c}_{\uparrow} \)  

**two-particle interaction potential**

**pair creation and annihilation operators**

\[
H_{\text{BCS}} = \sum_{\sigma} \sum_{k} \varepsilon_k \hat{c}^\dagger_{k\sigma} \hat{c}_{k\sigma} + \sum_{k,k'}^N V_{k,k'} \hat{c}^\dagger_{k_1} \hat{c}^\dagger_{-k_1} \hat{c}_{-k_1} \hat{c}_{k_1} \\
\]

often the energy is given with respect to chemical potential \( \mu \)

\[\varepsilon_k = \frac{\hbar^2 k^2}{2m^*} \text{ is replaced by } \xi_k = \varepsilon_k - \mu\]
4.2 The BCS Ground State

**basic definitions, abbreviations, assumptions, ...**

1. weak isotropic interaction:
   \[ V_{k,k'} = \begin{cases} -V_0 & \text{for } |\xi_k|, |\xi_{k'}| < \hbar \omega_D \\ 0 & \text{else} \end{cases} \quad V_0 D (E_F) \ll 1 \]

2. pairing (Gorkov) amplitude:
   \[ g_{k\sigma_1 \sigma_2} \equiv \langle c_{-k\sigma_1} c_{k\sigma_2} \rangle \neq 0 \]
   \[ g^*_{k\sigma_1 \sigma_2} \equiv \langle c_{-k\sigma_1}^\dagger c_{k\sigma_2}^\dagger \rangle \neq 0 \]

3. Pauli principle: pairing amplitude is antisymmetric for interchanging spins and wave vector:
   \[ g_{k\sigma_1 \sigma_2} = -g_{-k \sigma_2 \sigma_1} \]

4. spin part allows to distinguish between singlet and triplet pairing:
   \[ S = \begin{cases} 0 & m_s = 0 \quad \text{singlet pairing} \\ 1 & m_s = -1,0, +1 \quad \text{triplet pairing} \end{cases} \]

5. pairing potential:
   \[ \Delta_{k\sigma_1 \sigma_2} \equiv -\sum_{k'} V_{k,k'} g_{k'\sigma_1 \sigma_2} \]
   expectation value of pairing interaction
   \[ \Delta^*_{k'\sigma_1 \sigma_2} \equiv -\sum_k V_{k,k'} g^*_{k\sigma_1 \sigma_2} \]
4.2 The BCS Ground State

calculation of the ground state energy

- **Hamilton operator:**
  \[
  \mathcal{H}_{BCS} = \sum_{\sigma} \sum_{k} \varepsilon_k \hat{c}_{k\sigma}^{\dagger} \hat{c}_{k\sigma} + \sum_{k,k'} V_{k,k'} \hat{c}_{k\uparrow}^{\dagger} \hat{c}_{-k\downarrow}^{\dagger} \hat{c}_{-k'\downarrow} \hat{c}_{k'\uparrow}
  \]

  \( n_{k\sigma} \) = particle number operator

- how to solve the **Schrödinger equation**?

  → most general form of \( N \)-electron wave function:

  \[
  |\Psi_N\rangle = \sum g(k_i, ..., k_l) \hat{c}^{\dagger}_{k_1 \uparrow} \hat{c}^{\dagger}_{-k_1 \downarrow} ... \hat{c}^{\dagger}_{k_l \uparrow} \hat{c}^{\dagger}_{-k_l \downarrow} |0\rangle
  \]

  **problem:** huge number of possible realizations, typically \( 10^{10^{20}} \)

  → **mean field approach:** occupation probability of state \( k \) only depends only on **average occupation probability** of other states

  → **Bardeen, Cooper** and **Schrieffer** used the following Ansatz (mean-field approach):

  \[
  |\Psi_{BCS}\rangle = \prod_{k=k_1, ..., k_M} \left( u_k + v_k \hat{c}^{\dagger}_{k \uparrow, -k \downarrow} \right) |0\rangle
  \]

  \(|u_k|^2\): probability that pair state \( (k \uparrow, -k \downarrow) \) is empty

  \(|v_k|^2\): probability that pair state \( (k \uparrow, -k \downarrow) \) is occupied

  \(|u_k|^2 + |v_k|^2 = 1\)

  \[\varepsilon_k = \frac{\hbar^2 k^2}{2m^*} = \xi_k + \mu\]

  \# of possibilities to place \( N/2 \) particles on \( M \) sites:

  \[
  \frac{M!}{[M - (N/2)]! (N/2)!}
  \]
4.2 The BCS Ground State

How to guess the BCS many particle wavefunction?

\[ |\Psi_{\text{BCS}}\rangle = \prod_{k=k_1,\ldots,k_M} \left( u_k + v_k c_k^\dagger c_{-k}^\dagger \right) |0\rangle \]

Wave function assumed by Bardeen, Cooper and Schrieffer

assume that the macroscopic wave function \( \psi(\mathbf{r}, t) = \psi_0(\mathbf{r}, t)e^{i\theta(\mathbf{r}, t)} \) can be described by a \textit{coherent many particle state of fermions} (motivated by strong overlap of Cooper pairs)

• \textit{coherent state of bosons}

Discussed first by \textit{Erwin Schrödinger} in 1926 when searching for a state of the quantum mechanical harmonic oscillator approximating best the behavior of a classical harmonic oscillator

E. Schrödinger, Der stetige Übergang von der Mikro- zur Makromechanik, Die Naturwissenschaften 14, 664-666 (1926).

Transferred later by \textit{Roy J. Glauber} to Fock state representation


Nobel Prize in Physics 2005 "\textit{for his contribution to the quantum theory of optical coherence}" with the other half shared by John L. Hall and Theodor W. Hänsch.
4.2 The BCS Ground State

- **Fock state representation of coherent state of bosons** (e.g. laser light)

Coherent state $|\alpha\rangle$ is expressed as an infinite linear combination of number (Fock) states

$$|\phi_n\rangle = \frac{1}{\sqrt{n!}} (a^\dagger)^n |0\rangle$$

where $a^\dagger$ is the boson creation operator and $|0\rangle$ is the vacuum state.

$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |\phi_n\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{(aa^\dagger)^n}{n!} |0\rangle = e^{-|\alpha|^2/2} e^{(aa^\dagger)} |0\rangle$

Schrödinger (1926)

Normalization

$\alpha = |\alpha| e^{i\phi}$ is a complex number.

Probability for occupation of $n$ particles is given by Poisson distribution

$$P(n) = |\langle \phi_n | \alpha \rangle|^2 = \frac{|\alpha|^{2n}}{n!} e^{-|\alpha|^2} = \frac{\langle n \rangle^n}{n!} e^{-\langle n \rangle}$$

- Expectation value of number operator:
  $$\langle n \rangle = \bar{N} = |\alpha|^2$$
  $$(\Delta N)^2 = \text{var}(n) = |\alpha|^2 = \bar{N} \gg 1$$

- Relative standard deviation:
  $$\frac{\Delta N}{\bar{N}} = \frac{1}{\sqrt{\bar{N}}} \ll 1 \quad \text{(as } \bar{N} \gg 1\text{)}$$

- Uncertainty relation:
  $$\Delta N \Delta \phi \geq \frac{1}{2}, \quad \Delta \phi \ll 1$$

Application: **coherent photonic state generated by laser**
4.2 The BCS Ground State

- Poisson distribution

\[
P(n) = |\langle \phi_n | \alpha \rangle|^2 = \frac{|\alpha|^{2n}}{n!} e^{-|\alpha|^2}
\]

\[
\bar{N} = |\alpha|^2 = \begin{pmatrix} 5 \\ 10 \\ 20 \end{pmatrix}
\]
4.2 The BCS Ground State

• Poisson and normal distribution

For large $\bar{N} = |\alpha|^2$ the Poisson distribution approaches the normal (Gaussian) distribution:

$$P_{\bar{N}}(n) = \frac{1}{\sqrt{2\pi \bar{N}}} e^{-\frac{(n - \bar{N})^2}{2\bar{N}}}$$

$$P(n) = |\langle \phi_n | \alpha \rangle|^2 = \frac{|\alpha|^{2n}}{n!} e^{-|\alpha|^2}$$

$\bar{N} = 50$
4.2 The BCS Ground State

- **Fock state representation of coherent state of fermions**

  starting point: coherent bosonic state

  \[ |\alpha\rangle = e^{-|\alpha|^2/2} \exp(\alpha a^\dagger) |0\rangle \]

  in analogy: coherent fermionic state

  \[ |\Psi_{\text{BCS}}\rangle = c_1 \exp \left( \sum_k \alpha_k P_k^\dagger \right) |0\rangle \]

  summation over \( k \) since we have many fermionic modes

  ➢ we make use of the fact that higher powers of fermionic creation operators disappear due to **Pauli principle** (**key difference to bosonic system**):

  \[
P_{k_1}^\dagger P_{k_2}^\dagger = (P_k^\dagger)^2 = \hat{c}_{k_1}^\dagger \hat{c}_{-k_1}^\dagger \hat{c}_{k_1}^\dagger \hat{c}_{-k_1}^\dagger = -\hat{c}_{k_1}^\dagger \hat{c}_{-k_1}^\dagger \hat{c}_{k_1}^\dagger \hat{c}_{-k_1}^\dagger = 0
\]

  \[|\Psi_{\text{BCS}}\rangle = c_1 \exp \left( \sum_k \alpha_k P_k^\dagger \right) |0\rangle = c_1 \prod_k \exp(\alpha_k P_k^\dagger) |0\rangle = c_1 \prod_k (1 + \alpha_k P_k^\dagger) |0\rangle\]

  **normalization**: \([\Psi_{\text{BCS}}^* |\Psi_{\text{BCS}}\rangle = c_1^2 \langle 0 | \prod_k (1 + \alpha_k^* P_k ) (1 + \alpha_k P_k^\dagger) |0\rangle = 1 \quad \text{satisfied if all factors} = 1\]

  \[1 = c_1^2 \langle 0 | (1 + \alpha_k^* P_k ) (1 + \alpha_k P_k^\dagger) |0\rangle = c_1^2 (1 + |\alpha_k|^2) \]

  ➢ \[c_1 = \frac{1}{\sqrt{(1 + |\alpha_k|^2)}}\]
4.2 The BCS Ground State

- BCS ground state as coherent state of fermions

\[ |\Psi_{\text{BCS}}\rangle = c_1 \prod_k (1 + \alpha_k P_k^+) |0\rangle = \frac{1}{\sqrt{(1 + |\alpha_k|^2)}} \prod_k (1 + \alpha_k P_k^+) |0\rangle \]

\[ |\Psi_{\text{BCS}}\rangle = \prod_k (u_k + v_k \hat{c}_{k\uparrow} \hat{c}_{-k\downarrow}^+ ) |0\rangle \]

coherence factors

\[ u_k = \frac{1}{\sqrt{(1 + |\alpha_k|^2)}} \]
\[ v_k = \frac{\alpha_k}{\sqrt{(1 + |\alpha_k|^2)}} \]

coherent superposition of pair states \(\rightarrow\) only average pair number is fixed

\[ \Delta N = \sqrt{\bar{N}} \gg 1 \quad \frac{\Delta N}{\bar{N}} = \frac{1}{\sqrt{\bar{N}}} \ll 1 \quad \Delta N \Delta \varphi \geq \frac{1}{2} \Rightarrow \Delta \varphi \ll 1 \]

\(\Rightarrow\) uncertainties \(\Delta N/\bar{N}\) and \(\Delta \varphi/2\pi\) are very small for large average pair number \(\bar{N}\)

\[ u_k \text{ and } v_k \text{ are complex probability amplitudes:} \]

\[ |u_k|^2: \text{probability that pair state } (k \uparrow, -k \downarrow) \text{ is empty} \]
\[ |v_k|^2: \text{probability that pair state } (k \uparrow, -k \downarrow) \text{ is occupied} \]
\[ |u_k|^2 + |v_k|^2 = 1 \]
4.2 The BCS Ground State

- some expectation values (1):

  single spin particle number

\[
\langle n_{k\uparrow} \rangle = \langle \Psi_{BCS} | c_{k\uparrow}^\dagger c_{k\uparrow} | \Psi_{BCS} \rangle
\]

\[
= \langle 0 | (u_k^* + v_k \hat{c}_{-k\uparrow}^\dagger \hat{c}_{k\uparrow}) (u_k + v_k \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\uparrow}^\dagger) | 0 \rangle
\]

we use the identities:

- \( \langle O \phi | \Psi \rangle = \langle \phi | O^\dagger \Psi \rangle \)
- \( \langle \phi | (AB)^\dagger | \Psi \rangle = \langle \phi | B^\dagger A^\dagger | \Psi \rangle \)

(see exercise sheet No. 7 for detailed derivation)

\[
\langle n_{k\uparrow} \rangle = |u_k|^2 \langle 0 | \hat{c}_{k\uparrow}^\dagger \hat{c}_{k\uparrow} | 0 \rangle + u_k^* v_k \langle 0 | \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\uparrow}^\dagger \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\uparrow} | 0 \rangle + v_k^* u_k \langle 0 | \hat{c}_{-k\uparrow}^\dagger \hat{c}_{k\uparrow}^\dagger \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\uparrow} | 0 \rangle + |v_k|^2 \langle 0 | \hat{c}_{-k\uparrow}^\dagger \hat{c}_{k\uparrow}^\dagger \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\uparrow}^\dagger | 0 \rangle
\]

since \( n_{k\uparrow} | 0 \rangle = 0 | 0 \rangle \)

use even number of permutations to transform into terms \( n_{k\uparrow} | 0 \rangle = 0 | 0 \rangle \)

\[
\langle n_{k\uparrow} \rangle = |v_k|^2
\]

average total pair number

\[
\bar{N} = \langle \mathcal{N} \rangle = \sum_{k\sigma} \langle n_{k\sigma} \rangle = \sum_{k\sigma} |v_k|^2 = 2 \sum_k |v_k|^2 = \sum_k |v_k|^2 - |u_k|^2 + 1
\]
4.2 The BCS Ground State

• some expectation values (2a):

statistical fluctuation of average particle number

\[(\Delta N)^2 = (\langle N \rangle - \langle N \rangle)^2 = \langle N^2 \rangle - \langle N \rangle^2 \]

\[(\Delta N)^2 = \left( \sum_{k,\sigma} n_{k\sigma} \right)^2 - \left( \sum_{k,\sigma} n_{k\sigma} \right)^2 = 2 \sum_{k,k'} \langle n_k n_{k'} \rangle - 2 \sum_{k,k'} \langle n_k \rangle \langle n_{k'} \rangle \]

i. \( k \neq k' \) we obtain contributions \( \langle n_{k\sigma} n_{k'\sigma} \rangle \) and \( \langle n_{k\sigma} \rangle \langle n_{k'\sigma} \rangle \); since there is no correlation between the calculation of \( \sum_k \) and \( \sum_{k'} \) we obtain \( \langle n_{k\sigma} n_{k'\sigma} \rangle = \langle n_{k\sigma} \rangle \langle n_{k'\sigma} \rangle \)

\( \Rightarrow \) the contributions \( \langle n_{k\sigma} n_{k'\sigma} \rangle \) and \( \langle n_{k\sigma} \rangle \langle n_{k'\sigma} \rangle \) just cancel each other in the sums due to the minus sign

ii. \( k = k' \) we use \( \langle n_{k\sigma}^2 \rangle = \langle c_{k\sigma}^{+} c_{k\sigma} c_{k\sigma}^{+} c_{k\sigma} \rangle = \langle c_{k\sigma}^{+} (1 - c_{k\sigma}^{+} c_{k\sigma} c_{k\sigma}^{+} c_{k\sigma}) c_{k\sigma} \rangle = \frac{\langle c_{k\sigma}^{+} c_{k\sigma} \rangle - \langle c_{k\sigma}^{+} c_{k\sigma} c_{k\sigma} c_{k\sigma} \rangle}{|v_k|^{-2}} = -|v_k|^4 \)

\[(\Delta N)^2 = 2 \sum_k \langle n_k n_k \rangle - \sum_k \langle n_k \rangle \langle n_k \rangle = 2 \sum_k |v_k|^2 + |v_k|^4 - 2 \sum_k |v_k|^4 = 2 \sum_k |v_k|^2 \]

(see exercise sheet No. 7 for detailed derivation)
4.2 The BCS Ground State

- some expectation values (2b):

statistical fluctuation of average particle number

\[(\Delta N)^2 = 2 \sum_k |v_k|^2\]

\[\Delta N = \sqrt{2 \sum_k |v_k|^2} = \sqrt{\bar{N}}\]

\(\Delta N\) gets very large for large \(\bar{N}\), but relative fluctuation \(\Delta N/\bar{N}\) becomes vanishingly small !!

(see exercise sheet No. 7 for detailed derivation)
4.2 The BCS Ground State

- some expectation values (3):

  pairing or Gorkov amplitude

\[ g_{k\sigma_1\sigma_2} \equiv \langle \Psi_{\text{BCS}} | c_{-k\sigma_1} c_{k\sigma_2} | \Psi_{\text{BCS}} \rangle = u_k v_k^* \]

\[ g_{k\sigma_1\sigma_2}^\dagger \equiv \langle \Psi_{\text{BCS}} | c_{-k\sigma_1}^\dagger c_{k\sigma_2}^\dagger | \Psi_{\text{BCS}} \rangle = u_k^* v_k \]

BCS Hamiltonian

\[ \mathcal{H}_{\text{BCS}} = \sum_{\sigma} \sum_k \epsilon_k \hat{c}_{k\sigma}^\dagger \hat{c}_{k\sigma} + \sum_{k,k'} V_{k,k'} \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\uparrow} \hat{c}_{k'\downarrow}^\dagger \hat{c}_{-k'\downarrow} \]

\[ \langle \Psi_{\text{BCS}} | \hat{c}_{k\sigma}^\dagger \hat{c}_{k\sigma} | \Psi_{\text{BCS}} \rangle = |v_k|^2 \]

\[ \langle \Psi_{\text{BCS}} | \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\uparrow}^\dagger \hat{c}_{-k'\downarrow} \hat{c}_{k'\downarrow}^\dagger | \Psi_{\text{BCS}} \rangle = v_k v_{k'}^* u_{k'} u_k^* \]

\[ \langle \Psi_{\text{BCS}} | \mathcal{H}_{\text{BCS}} | \Psi_{\text{BCS}} \rangle = \frac{2}{N} \sum_k \epsilon_k |v_k|^2 + \sum_{k,k'} V_{k,k'} v_k v_{k'}^* u_{k'} u_k^* \]

(see exercise sheets for detailed derivation)
4.2 The BCS Ground State

Task: find the minimum of the expectation value \( \langle \Psi_{BCS} | \mathcal{H}_{BCS} | \Psi_{BCS} \rangle \) by variational method (\( @ T = 0 \))

we take the energy relative to the chemical potential \( \mu \)

\[
\langle E_{BCS} - \bar{N} \mu \rangle = \langle \Psi_{BCS} | \mathcal{H}_{BCS} - \bar{N} \mu | \Psi_{BCS} \rangle = 2 \sum_k (\xi_k + \mu) |v_k|^2 - \bar{N} \mu + \sum_{k,k'} V_{k,k'} v_k v_k^* u_{k'} u_{k'}^*
\]

\[
\langle E_{BCS} - \bar{N} \mu \rangle = \langle \Psi_{BCS} | \mathcal{H}_{BCS} - \bar{N} \mu | \Psi_{BCS} \rangle = 2 \sum_k \xi_k |v_k|^2 - \bar{N} \mu + \bar{N} \mu + \sum_{k,k'} V_{k,k'} v_k v_k^* u_{k'} u_{k'}^*
\]

\[
\delta \left\{ 2 \sum_k \xi_k |v_k|^2 + \sum_{k,k'} V_{k,k'} v_k v_k^* u_{k'} u_{k'}^* \right\} = 0
\]

minimization of expectation value by variation of the probability amplitudes yields expressions for \( |u_k|^2 \) and \( |v_k|^2 \)
4.2 The BCS Ground State

**Method 1:** we assume that $u_k$ and $v_k$ are real and satisfy $|u_k|^2 + |v_k|^2 = 1$ (Bardeen, Cooper, Schrieffer: 1957)

$$u_k = \sin \theta_k, \quad v_k = \cos \theta_k,$$

and

$$2 \sin \theta_k \cos \theta_k = \sin 2\theta_k$$

$$\langle E_{BCS} - \bar{N} \mu \rangle = 2 \sum_k \xi_k |v_k|^2 + \sum_{k,k'} V_{k,k'} v_k^* u_k^* = 2 \sum_k \xi_k \cos^2 \theta_k + \frac{1}{4} \sum_{k,k'} V_{k,k'} \sin 2\theta_k \sin 2\theta_k'$$

minimization

$$\frac{\partial \langle E_{BCS} - \bar{N} \mu \rangle}{\partial \theta_1} = 0$$

$$\frac{\partial \langle E_{BCS} - \bar{N} \mu \rangle}{\partial \theta_1} = 0 = 2\xi_1 (-2 \cos \theta_1 \sin \theta_1) + \frac{1}{4} \frac{\partial}{\partial \theta_1} \sum_k \sin 2\theta_k \sum_{k'} V_{k,k'} \sin 2\theta_k'$$

$$\frac{1}{4} (2 \cos \theta_1) \sum_{k'} V_{1k'} \sin 2\theta_{k'} + \sum_k \sin 2\theta_k V_{k,1} \cos 2\theta_1$$

$$2\xi_1 \sin 2\theta_1 = \frac{1}{2} \cos 2\theta_1 \left( \sum_{k'} V_{1k'} \sin 2\theta_{k'} + \sum_k \sin 2\theta_k V_{k,1} \right) \overset{V_{1k'} = V_{k,1}}{=} \cos 2\theta_1 \sum_{k'} V_{1k'} \sin 2\theta_{k'}$$

$$\tan 2\theta_1 = \frac{\sum_{k'} V_{1k'} \sin \theta_{k'} \cos \theta_{k'}}{\xi_k}$$
4.2 The BCS Ground State

- we switch back to old summation \((l \rightarrow k)\) and restore \(u_k = \sin \theta_k, \ v_k = \cos \theta_k\):

\[
\tan 2\theta_k = \frac{\sum_{k'} V_{k,k'} u_{k'} v_{k'}}{\xi_k}
\]

- we further use the pairing strength \(\Delta_k \equiv -\sum_{k'} V_{k,k'} u_{k'} v_{k'}\):

\[
\tan 2\theta_k = \frac{\sin 2\theta_k}{\cos 2\theta_k} = \frac{2\sin \theta_k \cos \theta_k}{\cos^2 \theta_k - \sin^2 \theta_k} = \frac{2u_k v_k}{u_k^2 - v_k^2}
\]

we obtain \(\tan 2\theta_k = -\frac{\Delta_k}{\xi_k}\)

- we define \(E_k \equiv \sqrt{\xi_k^2 + \Delta_k^2}\) and obtain the following expressions for \(u_k\) and \(v_k\) minimizing the energy

\[
|u_k|^2 = \frac{1}{2} \left[ 1 + \frac{\xi_k}{E_k} \right] \quad \quad |v_k|^2 = \frac{1}{2} \left[ 1 - \frac{\xi_k}{E_k} \right]
\]

\[
u_k v_k = g_k = \frac{\Delta_k}{2E_k}
\]

\(\Delta_k \equiv -\sum_{k'} V_{k,k'} \frac{\Delta_{k'}}{2E_{k'}}\)

pairing amplitude self-consistent gap equation

for \(k\)-independent \(\Delta_k\): minimum energy is \(E_k = \Delta\)
we will see later that \(E_k\) is the energy required to add a single excitation to the ground state

\(\Rightarrow\) minimum excitation energy is required, therefore \(\Delta\) represents an energy gap in the excitation spectrum
\[ |u_k|^2 = \frac{1}{2} \left[ 1 + \frac{\xi_k}{E_k} \right] \]

\[ |v_k|^2 = \frac{1}{2} \left[ 1 - \frac{\xi_k}{E_k} \right] \]

\[ u_k v_k = g_k = \frac{\Delta_k}{2E_k} \]

\[ |v_k|^2: \text{ probability that } \mathbf{k} \text{ is occupied} \]

\[ \rightarrow \text{ probability } |v_k|^2 \text{ is smeared out around Fermi level even at } T = 0: \text{ increase of kinetic energy} \]

\[ \rightarrow \text{ smearing is required to allow for pairing interaction: reduction of potential energy} \]

\[ \text{ increase of kinetic energy} \]

\[ |v_k|^2 \approx f(T = T_c) \]
4.2 The BCS Ground State

**Method 2:** we use the method of Lagrangian multipliers

- we use the following two constraints:
  \[ \phi_1 = 0 = \langle \mathcal{N} \rangle - 2 \sum_k |v_k|^2 = \langle \mathcal{N} \rangle - \sum_k |v_k|^2 - |u_k|^2 + 1 \]
  \[ \phi_2 = 0 = |u_k|^2 + |v_k|^2 - 1 = u_k u_k^* + v_k v_k^* - 1 \]

  \[ \mathcal{L}(u_k^*, v_k^*, \lambda_1, \lambda_2) = \langle E_{\text{BCS}} \rangle - \lambda_1 \phi_1 - \lambda_2 \phi_2 \]

  \[ \lambda_1, \lambda_2 : \text{Lagrangian multipliers} \]

  \[ \text{with } \langle E_{\text{BCS}} \rangle = 2 \sum_k \epsilon_k |v_k|^2 + \sum_{k,k'} V_{k,k'} v_k v_k^* u_{k'} u_k^* = 2 \sum_k \epsilon_k (|v_k|^2 - |u_k|^2 + 1) + \sum_{k,k'} V_{k,k'} v_k v_k^* u_{k'} u_k^* \]

- by setting the partial derivative of the Lagrangian function \( \mathcal{L} \) with respect to \( u_k^* \) and \( v_k^* \) to zero we obtain the eigenvalue eqns:

  \[ (\epsilon_k - \lambda_1) u_k + \Delta_k v_k - \lambda_2 u_k = 0 \]
  \[ \Delta_k^+ u_k - (\epsilon_k - \lambda_1) v_k - \lambda_2 v_k = 0 \]

- physical meaning of the Lagrangian multipliers
  i. \( \lambda_1 \) shifts the energy and corresponds to the chemical potential \( \mu \)
  ii. \( \lambda_2 \) corresponds to the eigenvalue of the the vector \( (u_k, v_k) \) and is given by the energy \( \pm E_k \) of the quasiparticles excited out of the condensate

- solving the eigenvalue eqns yields \( E_k \equiv \sqrt{\xi_k^2 + \Delta_k^2} \)
  \[ |u_k|^2 = \frac{1}{2} \left[ 1 + \xi_k \frac{E_k}{E_k} \right] \]
  \[ |v_k|^2 = \frac{1}{2} \left[ 1 - \xi_k \frac{E_k}{E_k} \right] \]
  \[ u_k u_k^* = g_k = \frac{\Delta_k}{2E_k} \]
  \[ v_k v_k^* = \frac{\delta_k}{2E_k} \]
4.2.1 The BCS Gap Equation

Solution of the self-consistent gap equation ($T = 0$)

\[
\Delta_k \equiv -\sum_{k'} V_{k,k'} \frac{\Delta_{k'}}{2E_{k'}} = -\sum_{k'} V_{k,k'} \frac{\Delta_{k'}}{2\sqrt{\xi_{k'}^2 + |\Delta_{k'}|^2}}
\]

cannot be solved analytically in the general case.

- simple solution only if the gap $\Delta_k$ and the interaction potential $V_{k,k'}$ are assumed $k$-independent: $\Delta_k = \Delta$, $V_{k,k'} = -V_0$

\[
1 = V_0 \sum_{k'} \frac{1}{2\sqrt{\xi_{k'}^2 + |\Delta|^2}}
\]

transforming sum into integration with pair density $\bar{D}(E) \approx D(E_F)/2$

\[
1 = \frac{V_0 D(E_F)}{2} \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{d\xi}{2\sqrt{\xi^2 + |\Delta|^2}}
\]

- with $\int \frac{dx}{\sqrt{x^2 + a^2}} = \arcsinh \left( \frac{x}{a} \right)$ we obtain

\[
1 = \frac{V_0 D(E_F)}{4} \left[ \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{d\xi}{\sqrt{\xi^2 + |\Delta|^2}} \right] = \frac{V_0 D(E_F)}{4} \arcsinh \left( \frac{\hbar\omega_D}{\Delta} \right)_{-\hbar\omega_D}^{\hbar\omega_D} = \frac{V_0 D(E_F)}{2} \arcsinh \left( \frac{\hbar\omega_D}{\Delta} \right)
\]

energy gap corresponds to binding energy estimated for single Cooper pair

factor 2 in argument of exp. function is missing, since we have assumed that the two additional electrons are in the interval $[E_F - \hbar\omega_D, E_F + \hbar\omega_D]$ and not in $[E_F, E_F + \hbar\omega_D]$ as assumed previously in „Gedanken“ experiment

\[
\Delta = \frac{\hbar\omega_D}{\sinh \left( 2/V_0 D(E_F) \right)} \approx 2\hbar\omega_D e^{-2/V_0 D(E_F)}
\]

$V_0 D(E_F) \ll 1$: weak coupling approximation, $\sinh x \approx \frac{1}{2} \exp x$
4.2.2 Ground State Energy

calculation of the BCS condensation energy

- calculate expectation value of BCS Hamiltonian for \( T = 0 \)

\[
E_{\text{BCS}} = \langle \Psi_{\text{BCS}} | \mathcal{H}_{\text{BCS}} - \mu N | \Psi_{\text{BCS}} \rangle = 2 \sum_{k} \xi_{k} |v_{k}|^{2} + \sum_{k,k'} V_{k,k'} v_{k} v_{k'}^{*} u_{k'} u_{k}^{*}
\]

- we plug in the results for the coherence factors and the pair amplitude

\[
|u_{k}|^{2} = \frac{1}{2} \left[ 1 + \frac{\xi_{k}}{E_{k}} \right], \quad |v_{k}|^{2} = \frac{1}{2} \left[ 1 - \frac{\xi_{k}}{E_{k}} \right], \quad u_{k} v_{k}^{*} = g_{k}^{*} = \frac{\Delta_{k}^{*}}{2E_{k}}, \quad u_{k}^{*} v_{k} = g_{k} = \frac{\Delta_{k}}{2E_{k}}
\]

\[
E_{\text{BCS}} = \sum_{k} \left( \xi_{k} - \frac{\xi_{k}^{2}}{E_{k}} \right) - \sum_{k} g_{k}^{*} \Delta_{k} = \sum_{k} \left( \xi_{k} - \frac{\xi_{k}^{2}}{E_{k}} \right) - 2 \sum_{k} g_{k}^{*} \Delta_{k} + \sum_{k} g_{k}^{*} \Delta_{k}
- \sum_{k} \frac{\Delta_{k}^{2}}{2E_{k}}
\]

\[
E_{\text{BCS}} = \sum_{k} \left( \xi_{k} - E_{k} \right) + \sum_{k} g_{k}^{*} \Delta_{k}
\]

energy relative to chemical potential

\[
\xi_{k} = \varepsilon_{k} - \mu
\]

(see exercise sheet No. 8 for detailed derivation)
4.2.2 Ground State Energy

- for simplicity we assume for $V_{k,k'} = -V_0$ and $\Delta_k = \Delta$

$$E_{BCS} = \langle \Psi_{BCS} | \mathcal{H}_{BCS} - N\mu | \Psi_{BCS} \rangle = \sum_k \{\xi_k - E_k + g_k^*\Delta\}$$

- subtract mean energy of normal state at $T = 0$ (making use of symmetry around $\mu$)

$$\langle \Psi_{BCS} | \mathcal{H}_n - N\mu | \Psi_{BCS} \rangle = \lim_{\Delta \to 0} \langle \Psi_{BCS} | \mathcal{H}_{BCS} - N\mu | \Psi_{BCS} \rangle = \sum_k \xi_k - |\xi_k| = 2 \sum_{|k|<k_F} \xi_k$$

$$\Delta E = \sum_{|k|<k_F} \xi_k - E_k + \Delta g_k^* - 2\xi_k + \sum_{|k|\geq k_F} \xi_k - E_k + \Delta g_k^*$$

- we use $-\xi_k = |\xi_k|$ for $|k| < k_F$ and $E_k = \sqrt{\xi_k^2 + |\Delta|^2}$

$$\Delta E = 2 \sum_{|k|\geq k_F} \left( \xi_k - \sqrt{\xi_k^2 + |\Delta|^2} + \Delta g_k^* \right) \overset{\Delta g_k^* = \frac{\Delta^2}{2\sqrt{\xi_k^2 + |\Delta|^2}}}{=} 2 \sum_{|k|\geq k_F} \left( \xi_k - \sqrt{\xi_k^2 + |\Delta|^2} + \frac{\Delta^2}{2\sqrt{\xi_k^2 + |\Delta|^2}} \right)$$
4.2.2 Ground State Energy

\[
\Delta E = 2 \sum_{|k| \geq k_F} \left( \xi_k - \sqrt{\xi_k^2 + |\Delta|^2} + \frac{\Delta^2}{2 \sqrt{\xi_k^2 + |\Delta|^2}} \right)
\]

- replace summation by integration ...... after some algebra (see appendix H.3 in R. Gross, A. Marx, Festkörperphysik, 4. Auflage, de Gruyter (2022)):

\[
\Delta E = E_{\text{cond}}(0) = -\frac{1}{4} D(E_F) \Delta^2(0)
\]

\[
D(E_F) = \text{DOS for both spin directions}
\]

- interpretation of the result:
  - number of Cooper pairs: \( \frac{D(E_F)}{2} \Delta(0) \)
  - average energy gain per Cooper pair: \(-\frac{\Delta(0)}{2}\)

- compare to \( g_s - g_n = E_{\text{cond}}(0) = -B_{\text{cth}}^2(0)/2\mu_0 \) (thermodynamics)

\[
B_{\text{cth}}(0) = \sqrt{\frac{\mu_0 D(E_F)\Delta^2(0)}{2V}}
\]
4.2.2 Ground State Energy

• condensation energy per volume:

\[
\frac{E_{\text{cond}}(0)}{V} = -\frac{1}{4} \frac{D(E_F)}{V} \Delta^2(0) = -\frac{1}{4} N(E_F) \Delta^2(0)
\]

with \( N(E_F) = \frac{3n}{2E_F} \) and \( \frac{\Delta(0)}{k_B T_c} = \frac{\pi}{e \gamma} = 1.7638 \ldots \) we obtain (result is derived later)

\[
\frac{E_{\text{cond}}(0)}{V} = -\frac{3}{8} n \frac{\Delta^2(0)}{E_F} = \frac{3}{8} \left( \frac{\pi}{e \gamma} \right)^2 \frac{(k_B T_c)^2}{E_F} = -1.167 \, n \frac{(k_B T_c)^2}{E_F}
\]

⇒ average condensation energy per electron is of the order of \((k_B T_c)^2/E_F\)

⇒ plausibility:
only a small fraction \( k_B T_c/E_F \) of the electrons is participating in pairing process and the average energy reduction per electron is about \( k_B T_c \)
**Summary of Lecture No. 8 (1)**

- **BCS Hamilton operator:**

  \[
  \mathcal{H}_{\text{BCS}} = \sum_{\sigma} \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{k}, \mathbf{k}'} V_{\mathbf{k}, \mathbf{k}'} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{-\mathbf{k}\sigma} \hat{c}_{-\mathbf{k}'\sigma} \hat{c}_{\mathbf{k}'\sigma}
  \]

  \[\hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} = n_{\mathbf{k}\sigma} = \text{particle number operator}\]

  \[\varepsilon_{\mathbf{k}} = \xi_{\mathbf{k}} + \mu = \frac{\hbar^2 \mathbf{k}^2}{2m^*}\]

- **Bardeen, Cooper and Schrieffer** used the following Ansatz for the ground state wave function (mean-field approach):

  \[|\Psi_{\text{BCS}}\rangle = \prod_{\mathbf{k} = \mathbf{k}_1, \ldots, \mathbf{k}_M} (u_{\mathbf{k}} + v_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger) |0\rangle\]

  coherent fermionic state

  \[|u_{\mathbf{k}}|^2: \text{probability that pair state } (\mathbf{k} \uparrow, -\mathbf{k} \downarrow) \text{ is empty}\]

  \[|v_{\mathbf{k}}|^2: \text{probability that pair state } (\mathbf{k} \uparrow, -\mathbf{k} \downarrow) \text{ is occupied}\]

  \[|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1\]

- **Expectation values:**

  \[\langle \Psi_{\text{BCS}} | \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} | \Psi_{\text{BCS}} \rangle = |v_{\mathbf{k}}|^2\]

  \[\langle \Psi_{\text{BCS}} | \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{\mathbf{k}\downarrow} \hat{c}_{-\mathbf{k}\uparrow} \hat{c}_{-\mathbf{k}\downarrow} | \Psi_{\text{BCS}} \rangle = v_{\mathbf{k}}^* u_{\mathbf{k}} u_{\mathbf{k}}^* v_{\mathbf{k}}\]

  determination of \(u_{\mathbf{k}}, v_{\mathbf{k}}\) by minimization of expectation value

  \[
  \langle \Psi_{\text{BCS}} | \mathcal{H}_{\text{BCS}} | \Psi_{\text{BCS}} \rangle = 2 \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} |v_{\mathbf{k}}|^2 + \sum_{\mathbf{k}, \mathbf{k}'} V_{\mathbf{k}, \mathbf{k}'} v_{\mathbf{k}}^* u_{\mathbf{k}} u_{\mathbf{k}}^* v_{\mathbf{k}'}^* u_{\mathbf{k}'} u_{\mathbf{k}'}^* u_{\mathbf{k}} u_{\mathbf{k}}^*
  \]

  (kinetic energy)

  interaction energy
Summary of Lecture No. 8 (2)

- **minimization of expectation value**

\[
|u_k|^2 = \frac{1}{2} \left[ 1 + \frac{\xi_k}{E_k} \right] \quad |v_k|^2 = \frac{1}{2} \left[ 1 - \frac{\xi_k}{E_k} \right]
\]

\[
u_k u_k^* = g_k^* = \frac{\Delta_k^*}{2E_k}
\]

\[
u_k^* v_k = g_k = \frac{\Delta_k}{2E_k}
\]

probability that pair state \((k \uparrow, -k \downarrow)\) is empty/occupied

- **pairing amplitude**

\[
\Delta_k \equiv - \sum_{k'} V_{k,k'} g_{k'} = - \sum_{k'} V_{k,k'} \frac{\Delta_{k'}}{2E_{k'}}
\]

\[
\Delta_k^\dagger \equiv - \sum_{k'} V_{k,k'} g_{k'}^* = - \sum_{k'} V_{k,k'} \frac{\Delta_{k'}}{2E_{k'}}
\]

self-consistent gap equation

- **gap equation for \(T = 0\)**

\[
\Delta = \frac{\hbar \omega_D}{\sinh(2/V_0 D(E_F))} \approx 2 \hbar \omega_D e^{-2/V_0 D(E_F)}
\]

energy gap corresponds to binding energy estimated for single Cooper pair

\[
V_0 D(E_F) \ll 1: \text{weak coupling approximation, } \sinh x \approx \frac{1}{2} \exp x
\]
Superconductivity
and
Low Temperature
Physics I

Lecture No. 9

R. Gross
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Chapter 4

4. Microscopic Theory

4.1 Attractive Electron-Electron Interaction
   4.1.1 Phonon Mediated Interaction
   4.1.2 Cooper Pairs
   4.1.3 Symmetry of Pair Wavefunction

4.2 BCS Ground State
   4.2.1 The BCS Gap Equation
   4.2.2 Ground State Energy
   4.2.3 Bogoliubov-Valatin Transformation and Quasiparticle Excitations

4.3 Thermodynamic Quantities

4.4 Determination of the Energy Gap
   4.4.1 Specific Heat
   4.4.2 Tunneling Spectroscopy

4.5 Coherence Effects
4.2.3 The Bogoliubov-Valatin Transformation

- so far we have found the BCS ground state wave function and the energy gap at zero temperature

- next step:
  - determine the properties of the superconducting state at finite temperature
  - determine the energy of excitations out of the ground state

- how to proceed?
  - use BCS ground state as reference state
  - discuss effect of small deviations (e.g. by adding a small number of excitations to the ground state)

- we use the identities (with $\delta g_k$, $\delta g_k^*$ being small)

\[
\hat{c}_{-k\downarrow} \hat{c}_{k\uparrow} = \frac{\langle \hat{c}_{-k\downarrow} \hat{c}_{k\uparrow} \rangle}{\delta g_k} + \frac{\langle \hat{c}_{-k\downarrow} \hat{c}_{k\uparrow} \rangle}{\delta g_k^*} - \frac{\langle \hat{c}_{-k\downarrow} \hat{c}_{k\uparrow} \rangle}{\delta g_k^*}
\]

as the particle number is usually very large, the fluctuations $\delta g_k$, $\delta g_k^*$ are very small and we can neglect quadratic terms in $\delta g_k$, $\delta g_k^*$
4.2.3 The Bogoliubov-Valatin Transformation

- rewriting of pair creation and annihilation operators in

$$\hat{c}_{-k\downarrow} \hat{c}_{k\uparrow} = \frac{\langle \hat{c}_{-k\downarrow} \hat{c}_{k\uparrow} \rangle}{g_k} + \frac{\hat{c}_{-k\downarrow} \hat{c}_{k\uparrow}}{\delta g_k}$$

$$\hat{c}_{k\uparrow} \hat{c}_{-k\downarrow} = \frac{\langle \hat{c}_{k\uparrow} \hat{c}_{-k\downarrow} \rangle}{g_k} + \frac{\hat{c}_{k\uparrow} \hat{c}_{-k\downarrow}}{\delta g_k}$$

- insert into Hamiltonian and consider only terms linear in $\delta g_k^{(*)}$ (and after some math)

$$\mathcal{H}_{BCS} - N\mu = \sum_{k,\sigma} \tilde{\xi}_k \tilde{n}_{k\sigma} + \sum_{k,k'} V_{k,k'} \left[ g^*_k \tilde{c}_{-k'\downarrow} \hat{c}_{k'\uparrow} + g_k \tilde{c}_{k\uparrow} \hat{c}_{-k'\downarrow} - g_k g^*_k \right]$$

- make use of pair potential

$$\Delta_k \equiv - \sum_{k'} V_{k,k'} g_k$$

$$\Delta^*_k \equiv - \sum_{k'} V_{k,k'} g^*_k$$

$$\mathcal{H}_{BCS} - N\mu = \sum_{k,\sigma} \tilde{\xi}_k \tilde{n}_{k\sigma} - \sum_k \left[ \Delta^*_k \tilde{c}_{-k'\downarrow} \hat{c}_{k'\uparrow} + \Delta_k \tilde{c}_{k\uparrow} \hat{c}_{-k'\downarrow} - \Delta_k g^*_k \right]$$
4.2.3 The Bogoliubov-Valatin Transformation

- we use

\[
\sum_{k,\sigma} \xi_k n_{k\sigma} = \sum_{k} \xi_k \left( \hat{c}_{k\uparrow}^\dagger \hat{c}_{k\uparrow} + \hat{c}_{-k\downarrow}^\dagger \hat{c}_{-k\downarrow} \right) = 1 - \hat{c}_{-k\downarrow}^\dagger \hat{c}_{-k\downarrow}^\ddagger
\]

\[
\sum_{k,\sigma} \xi_k n_{k\sigma} = \sum_{k} \xi_k \hat{c}_{k\uparrow}^\dagger \hat{c}_{k\uparrow} - \xi_k \hat{c}_{-k\downarrow}^\dagger \hat{c}_{-k\downarrow}^\ddagger + \xi_k
\]

\[
\mathcal{H}_{BCS} - N\mu = \sum_{k,\sigma} \xi_k n_{k\sigma} - \sum_{k} \left[ \Delta_k \hat{c}_{-k\downarrow}^\dagger \hat{c}_{k\uparrow}^\dagger + \Delta_k \hat{c}_{k\uparrow} \hat{c}_{-k\downarrow} - \Delta_k g_k \right]
\]

- due to finite \( \Delta_k, \Delta_k^* \), the Hamiltonian describes interacting electron gas with new quasiparticles consisting of superposition of electron and hole states

- derive excitation energies by diagonalization of Hamiltonian

\( \to \) Bogoliubov-Valatin transformation

\( \to \) define new fermionic operators \( \alpha_k, \beta_k^\dagger \) and \( \alpha_k^\dagger, \beta_k \) by unitary transformation (rotation)
4.2.3 The Bogoliubov-Valatin Transformation

- use unitarian matrix to rotate the energy matrix into eigenbasis of Bogoliubov quasiparticles

\[
\mathcal{H}_{BCS} - N\mu = \sum_k \left\{ \xi_k + \Delta_k g_k^* + \left( \begin{array}{c} \hat{c}_k^+ \hat{c}_{-k} \\ \hat{c}_{k} \end{array} \right) \begin{pmatrix} \xi_k & -\Delta_k \\ -\Delta_k^* & -\xi_k \end{pmatrix} \begin{pmatrix} \hat{c}_k^+ \\ \hat{c}_{-k} \end{pmatrix} \right\}
\]

spinors

energy matrix

appropriate unitary matrix to make transformed energy matrix \( \hat{\mathcal{E}}_k = \mathcal{U}_k \mathcal{E}_k \mathcal{U}_k^+ \) diagonal:

\[
\mathcal{U}_k = \begin{pmatrix} u_k & v_k^* \\ -v_k & u_k^* \end{pmatrix} \quad \mathcal{U}_k^+ = \begin{pmatrix} u_k^* & -v_k^* \\ v_k & u_k \end{pmatrix} \quad \mathcal{U}_k^+ \mathcal{E}_k \mathcal{U}_k = \hat{\mathcal{E}}_k = \begin{pmatrix} E_k & D_k \\ -D_k & -E_k \end{pmatrix}
\]

choose \( u_k \) and \( v_k \) such that off-diagonal terms vanish

\[
\mathcal{H}_{BCS} - N\mu = \sum_k \left\{ \xi_k + \Delta_k g_k^* + \left( \begin{array}{c} \alpha_k^+ \beta_{-k} \end{array} \right) \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} \begin{pmatrix} \alpha_k^+ \\ \beta_{-k} \end{pmatrix} \right\}
\]

eigenenergies \( \pm E_k \)
4.2.3 The Bogoliubov-Valatin Transformation

\[
\mathcal{B}_k^\dagger = (\alpha_k^\dagger, \beta_{-k}) = \mathcal{C}_k^\dagger \mathcal{U}_k = \mathcal{U}_k^T \mathcal{C}_k
\]

\[
\mathcal{B}_k = (\alpha_k, \beta_{-k}^\dagger) = \mathcal{U}_k^\dagger \mathcal{C}_k
\]

creation and annihilation operators for Bogoliubov quasiparticles: symmetric and anti-symmetric superposition of electron and hole states with opposite momentum and spin

- operators satisfy fermionic anti-commutation rules: \(\{\alpha_k, \beta_{-k}^\dagger\} = \delta_{kk'}\) and \(\{\alpha_k, \alpha_{k'}\} = \{\alpha_k^\dagger, \alpha_{k'}^\dagger\} = 0\)

\[
\mathcal{B}_k^\dagger \mathcal{U}_k^\dagger = \mathcal{C}_k^\dagger \mathcal{U}_k = \mathcal{C}_k^\dagger \Rightarrow \mathcal{C}_k^\dagger = (\mathcal{U}_k^\dagger)^T \mathcal{B}_k^\dagger \Rightarrow (\hat{\mathcal{C}}_k^\dagger, \hat{\mathcal{C}}_{-k}) = \left(\begin{array}{c} u_k^* & v_k \\ v_k^* & u_k \end{array}\right) \left(\begin{array}{c} \alpha_k^\dagger \\ \beta_{-k} \end{array}\right)
\]

\[
\mathcal{U}_k \mathcal{B}_k = \mathcal{U}_k \mathcal{C}_k = \mathcal{C}_k = \mathcal{U}_k \mathcal{B}_k \Rightarrow (\hat{\mathcal{C}}_k^\dagger, \hat{\mathcal{C}}_{-k}) = \left(\begin{array}{c} u_k^* & v_k \\ v_k^* & u_k \end{array}\right) \left(\begin{array}{c} \alpha_k \\ \beta_{-k} \end{array}\right)
\]
4.2.3 The Bogoliubov-Valatin Transformation

Bogoliubov quasiparticles

\[ \begin{align*}
\alpha_k &= u_k^* \hat{c}_{k \uparrow} - v_k^* \hat{c}_{-k \downarrow} \\
\beta_{-k}^\dagger &= v_k \hat{c}_{k \downarrow} + u_k \hat{c}_{-k \uparrow} \\
\alpha_{-k}^\dagger &= u_k \hat{c}_{k \uparrow}^\dagger - v_k \hat{c}_{-k \downarrow}^\dagger \\
\beta_{-k} &= v_k^* \hat{c}_{k \downarrow}^\dagger + u_k^* \hat{c}_{-k \uparrow}^\dagger
\end{align*} \]

\[ |u_k|^2 = |v_k|^2 = \frac{1}{2} \]

- symmetric and anti-symmetric superposition of electron and hole states with opposite spin direction

- \(|u_k|^2 = \text{hole fraction}, |v_k|^2 = \text{electron fraction}\)

\[ \xi_k = 0 \]

\[ \begin{align*}
\alpha_k &= 1/\sqrt{2}(\hat{c}_{k \uparrow} - \hat{c}_{-k \downarrow}) \\
\beta_{-k}^\dagger &= 1/\sqrt{2}(\hat{c}_{k \downarrow} + \hat{c}_{-k \uparrow}) \\
\alpha_{-k}^\dagger &= 1/\sqrt{2}(\hat{c}_{k \uparrow}^\dagger - \hat{c}_{-k \downarrow}^\dagger) \\
\beta_{-k} &= 1/\sqrt{2}(\hat{c}_{k \downarrow}^\dagger + \hat{c}_{-k \uparrow}^\dagger)
\end{align*} \]

\[ \mathcal{U}_k \]

\[ \mathcal{V}_k \]

\[ \mathcal{W}_k \]

\[ \mathcal{X}_k \]

\[ \mathcal{Y}_k \]

\[ \mathcal{Z}_k \]

\[ \mathcal{A}_k \]

\[ \mathcal{B}_k \]

\[ \mathcal{C}_k \]

\[ \mathcal{D}_k \]

\[ \mathcal{E}_k \]

\[ \mathcal{F}_k \]

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\[ \mathcal{M}_k \]
4.2.3 The Bogoliubov-Valatin Transformation

determine $|u_k|^2$ and $|v_k|^2$ by Bogoliubov-Valatin transformation

BCS Hamiltonian

$$\mathcal{H}_{BCS} - N\mu = \sum_k \left\{ \xi_k + \Delta_k g_k^* + \left( \hat{c}_{k\uparrow}^\dagger, \hat{c}_{-k\downarrow} \right) \left( \begin{array}{cc} \xi_k & -\Delta_k \\ -\Delta_k^* & -\xi_k \end{array} \right) \left( \begin{array}{c} \hat{c}_{k\uparrow}^\dagger \\ \hat{c}_{-k\downarrow} \end{array} \right) \right\}$$

- replace operators by Bogoliubov quasiparticle operators $\Rightarrow$ resulting Hamiltonian:

$$\mathcal{H}_{BCS} - N\mu = \sum_k \left[ 2\xi_k v_k^2 - \Delta_k u_k v_k^* - \Delta_k^* u_k^* v_k + \Delta_k g_k^* \right]$$

$$+ \sum_k \left[ \xi_k (u_k^2 - v_k^2) + \Delta_k u_k v_k^* + \Delta_k^* u_k^* v_k \right] \alpha_k^\dagger \alpha_k$$

$$+ \sum_k \left[ \xi_k (u_k^2 - v_k^2) + \Delta_k u_k v_k^* + \Delta_k^* u_k^* v_k \right] \beta_{-k}^\dagger \beta_{-k}$$

$$+ \sum_k \left[ 2\xi_k u_k^* v_k^* + \Delta_k v_k^2 - \Delta_k^* u_k^2 \right] \beta_{-k} \alpha_k$$

$$+ \sum_k \left[ 2\xi_k u_k v_k + \Delta_k^* v_k^2 - \Delta_k u_k^2 \right] \alpha_k^\dagger \beta_{-k}^\dagger \right\} \quad [\ldots] = 0!$$

- we have to set expressions marked in red to zero to keep only diagonal terms
- $\alpha_k^\dagger \alpha_k$ and $\beta_{-k}^\dagger \beta_{-k}$ = quasiparticle number operators

\[ \hat{c}_{k\uparrow}^\dagger = u_k^* \alpha_k^\dagger + v_k \beta_{-k} \]
\[ \hat{c}_{-k\downarrow} = -v_k^* \alpha_k^\dagger + u_k \beta_{-k} \]
\[ \hat{c}_{k\uparrow} = u_k \alpha_k + v_k^* \beta_{-k}^\dagger \]
\[ \hat{c}_{-k\downarrow} = -v_k \alpha_k + u_k^* \beta_{-k}^\dagger \]
• multiply by $\Delta^*_k / u_k^2$, solve the resulting quadratic eqn. for $\Delta^*_k v_k / u_k$ ($\Delta_k v_k^*/u_k^*$)

$$2\xi_k u_k v_k + \Delta_k v_k^2 - \Delta_k u_k^2 = 0$$

$$2\xi_k u_k^* v_k^* + \Delta_k v_k^* - \Delta_k u_k^2 = 0$$

\[
\begin{pmatrix}
\Delta^*_k v_k \\
u_k
\end{pmatrix}_{1,2} = \begin{pmatrix}
\Delta^*_k v_k \\
u_k
\end{pmatrix}_{1,2} = -\xi_k \pm \sqrt{\xi_k^2 + |\Delta_k|^2} = -\xi_k + E_k
\]

\[
E_k = \sqrt{\xi_k^2 + |\Delta_k|^2}
\]

note that the phases of $u_k, v_k$ and $\Delta^*_k$ ($u_k^*, v_k^*$ and $\Delta_k$), although arbitrary, are related, since the quantity on the r.h.s. is real

- the relative phase of $u_k$ and $v_k$ must be fixed and must be the phase of $\Delta^*_k$
- we can choose $u_k$ real and use $v_k = |v_k|e^{i\phi}$, the phase of $v_k$ corresponds to that of $\Delta_k$

\[
\left|\frac{v_k}{u_k}\right| = \frac{E_k - \xi_k}{|\Delta_k|}
\]
with the condition \( \frac{|u_k|}{u_k} = \frac{E_k - \xi_k}{|\Delta_k|} \) and the normalization condition \( |u_k|^2 + |v_k|^2 = 1 \) we obtain

\[
|u_k|^2 = \frac{1}{2} \left[ 1 + \frac{\xi_k}{E_k} \right] \quad |v_k|^2 = \frac{1}{2} \left[ 1 - \frac{\xi_k}{E_k} \right]
\]

\[
u_k^* v_k = g_k = \frac{\Delta_k}{2E_k} \quad u_k^* v_k = g_k = \frac{\Delta_k}{2E_k}
\]

The Bogoliubov-Valatin Transformation

\[
\Delta_k \equiv - \sum_{k'} V_{k,k'} g_k' = - \sum_{k'} V_{k,k'} \frac{\Delta_k'}{2E_k'}
\]

\[
\Delta_k^* \equiv - \sum_{k'} V_{k,k'} g_k'^* = - \sum_{k'} V_{k,k'} \frac{\Delta_k'}{2E_k'}
\]

probability that pair state \((k \uparrow, -k \downarrow)\) is empty/occupied

pairing amplitude

\[
E_k = \sqrt{\xi_k^2 + |\Delta_k|^2}
\]

self-consistent gap equation
4.2.3 The Bogoliubov-Valatin Transformation

excitation spectrum of Bogoliubov quasiparticles and energy gap

![Diagram showing excitation spectrum of Bogoliubov quasiparticles and energy gap.](image)

**quasiparticle excitations: superposition of electron and hole states**

**reason:** single particle excitation with wave vector $\mathbf{k}$ can only exist if at the same time, if there is a hole with wave vector $-\mathbf{k}$, otherwise there would be a pair state

$$E_k = \pm \sqrt{\xi_k^2 + |\Delta_k|^2}$$

**excitation energy**

![Graph showing excitation energy.](image)
4.2.3 The Bogoliubov-Valatin Transformation

\[ \frac{E_k}{E_F}, \frac{\xi_{k,h}}{E_F}, \frac{\xi_{k,e}}{E_F} \] 
\[ \frac{(k-k_F)}{k_F} \]
4.2.3 The Bogoliubov-Valatin Transformation

reformulation of the BCS Hamilton operator

- we start from the Hamiltonian $\mathcal{H}_{BCS} - \mathcal{N}\mu = \sum_k \left\{ \xi_k + \Delta_k g_k^* + \begin{pmatrix} \alpha_k^+, \beta_{-k}^- \end{pmatrix} \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} \begin{pmatrix} \alpha_k^- \\ \beta_{-k}^+ \end{pmatrix} \right\}$

$$\mathcal{H}_{BCS} - \mathcal{N}\mu = \sum_k \{\xi_k + \Delta_k g_k^*\} + \sum_k \left\{ E_k\alpha_k^+\alpha_k^- - E_k\beta_{-k}^+\beta_{-k}^- \right\}$$

$$= \sum_k \{\xi_k + \Delta_k g_k^*\} + \sum_k \{ E_k\alpha_k^+\alpha_k^- - E_k + E_k\beta_{-k}^+\beta_{-k}^- \}$$

mean-field contribution ($T = 0$)

differs from the normal state value by the condensation energy

$\Rightarrow$ minimization of free energy yields BCS gap equation for finite $T$

contribution of spinless Fermion system with two kind of quasiparticles described by operators $\alpha_k^+, \alpha_k^-$ and $\beta_{-k}^+, \beta_{-k}^-$ and excitation energies $\pm E_k$

spinless quasiparticles since they consist of superposition of spin-↑ and spin-↓ electrons
4.2.3 The Bogoliubov-Valatin Transformation

- note that the Bogoliubov quasiparticles are not part of the BCS ground state, as is evident from

\[
\alpha_k |\Psi_{BCS}\rangle = 0
\]
\[
\beta_{-k} |\Psi_{BCS}\rangle = 0
\]

- the occupation probability of the Bogoliubov particles is given by the Fermi-Dirac distribution

\[
\langle \alpha_k^\dagger \alpha_k \rangle = \langle \beta_{-k}^\dagger \beta_{-k} \rangle = f(E_k) = \frac{1}{\exp(E_k/k_B T) + 1}
\]
determination of temperature dependence of $\Delta$ by minimization of free energy

- Hamiltonian has two terms: $\mathcal{H}_{\text{BCS}} - N \mu = \sum_k \{ \xi_k - E_k + \Delta_k g_k^* \} + \sum_k \{ E_k \alpha_k^+ \alpha_k + E_k \beta_{-k}^+ \beta_{-k} \}$

  \[ \text{constant term } \mathcal{H}_0 \]

  \[ \text{term of free Fermi gas composed of two kind of fermions with energy } E_k \]

- grand canonical partition function:

  \[ Z = e^{-\mathcal{H}_0/k_B T} \prod_k \left(1 + e^{-E_k/k_B T}\right) \left(1 + e^{E_k/k_B T}\right) = e^{-\mathcal{F}/N k_B T} \]

  (since $\mathcal{F} = -N k_B T \ln Z$)

- solve for free energy $\mathcal{F}$:

  \[ \frac{\mathcal{F}}{N} = \mathcal{H}_0 - k_B T \sum_k \left[ \ln \left(1 + e^{-E_k/k_B T}\right) + \ln \left(1 + e^{E_k/k_B T}\right) \right] \]

- minimize free energy regarding variation of $\Delta_k$:

  \[ \frac{\partial \mathcal{F}}{\partial \Delta_k} = 0, \quad \frac{\partial \mathcal{F}}{\partial \Delta_k^+} = 0 \]
4.2.3 The BCS Gap Equation and QP Excitations

\[
\frac{\partial (F/N)}{\partial \Delta_k} = 0 = \frac{\partial}{\partial \Delta_k} \left\{ \mathcal{H}_0 - k_B T \sum_k [\ln(1 + e^{-E_k/k_B T}) + \ln(1 + e^{E_k/k_B T})] \right\}
\]

\[
\mathcal{H}_0 = \xi_k - E_k + \Delta_k g^*_k
\]

\[
g^*_k + \frac{\partial E_k}{\partial \Delta_k} \left[ \frac{e^{-E_k/k_B T}}{1 + e^{-E_k/k_B T}} - \frac{e^{E_k/k_B T}}{1 + e^{E_k/k_B T}} \right] = 0
\]

\[
\Delta_k \equiv - \sum_{k'} V_{k,k'} g^*_k = - \sum_{k'} V_{k,k'} \frac{\Delta_{k'}}{2E_{k'}}
\]

\[
g^*_k = \frac{\Delta^*_k}{2E_k} \tanh \left( \frac{E_k}{2k_B T} \right) = u_k v^*_k \tanh \left( \frac{E_k}{2k_B T} \right)
\]

pairing susceptibility/amplitude: ability of the electron system to form pairs

- we use \( \Delta^*_k \equiv - \sum_{k'} V_{k,k'} g^*_k \) and obtain:

\[
\Delta^*_k = - \sum_{k'} V_{k,k'} \frac{\Delta^*_{k'}}{2E_{k'}} \tanh \left( \frac{E_{k'}}{2k_B T} \right)
\]

BCS gap equation

- set of equations for variables \( \Delta_k \)
- equations are nonlinear, since \( E_k \) depends on \( \Delta_k \)
- solve numerically, analytical solutions in limiting cases
4.2.3 The BCS Gap Equation and QP Excitations

**energy gap $\Delta$ and transition temperature $T_c$**

- trivial solution: $\Delta_k = 0$, results in $\nu_k = 1$ for $\xi_k < 0$ and $\nu_k = 0$ for $\xi_k > 0$

  $\rightarrow$ intuitive expectation for normal state

- non-trivial solution: we use approximations $V_{k,k'} = -V_0$ and $\Delta_k = \Delta$

  \[
  \Delta_k^* = -\sum_{k'} V_{k,k'} \frac{\Delta_{k'}^*}{2E_{k'}} \tanh \left( \frac{E_{k'}}{2k_B T} \right)
  \]

  \[
  1 = V_0 \sum_{k'} \frac{1}{2E_{k'}} \tanh \left( \frac{E_{k'}}{2k_B T} \right)
  \]

  - we use pair density of states $\tilde{D}(E) = D(E)/2$ and change from summation to integration

  simple solutions for
  
  (i) $T \to 0$
  
  (ii) $T \to T_c$
4.2.3 The BCS Gap Equation and QP Excitations

i. solution for \( T \to 0 \):

(already discussed above for \( V_{k,k'} = -V_0 \) and \( \Delta_k = \Delta \))

\[
1 = V_0 \sum_{k'} \frac{1}{2E_{k'}} \tanh \left( \frac{E_{k'}}{2k_B T} \right) \quad \text{transforming sum into integration}
\]

\[
1 = \frac{V_0 D(E_F)}{4} \int_{-\hbar \omega_D}^{\hbar \omega_D} \frac{d\xi}{\sqrt{\xi^2 + |\Delta(0)|^2}} = \frac{V_0 D(E_F)}{4} \arcsinh \left( \frac{\hbar \omega_D}{\Delta(0)} \right)_{-\hbar \omega_D}^{\hbar \omega_D} = \frac{V_0 D(E_F)}{2} \arcsinh \left( \frac{\hbar \omega_D}{\Delta(0)} \right)
\]

- solve for \( \Delta \):

\[
\Delta(0) = \frac{\hbar \omega_D}{\sinh \left( \frac{2}{V_0 D(E_F)} \right)} \approx 2\hbar \omega_D e^{-2/V_0 D(E_F)}
\]

\( V_0 D(E_F) \ll 1 \): weak coupling approximation

- compare to expression derived for energy of two interacting electrons ("Gedanken" experiment):

\[
E \approx 2E_F - 2\hbar \omega_D e^{-4/V_0 D(E_F)}
\]

factor 2 in argument of exponential function since we have assumed that the two additional electrons are in interval between \( E_F \) and \( E_F + \hbar \omega_D \) and not between \( E_F - \hbar \omega_D \) and \( E_F + \hbar \omega_D \)
ii. solution for $T \to T_c$: $E_k \to |\xi_k|$ since $\Delta_k \to 0$

\[
1 = V_0 \sum_{k'} \frac{1}{2E_{k'}} \tanh \left( \frac{E_{k'}}{2k_B T} \right) \Rightarrow 1 = V_0 \sum_{k'} \frac{1}{2\xi_{k'}} \tanh \left( \frac{\xi_{k'}}{2k_B T} \right)
\]

\[
1 = \frac{V_0 D(E_F)}{4} \int_{-\hbar \omega_D}^{\hbar \omega_D} \frac{1}{\xi_{k'}} \tanh \left( \frac{\xi_{k'}}{2k_B T_c} \right) d\xi = \frac{V_0 D(E_F)}{4} \int_{-\hbar \omega_D/2k_B T_c}^{\hbar \omega_D/2k_B T_c} \tanh \frac{x}{x} dx \quad \text{with } x = \xi_k / 2k_B T_c
\]

• integral gives $2 \ln(p \hbar \omega_D / 2k_B T_c)$ with $p = \frac{2e^r}{\pi} \approx 1.13$ and $r = 0.577 \ldots$ (Euler constant)

\[
k_B T_c = 1.13 \hbar \omega_D e^{-2/V_0 D(E_F)}
\]

critical temperature is proportional to Debye frequency $\omega_D \propto 1/\sqrt{M}$

$\Rightarrow$ explains isotope effect!!
relation between energy gap at zero temperature and critical temperature

\[ \Delta(0) \approx 2\hbar \omega_D e^{-2/V_0D(E_F)} \]

key prediction of BCS theory

\[ k_B T_c = \frac{2e^\gamma}{\pi} \hbar \omega_D e^{-2/V_0D(E_F)} \]

| Material | \( T_c \) (K) | \( 2\Delta(0) \) (meV) | \( 2\Delta(0)/k_B T_c \) |
|----------|----------------|--------------------------|
| Al       | 1.19           | 0.36                     | 3.5 ± 0.1                |
| Nb       | 9.2            | 2.90                     | 3.6                      |
| Pb       | 7.2            | 2.70                     | 4.3 ± 0.05               |
| Ta       | 4.29           | 1.30                     | 3.5 ± 0.1                |
| NbN      | 15             | 4.65                     | 3.6                      |
| NbSe\(_2\) | 7             | 2.2                      | 3.7                      |
| In       | 3.4            | 1.05                     | 3.5 ± 0.1                |
| Hg       | 4.15           | 1.65                     | 4.6 ± 0.1                |
| Sn       | 3.72           | 1.15                     | 3.5 ± 0.1                |
| Tl       | 2.39           | 0.75                     | 3.6 ± 0.1                |
| Nb\(_3\)Sn | 18         | 6.55                     | 4.2                      |
| MgB\(_2\) | 40            | 3.6-15                   | 1.1 − 4.5                |

considerable deviations for “strong-coupling” superconductors:

\[ V_0D(E_F) \ll 1 \] is no longer a good approximation
solution for $0 < T < T_c$ (numerical solution of integral)

$$1 = V_0 \sum_{k'} \frac{1}{2E_{k'}} \tanh \left( \frac{E_{k'}}{2k_B T} \right) \text{ sum } \Rightarrow \text{ integral } \quad 1 = \frac{V_0 D(E_F)}{2} \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{1}{2E_k} \tanh \left( \frac{E_k}{2k_B T} \right) d\xi_k$$

good approximation close to $T_c$:

$$\frac{\Delta(T)}{\Delta(0)} \approx 1.74 \left( 1 - \frac{T}{T_c} \right)^{1/2}$$ (characteristic result of mean-field theory)

### 4.2.3 The BCS Gap Equation and QP Excitations

**strong electron-phonon coupling**

- BCS results are valid only for weak coupling: $V_0 D(E_F) \ll 1$
- for $V_0 D(E_F) \gtrsim 0.2$ a more elaborate treatment is required

**phonons have influence on electrons but also electrons change e.g. phonon frequencies**

- **Eliashberg theory**
  - replace coupling constant $\lambda = V_0 D(E_F)$ by
  $$
  \lambda(\omega) = 2 \int_0^{\infty} \frac{\alpha^2(\omega) F(\omega)}{\omega} \, d\omega
  $$

- **McMillan approximation**
  - several attempts have been made to improve prediction for $T_c$ using strong coupling theory, e.g. by McMillan:
  $$
  T_c = \frac{\hbar \omega_D}{1.45} \exp \left( \frac{1.04(1 + \lambda)}{\lambda - \mu^*(1 + 0.62 \lambda)} \right)
  $$

---

$F(\omega)$: phonon density of states  
$\alpha(\omega)$: matrix element of the electron-phonon interaction


4.2.3 Energy Gap and Excitation Spectrum

dispersion of excitations (Bogoliubov quasiparticles) from the superconducting ground state

→ excitations represent superpositions of electron- and hole-type single particle states
(reason: single particle excitation with \( \mathbf{k} \) can only exist if there is hole with \(-\mathbf{k}\), if not, Cooper pair would form)

\[
e_{\mathbf{k}} = E_{-\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}
\]

- break up of Cooper pair requires energy \(2E_{\mathbf{k}}\)
- \(\Delta\) represents energy gap for quasiparticle excitation from ground state
  ⇒ minimum excitation energy

equal superposition of electron with wave vector \( \mathbf{k} \)
and hole with wave vector \(-\mathbf{k}\)
4.2.3 Energy Gap and Excitation Spectrum

density of states

- conservation of states on transition to sc state requires \( D_s(E_k) dE_k = D_n(\xi_k) d\xi_k \)
- close to \( E_F \): \( D_n(\xi_k) \approx D_n(E_F) = \text{const.} \)

\[
D_s(E_k) = D_n(\xi_k) \frac{d\xi_k}{dE_k} = \begin{cases} 
D_n(E_F) \frac{E_k}{\sqrt{E_k^2 - \Delta^2}} & \text{for } E_k > \Delta \\
0 & \text{for } E_k < \Delta 
\end{cases}
\]

\( I. \) Giaever, 

- measurement by tunneling spectroscopy

\( \Delta = 1.34 \text{ meV} \)
\( T = 0.33 \text{ K} \)
4.3 Thermodynamic Quantities

- occupation probability of qp-excitations is given by \( f(E_k) = \frac{\exp(E_k/k_B T) + 1}{\exp(E_k/k_B T) + 1} \)

\[ \rightarrow \text{i.e. by } \Delta_k(T), \text{ which is contained in } E_k = \sqrt{\xi_k^2 + |\Delta_k|^2(T)} \]

- **entropy of electronic system** (determined only by the occupation probability \( \rightarrow \) is fixed by \( \Delta_k \))

\[ S_s = -2k_B \sum_k \left\{ \left[ 1 - f(E_k) \right] \ln \left[ 1 - f(E_k) \right] + f(E_k) \ln [f(E_k)] \right\} \]

- **heat capacity**: \( C_S = T \left( \frac{\partial S_s}{\partial T} \right) \)

\[ C_S = \frac{2}{T} \sum_k \left( \frac{\partial f(E_k)}{\partial E_k} \left( E_k^2 - \frac{1}{2} \frac{d\Delta_k^2(T)}{dT} \right) \right) \]

\[ \text{results from redistribution of qp on available energy levels} \]
\[ \text{results from } T\text{-dependence of energy gap} \]

Yosida function:

\[ Y(T) = \frac{1}{D(E_F)} \sum_k \frac{\partial f(E_k, T)}{\partial E_k} = \frac{1}{4k_B T} \int_\mu^\infty \frac{d\xi_k}{\cosh^2(\xi_k/2k_B T)} \]

\[ Y(T) \text{ describes the } T\text{-dependence of the qp excitations (normal fluid density): } n_n(T) = n Y(T) \]
4.3 Thermodynamic Quantities

Discussion of limiting cases

\[ T \ll T_c: \]

- Since \( \Delta_k(T) \approx \Delta_k(0) \gg k_B T \), there are only a few thermally excited qp.

- We use approximations \( d\Delta_k^2(T)/dT \approx 0 \) and \( f(E_k) = [\exp(E_k/k_B T) + 1]^{-1} \approx \exp(-E_k/k_B T) \).

- We assume \( \Delta_k = \Delta \) for simplicity and transfer sum into an integration.

\[
C_s = \frac{2}{T} \sum_k - \frac{\partial f(E_k)}{\partial E_k} \left( E_k^2 - \frac{1}{2} T \frac{d\Delta_k^2(T)}{dT} \right) \approx \frac{D(E_F)}{k_B T^2} \Delta^2(0) \int_0^\infty e^{-\Delta^2 + \xi_k^2/k_B T} d\xi_k \\
C_s \approx \frac{D(E_F)}{k_B T^2} \Delta^2(0) e^{-\Delta(0)/k_B T} \int_0^\infty e^{-\xi_k^2/2\Delta(0)/k_B T} d\xi_k
\]

\[
C_s \propto T^{-\frac{3}{2}} e^{-\frac{\Delta(0)}{k_B T}} \propto T^{-\frac{3}{2}} e^{-1.76 \frac{T_c}{T}} \text{ at } T \ll T_c
\]

Exponential decrease of heat capacity at low \( T \)
specific heat of superconductors at $T \ll T_c$:

exponential decrease of $C_s$ with decreasing $T$:

$$C_s \propto T^{-\frac{3}{2}} e^{-\frac{\Delta(0)}{k_B T}} \propto T^{-\frac{3}{2}} e^{-1.76 \frac{T_c}{T}} \quad @ \ T \ll T_c$$

$M. \ A. \ Biondi, \ A. \ T. \ Forrester, \ M. \ P. \ Garfunkel, \ C. \ B. \ Satterthwaite, \ Rev. \ Mod. \ Phys. 30, 1109-1136 (1958)$
ii. $0.5 < T/T_c < 1$:

$\Delta(T)$ decreases with increasing $T \Rightarrow$ there is a rapid increase of the number of thermally excited quasiparticles

$\Rightarrow \frac{\partial S_{s}}{\partial T} > \frac{\partial S_{n}}{\partial T} \Rightarrow C_s$ is getting larger than $C_n$
4.3 Thermodynamic Quantities

iii. $T \approx T_c$:

$\Delta(T) \rightarrow 0 \Rightarrow$ we can replace $E_k$ by $|\xi_k|$: 

$$C_s = \frac{2}{T} \sum_k - \frac{\partial f(\xi_k)}{\partial \xi_k} \left( \xi_k^2 - \frac{1}{2} T \frac{d\Delta^2(T')}{dT} \right)$$

normal state specific heat $C_n = \frac{\pi^2}{3} D(E_F) k_B^2 T$

finite for $T < T_c$

zero for $T > T_c$

$\left\{ \text{jump of specific heat} \right\}$

Vanadium ($B_{ext} > B_{cth}$)

Vanadium ($B_{ext} = 0$)

Vanadium

Zinn

$\propto 9.17 \exp\left(-1.5 \frac{T_c}{T} \right)$

M. A. Biondi et al., Rev. Mod. Phys. 30, 1109-1136 (1958)
4.3 Thermodynamic Quantities

iii. $T \approx T_c$: jump of specific heat (we can replace $E_k$ by $|\xi_k|$)

\[ \Delta C = (C_S - C_n)_{T=T_c} = \frac{2}{T} \sum_k - \frac{\partial f(\xi_k)}{\partial \xi_k} \left( - \frac{1}{2} T \frac{d^2(T')}{dT'^2} \right)_{T=T_c} \]

\[ \Delta C = D(E_F) \left( - \frac{d^2(T')}{dT'} \right)_{T=T_c} \int_{-\infty}^{\infty} - \frac{\partial f(\xi_k)}{\partial \xi_k} d\xi_k = 1 \]

we use $\Delta(T') \approx 1.74 \left( 1 - \frac{T}{T_c} \right)^{1/2}$ for $T$ close to $T_c$ and $\Delta(0) = 1.76 k_B T_c$ and obtain

\[ \Delta C \approx 4.7 D(E_F) k_B^2 T_c \]

with $C_n(T_c) = \frac{\pi^2}{3} D(E_F) k_B^2 T_c = \gamma T_c$ we finally obtain

\[ \left( \frac{\Delta C}{C_n} \right)_{T=T_c} \approx \frac{4.7}{\pi^2/3} = 1.43 \]

result from phenomenological treatment: \( \left( \frac{\Delta C}{C_n} \right)_{T=T_c} = \frac{1}{C_n \mu_0} \left( \frac{\partial B_{\text{ch}}}{\partial T} \right)_{T=T_c}^2 = \frac{1}{C_n T_c} \frac{B^2_{\text{ch}}(0)}{2 \mu_0} = \frac{8}{\pi^2} \frac{B^2_{\text{ch}}(0)}{2 \mu_0} = \frac{6}{\pi^2} \left( \frac{\Delta(0)}{k_B T_c} \right)^2 = \frac{6}{\pi^2} (1.76)^2 = 1.88 \]

(Rutgers formula)

"further key prediction of BCS theory (in good agreement with experiment)"

\[ \left. \frac{1}{4} D(E_F) \Delta^2(0) \right| \]

difference comes from $B_{\text{ch}}(T)$
4.3 Thermodynamic Quantities

N.E. Phillips,
Phys. Rev. 114, 676 (1959)

M. A. Biondi et al.,
Rev. Mod. Phys. 30, 1109-1136 (1958)
Bogoliubov-Valatin transformation → BCS Gap Equation and Excitation Spectrum

\[
\mathcal{H}_{BCS} - N \mu = \sum_k \left\{ \xi_k + \Delta_k g_k^* + \frac{C_{k+}^* C_{k-}}{B_k^*} u_k^* u_k \left( \frac{\xi_k}{-\Delta_k} \right) u_k^* \right\} = \sum_k \left\{ \xi_k + \Delta_k g_k^* + D_k^* u_k^* \xi_k u_k \right\}
\]

Bogoliubov quasiparticles: → superposition of electron and hole states with opposite momentum and spin

Task: find unitary matrix \((u_k u_k^* = 1)\) that makes the transformed energy matrix \(u_k^* \xi_k u_k\) diagonal:

\[
u_k = \begin{pmatrix} u_k & v_k^* \\ -v_k & u_k^* \end{pmatrix}, \quad \xi_k = \sum_k \left\{ \xi_k + \Delta_k g_k^* + D_k^* u_k^* \xi_k u_k \right\}
\]

reformulation of the BCS Hamilton operator

\[
\mathcal{H}_{BCS} - N \mu = \sum_k \left\{ \xi_k - E_k + \Delta_k g_k^* \right\} + \sum_k \left\{ E_k \alpha_k^+ \alpha_k + E_k \beta_k^+ \beta_k \right\}
\]

mean-field contribution

differs from the normal state value by the condensation energy (see below)

contribution of spinless Fermion system with two kind of quasiparticles described by operators \(\alpha_k^+, \alpha_k\) and \(\beta_k^+, \beta_k\) and excitation energies \(\pm E_k\)

spinless quasiparticles since they consist of superposition of spin-↑ and spin-↓ electrons

minimization of free energy yields BCS gap equation for finite T
Summary of Lecture No. 9 (2)

- **minimization of free energy yields BCS gap equation:**

  \[
  1 = V_0 \sum_{\mathbf{k}' k} \frac{1}{2E_{\mathbf{k}'}^2} \tanh \left( \frac{E_{\mathbf{k}'}^2}{2k_B T} \right)
  \]

  **BCS gap equation**

- **analytical solution with simplifications:** \( V_{\mathbf{k} k'} = -V_0, \Delta_{\mathbf{k}} = \Delta, V_0 D(E_F) \ll 1 \): weak coupling approximation

  - \( T \ll T_c \)
    \[
    \Delta(0) \approx 2 \hbar \omega_D e^{-\frac{2}{V_0 D(E_F)}}
    \]
  
  - \( T \approx T_c \)
    \[
    \frac{\Delta(0)}{k_B T_c} = \frac{\pi}{\text{e}^\gamma} = 1.764
    \]

- **condensation energy at \( T = 0 \)** \( V_{\mathbf{k} k'} = -V_0, \Delta_{\mathbf{k}} = \Delta, V_0 D(E_F) \ll 1 \): weak coupling approximation

  \[
  E_{\text{kond}}(0) = \langle H_{\text{BCS}} \rangle - \langle H_n \rangle = -D(E_F)\Delta^2(0)/4
  \]

  comparison to \( E_{\text{cond}}(0) = -B_{\text{cth}}^2(0)/2\mu_0 \) (thermodynamics) yields

  \[
  B_{\text{cth}}(0) = \sqrt{\frac{\mu_0 D(E_F)\Delta^2(0)}{2V}}
  \]
Summary of Lecture No. 9 (3)

- **density of states:**

\[
D_s(E_k) = D_n(\xi_k) \frac{d\xi_k}{dE_k} = \begin{cases} 
D_n(E_F) \frac{E_k}{\sqrt{E_k^2 - \Delta^2}} & \text{for } E_k > \Delta \\
0 & \text{for } E_k < \Delta 
\end{cases}
\]

- **BCS prediction for thermodynamic quantities**

\[
S_s = -2k_B \sum_k \left\{ \frac{1 - f(E_k)}{\ln(1 - f(E_k))} + \frac{f(E_k) \ln(f(E_k))}{\ln(1 - f(E_k))} \right\}
\]

\[
C_s = \frac{2}{T} \sum_k \frac{\partial f(E_k)}{\partial E_k} \left( E_k^2 - \frac{1}{2} T \frac{d\Delta_k^2(T)}{dT} \right)
\]

\[
C_s \propto T^{-\frac{3}{2}e} \frac{\Delta(0)}{k_BT} \propto T^{-\frac{3}{2}e} -1.76 \frac{T}{T_c} \text{ at } T \ll T_c
\]

- **entropy**

- **heat capacity**

- **exponential decrease of heat capacity at low T**
Superconductivity and Low Temperature Physics I

Lecture No. 10

R. Gross
© Walther-Meißner-Institut
Chapter 4

4. Microscopic Theory

4.1 Attractive Electron-Electron Interaction
   4.1.1 Phonon Mediated Interaction
   4.1.2 Cooper Pairs
   4.1.3 Symmetry of Pair Wavefunction

4.2 BCS Ground State
   4.2.1 The BCS Gap Equation
   4.2.2 Ground State Energy
   4.2.3 Bogoliubov-Valatin Transformation and Quasiparticle Excitations

4.3 Thermodynamic Quantities

4.4 Determination of the Energy Gap
   4.4.1 Specific Heat
   4.4.2 Tunneling Spectroscopy

4.5 Coherence Effects
4.4 Determination of the Energy Gap

- Energy gap determines excitation spectrum of superconductors
  ➔ we can use quantities that depend on excitation spectrum to determine $\Delta$

  1. Specific heat
  2. Tunneling conductance
  3. Microwave and infrared absorption
  4. Ultrasound attenuation
  5. ..... 

- We concentrate on tunneling spectroscopy in the following
  (specific heat already discussed in previous subsection)
4.4.2 Tunneling Spectroscopy

tunneling of quasiparticle excitations between two superconductors separated by thin tunneling barrier

- SIS tunnel junction:

![SIS tunnel junction](image)

- fabrication by thin film technology and patterning techniques
  
  by shadow masks \((\approx \text{mm})\)
  
  by optical lithography \((\approx \text{μm})\)
  
  by e-beam lithography \((\approx 10\, \text{nm})\)

- sketch:

![Sketch of SIS tunnel junction](image)
4.4.2 Tunneling Spectroscopy

- Tunneling processes result in finite coupling of SC 1 and SC 2, described by tunneling Hamiltonian

\[ \mathcal{H}_{\text{tun}} = \sum_{kq\sigma} T_{kq} c_{k\sigma}^+ c_{q\sigma} + \text{c.c.} \]

- Tunnel matrix element describes the creation of electron \(|k\sigma\rangle\) in one SC and the annihilation of electron \(|q\sigma\rangle\) in the other

- Tunneling into state \(|k\sigma\rangle\) only possible if pair state \((k \uparrow, -k \downarrow)\) is empty

\[ \Rightarrow \text{resulting tunneling probability is } \propto |u_k|^2 |T_{kq}|^2 \]

- For each state \(|k\sigma\rangle\) there exists a state \(|k'\sigma\rangle\) with \(E_k = E_{k'}\) but with \(\xi_{k'} = -\xi_k\)

\[ \Rightarrow \text{resulting tunneling probability is } \propto |u_{k'}|^2 |T_{k'q}|^2 \]

\[ = \frac{|v_k|^2 |T_{k'q}|^2}{|u(-\xi_k)| = |v(\xi_k)|} \]

- Total tunneling probability \(\propto (|u_k|^2 + |v_k|^2) |T_{kq}|^2 = |T_{kq}|^2\) does not depend on coherence factors

\[ \Rightarrow \text{simple } \mu \text{"semiconductor model" for quasiparticle tunneling is applicable} \]
4.4.2 Tunneling Spectroscopy

elastic tunneling between two metals (NIN):

\[ I_{1 \rightarrow 2} = C \int_{-\infty}^{\infty} |T|^2 \frac{D_1(E)f(E)}{\text{occupied states in } N_1} \frac{D_2(E + eV) [1 - f(E + eV)]}{\text{empty states in } N_2} \, dE \]

- net tunneling current:

\[ I_{nn}(V) = C \int_{-\infty}^{\infty} |T|^2 D_1(E)D_2(E + eV) [f(E) - f(E + eV)] \, dE \]

- for \( eV \ll \mu \) and \( \mu \approx E_F \) we can use \( D_n(E + eV) \approx D_n(E_F) = \text{const.} \)

\[ I_{nn}(V) = C |T|^2 D_{n1}(E_F)D_{n2}(E_F) \int_{-\infty}^{\infty} [f(E) - f(E + eV)] \, dE = eV \]

\[ I_{nn}(V) = C |T|^2 D_{n1}(E_F)D_{n2}(E_F) e V = G_{nn} V \]
4.4.2 Tunneling Spectroscopy

elastic tunneling between N and S (NIS junction):

\[
I_{ns}(V) = \frac{C|T|^2 D_{n1}(E_F)D_{n2}(E_F)}{G_{nn}/e} \int_{-\infty}^{\infty} \frac{D_{s2}(E)}{D_{n2}(E_F)} [f(E) - f(E + eV)] \, dE
\]

\[
I_{ns}(V) = \frac{G_{nn}}{e} \int_{-\infty}^{\infty} \frac{D_{s2}(E)}{D_{n2}(E_F)} [f(E) - f(E + eV)] \, dE
\]

- analytical solution for \( T = 0 \)

\[
I_{ns}(V) = \frac{G_{nn}}{e} \int_{-\infty}^{\infty} \frac{|E|}{|E^2 - \Delta^2|^{1/2}} [f(E) - f(E + eV)] \, dE
\]

\[
I_{ns}(V) = \begin{cases} 
0 & |eV| < \Delta \\
\frac{G_{nn}}{e} [(eV)^2 - \Delta^2]^{1/2} & |eV| \geq \Delta
\end{cases}
\]
4.4.2 Tunneling Spectroscopy

$$\frac{I_{ns}}{G_{nff}/e \Delta(0)}$$

$T > T_c$

$T = 0$

$$\frac{\mu_1}{2\Delta}$$

$$\frac{\mu_2}{2\Delta}$$

$N/S$
4.4.2 Tunneling Spectroscopy

differential tunneling conductance of NIS junction

\[ I_{ns}(V) = \frac{G_{nn}}{e} \int_{-\infty}^{\infty} \frac{D_{s2}(E)}{D_{n2}(E_F)} \left[ f(E) - f(E + eV) \right] dE \]

\[ G_{ns}(V) = \frac{\partial I_{ns}(V)}{\partial V} = G_{nn} \int_{-\infty}^{\infty} \frac{D_{s2}(E)}{D_{n2}(E_F)} \left[ \frac{\partial f(E + eV)}{\partial (eV)} \right] dE \]

Bell-shaped weighting function with width \( \approx 4k_B T \) peaked at \( E = eV \)
\( \rightarrow \) approaches \( \delta \)-function for \( T \rightarrow 0 \)

\[ G_{ns}(V) = G_{nn} \frac{D_{s2}(eV)}{D_{n2}(E_F)} \]

@ \( T = 0 \) measurement of \( G_{ns}(V) \) allows determination of \( D_{s2}(eV) \) and \( \Delta \), for \( T > 0 \), \( G_{ns}(V) \) measures DOS smeared out by \( \pm k_B T \)

• at \( T > 0 \): finite conductance at \( eV \ll \Delta \) due to smeared Fermi distribution, calculation yields

\[ \frac{G_{ns}}{G_{nn}} \bigg|_{eV \ll \Delta} = \left( \frac{2\pi \Delta}{k_B T} \right) e^{-\Delta/k_B T} \]

exponential \( T \)-dependence can be used for temperature measurement, particle detectors, ...
4.4.2 Tunneling Spectroscopy

4.4.2 Tunneling Spectroscopy

elastic tunneling between two superconductors: SIS junction

\[
I_{ss}(V) = \frac{G_{nn}}{e} \int_{-\infty}^{\infty} \frac{D_{s1}(E + eV)}{D_{n1}(E_F)} \frac{D_{s2}(E)}{D_{n2}(E_F)} [f(E) - f(E + eV)] dE
\]

- strong increase of \( I_{ss} @ eV = 2\Delta \)
- \( I_{ss} \to I_{nn} @ eV \gg 2\Delta \)
- \( I_{ss} \propto e^{-\Delta/k_B T} @ eV < 2\Delta \)
4.4.2 Tunneling Spectroscopy

interpretation of tunneling in SIS junction at $T = 0$

- single electron tunnels from left to right:

  before tunneling

  \[
  \left| \psi_k \right> \quad \text{occupied and empty pair state}
  \]

  after tunneling

  \[
  \left| \psi_k \right> \quad \text{two quasiparticles}
  \]

- energy balance:

  \[
  -E_{F}^{\text{(left)}} + E_{k}^{\text{(left)}} + E_{F}^{\text{(right)}} + E_{k}^{\text{(right)}}
  \]

  $e^{-}$ moves from left to right

  generation of two qp

- required voltage:

  \[
  eV = E_{k}^{\text{(left)}} + E_{k}^{\text{(right)}}
  \]

- minimal voltage:

  \[
  eV = \Delta_1 + \Delta_2 = 2\Delta \quad \text{for } \Delta_1 = \Delta_2
  \]
4.4.2 Tunneling Spectroscopy

current-voltage characteristics of SIS junction at finite temperatures

\[ I_{ss} \] (pA.. A)

\[ 2\Delta(T) \quad 2\Delta_0 \quad eV \ (\approx \text{few meV}) \]

\[ T = 0 \]

NIN

increasing \( T \)
4.4.2 Tunneling Spectroscopy

special case: SIS tunnel junction with $\Delta_1 \neq \Delta_2$

- at $eV = \Delta_2 - \Delta_1$ the two singularities in the DOS are facing each other

$\Rightarrow$ maximum of the tunneling current

$\Rightarrow$ negative differential resistance
4.5 Coherence Effects

- description of an external perturbation on the electrons in a metal

\[ \mathcal{H}_1 = \sum_{k\sigma, k'\sigma'} P_{k'\sigma', k\sigma} c_{k'\sigma'}^\dagger c_{k\sigma} \]

interaction hamiltonian

\[ |P_{k'\sigma', k\sigma}|^2 \] corresponds to transition probability

- description of the external perturbation on the electrons in a superconductor

⇒ more complicated since there is a coherent superposition of occupied one-electron states

\[ \hat{c}_{k\uparrow} = u_k^* \alpha_k^\dagger + v_k \beta_{-k} \]

\[ \hat{c}_{-k\downarrow} = -v_k^* \alpha_k^\dagger + u_k \beta_{-k} \]

\[ \hat{c}_{k\downarrow} = u_k \alpha_k + v_k^* \beta_{-k}^\dagger \]

\[ \hat{c}_{-k\uparrow} = -v_k \alpha_k + u_k^* \beta_{-k}^\dagger \]

\[ c_{k\uparrow}^\dagger c_{k\uparrow} = \left( u_k^* \alpha_k^\dagger + v_k \beta_{-k} \right) \left( u_k \alpha_k + v_k^* \beta_{-k}^\dagger \right) \]

connect the same qp states

⇒ matrix elements \( |P_{k'\sigma', k\sigma}|^2 \) have to be multiplied by so-called coherence factors

\[ \left( u_k u_{k'} + v_k v_{k'} \right)^2 \] for scattering of quasiparticles

\[ \left( v_k u_{k'} \pm u_k v_{k'} \right)^2 \] for creation or annihilation of quasiparticles

\( u_k, v_k \) are assumed real
see e.g.
M. Tinkham
Introduction to Superconductivity
temperature dependence of low-frequency absorption processes in superconductors

**Case I Coherence Factor**
- $\nu$ nuclear relaxation, electromagnetic absorption
- (for perturbation which are even under time reversal)

**Case II Coherence Factor**
- $\alpha_s/\alpha_n$
- (for perturbation which are odd under time reversal)

**BCS Theory** makes prediction for coherence factors

**Graph**: Two-fluid model

- $T/T_c$
4.5 Coherence Effects

![Graph showing ultrasound attenuation in Sr$_2$RuO$_4$]

**Hebel-Slichter peak**

*Ultrasound Attenuation in Sr$_2$RuO$_4$: An Angle-Resolved Study of the Superconducting Gap Function*

C. Lupien, W. A. MacFarlane, Cyril Proust, Louis Taillefer, Z. Q. Mao, and Y. Maeno


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