Superconductivity and Low Temperature Physics I

Lecture Notes
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Chapter 4

Microscopic Theory
Superconductivity and Low Temperature Physics I

Lecture No. 7

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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 $\sim \text{meV}$
      ➔ 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:

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

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

\[
\log \left( \frac{T_c}{K} \right) \propto \log \left( \frac{M}{\text{bel. Einh.}} \right)
\]

\[
\begin{array}{cccccccc}
\text{Element} & \text{Hg} & \text{Sn} & \text{Pb} & \text{Cd} & \text{Tl} & \text{Mo} & \text{Os} & \text{Ru} \\
\text{Isotop-exponent } \beta^* & 0.50 & 0.47 & 0.48 & 0.5 & 0.5 & 0.33 & 0.2 & 0.0 \\
\end{array}
\]
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: \( \approx 10^6 \text{ m/s} \approx 0.01 c \)
  - 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
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**

- 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): $\tau = 1/\omega_q$
  - $\omega_q \approx 10^{12} - 10^{13}$ s$^{-1}$ (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: \( v_F \approx \text{few } 10^6 \text{ m/s} \)

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

• important fact:
  - retarded reaction of slow ions results in large interaction range

\[ \Rightarrow \text{retarded interaction} \]
  - retarded interaction is essential for achieving attractive interaction

\[ \Rightarrow \text{without any retardation: } \text{short interaction range} \]
  - Coulomb repulsion between electrons dominates

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

\[ \Rightarrow \text{retarded interaction potential:} \]

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

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

- screened Coulomb potential
- correction term is negative for \( \omega < \tilde{\Omega}_p(q) \) → overscreening

- \( 1/k_s = \text{Thomas-Fermi screening length} \)
4.1.1 Phonon Mediated Interaction

The effective e-ph interaction potential is given by:

\[ V(q, \omega) = \frac{e^2}{\varepsilon(q, \omega)\varepsilon_0 q^2} \]

\[ = \left( \frac{e^2}{\varepsilon_0 (q^2 + k_s^2)} \right) \left( 1 + \frac{\Omega_p^2(q)}{\omega^2 - \Omega_p^2(q)} \right) \]
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 $\Delta t \lesssim \frac{1}{\omega_q}$

- 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 $\Delta k \simeq m \omega_D / \hbar k_F$
    - for given $K$ only specific wave vectors $k_1, k_2$ are allowed for interaction process
4.1.2 Cooper-Pairs

\[ K = k_1 + k_2 > 0 \]

possible phase space for interaction

\[ K = k_1 + k_2 = 0 \]

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: \((k, -k)\)

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

\[
\Delta k \approx \frac{m \omega_D}{\hbar k_F}
\]
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

\[ \psi(r_1, r_2) = a \exp(i k_1 \cdot r_1) \exp(i k_2 \cdot r_2) = a \exp(i k \cdot r) \quad \text{with} \quad k = k_1 = -k_2, \quad r = r_1 - r_2 \]

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

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

with \( k_F < k < k_F + \Delta k \),

since restriction to energies \( E_F < E < E_F + \hbar \omega_D \)

\[ |a_k|^2 : \text{probability for realization of pair} \ (k, -k) \]

• 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:

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

- 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 \( e^{-i\mathbf{k}^\prime \cdot \mathbf{r}} \) and integrate over sample volume \( \Omega \)

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

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

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

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

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

**scattering integral**
4.1.2 Cooper-Pairs

- we use abbreviation

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

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

- result

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

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

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

\[
a_k = \frac{-V_0}{E - (\hbar^2 k^2 / m)} \sum_{k' = k_F}^{k_F + \Delta k} a_{k'}
\]
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 $\bar{D}(E) = D(E)/2$: sum $\Rightarrow$ integral

$$(D(E) = \text{DOS for both spin directions})$$

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

with $\epsilon = \frac{\hbar^2 k^2}{2m}$
4.1.2 Cooper-Pairs

integration and resolving for $E$ results in

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

with $\int \frac{dx}{ax+b} = \frac{1}{a} \ln|ax + b|$

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

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

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

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 $\exp\left(-\frac{4}{V_0 D(E_F)}\right) \ll 1$ 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

- electron density in metal: \( D(E_F)/V \sim 10^{28} \text{ eV}^{-1}\text{m}^{-3} \)
- relevant energy interval: \( \hbar \omega_D \sim 0.01 - 0.1 \text{ eV} \)

\[ N = 10^{28} \cdot 0.1 \cdot \frac{4}{3} \pi \left(10^{-7}\right)^3 \sim 10^6 \]

\( \Rightarrow \) strong overlap of pairs

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

attactive 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

$$ V(q, \omega) = \frac{e^2}{\epsilon_0 (q^2 + k_s^2)} = \int \left( \frac{e^2}{4\pi \epsilon_0 r} e^{-ik_s r} \right) e^{-i q \cdot r} d^3r $$

positive matrix element $\Rightarrow$ repulsive interaction ($k_s = \text{Thomas-Fermi wave number}, k_s \sim \pi/a$)

- 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

Thomas-Fermi-wave vector

$q$-dependent plasma frequency of screened ions in metal

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

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 consistst 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

\[
S = \begin{cases} 
0 & m_s = 0 & \chi^a = \frac{1}{\sqrt{2}} (\uparrow\downarrow - \downarrow\uparrow) \\
1 & m_s = 1 & \chi^s = \frac{1}{\sqrt{2}} (\uparrow\downarrow + \downarrow\uparrow) \\
1 & m_s = -1 & \chi^s = \downarrow\downarrow \\
0 & m_s = +1 & \chi^s = \uparrow\uparrow 
\end{cases}
\]

\( \rightarrow \) **singlet pairing**, antisymmetric spin wavefunction

**symmetric orbital function**: \( L = 0, 2, \ldots \) \( (s, d, \ldots) \)

\( \rightarrow \) **triplet pairing**, symmetric spin wavefunction

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

What is the symmetry of the pair wavefunction?

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

$L = 0$
- s-wave superconductor

$L = 1$
- p-wave superconductor

$L = 2$:
- d-wave superconductor

- 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
  - \textit{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)

- \textit{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

\[ L = 0, S = 0 \]

\[ \Delta(k) = \Delta_m \]

\[ L = 2, S = 0 \]

\[ \Delta(k) = \frac{\Delta_m}{2} \left( \cos k_y a - \cos k_x a \right) \]

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 $s_\pm$-wave, e.g. in iron-based SC
4.1.3 Symmetry of Pair Wavefunction

Example: UPt$_3$

**phase diagram**


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

phase A

phase B
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 $T \sim 10^4 \text{K}$)
    (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 $R \simeq v_F \tau \simeq v_F/\omega_D$ ($\omega_D =$ Debye frequency)
    $v_F \simeq 10^6 \text{m/s}$, $\omega_D \simeq 10^{13} \text{s}^{-1}$  $\Rightarrow R \approx 100 \text{ nm}$
    $R \gg$ 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
    1. pure Coulomb interaction: \( V(q) = \frac{e^2}{\epsilon_0 q^2} \) (always positive \( \rightarrow \) repulsive interaction)
    2. screened Coulomb interaction: \( V(q, \omega) = \frac{e^2}{\epsilon(q, \omega) \epsilon_0 q^2} \left( 1 + \frac{\Omega_p^2(q)}{\omega^2 - \Omega_p^2(q)} \right) \)

  - for \( E_k - E_{k'} = h\omega < \hbar \Omega_p(q) \) of involved electrons: denominator becomes negative
  
  - cut-off frequency: \( \omega = \tilde{\Omega}_p \approx \omega_D \) (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:
    1. electron 1:
      \( k_1 \rightarrow k'_1 = k_1 + q \)
    2. electron 2:
      \( k_2 \rightarrow k'_2 = k_2 - q \)
    3. 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 \( k_F \leq k \leq k_F + \frac{\hbar \omega_D}{\hbar k_F} = k_F + \Delta k \)

  - 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: 
    \[ \Psi(r_1, r_2) = \sum_{k=k_F} a_k \exp(i k \cdot r) \]
  - 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: 
    \[ V_{k,k'} = \begin{cases} -V_0 & \text{for } k' > k_F, k < k_F + \Delta k \\ 0 & \text{else} \end{cases} \]
  - total energy: 
    \[ E \approx 2E_F - 2\hbar \omega_D \exp \left( -\frac{4}{V_0 D(E_F)} \right) \]
  - 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, \ldots )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triplet Pairing</td>
<td>( S = 1 )</td>
<td>( L = 1, 3, 5, \ldots )</td>
</tr>
</tbody>
</table>

\[ S = \begin{cases} 0 & m_s = 0 \quad \chi^s = \frac{1}{\sqrt{2}} (\uparrow\downarrow - \downarrow\uparrow) \\ -1 & m_s = -1 \quad \chi^s = \downarrow\downarrow \\ 0 & m_s = 0 \quad \chi^s = \frac{1}{\sqrt{2}} (\uparrow\downarrow + \downarrow\uparrow) \\ +1 & m_s = 1 \quad \chi^s = \uparrow\uparrow \end{cases} \]

- **examples**: metallic superconductors: \( S = 0 \), \( L = 0 \), high-temperature cuprate superconductors: \( S = 0 \), \( L = 2 \), superfluid \( ^3\text{He} \): \( S = 1 \), \( L = 1 \)
Superconductivity
and
Low Temperature
Physics I

Lecture No. 8

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 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
4.2 The BCS Ground State

**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

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

- 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 packets**

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

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

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

**annihilation operator**

(destroys state with wave number \( \mathbf{k} \))

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

**creation operator**

(creates state with wave number \( \mathbf{k} \))

\[
\hat{c}_\sigma^+(\mathbf{k}) = \hat{c}_{k\sigma}^+ = \frac{1}{\sqrt{V}} \sum_k \hat{\Phi}_\sigma^+ \ e^{i\mathbf{k} \cdot \mathbf{r}}
\]
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):

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

\[
\hat{c}^\dagger_{k\sigma}\hat{c}_{k\sigma} = n_{k\sigma} \quad \hat{c}_{k\sigma}\hat{c}^\dagger_{k\sigma} = 1 - n_{k\sigma} \quad \langle 0|n_{k\sigma}|0\rangle = 0; \quad \langle 1|n_{k\sigma}|1\rangle = 1 \quad \text{particle number operator}
\]

\[
\hat{c}^\dagger_{k\sigma}\hat{c}^\dagger_{k\sigma} = 0 \quad \hat{c}_{k\sigma}\hat{c}_{k\sigma} = 0
\]

Pauli exclusion principle

anti-commutation relations (for fermions):

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

\[
\{\hat{c}_{k\sigma}, \hat{c}_{k'\sigma'}\} = \{\hat{c}^\dagger_{k\sigma}, \hat{c}^\dagger_{k'\sigma'}\} = 0
\]
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:**

\[
p_k^\dagger = \hat{c}_{k\uparrow}^\dagger \hat{c}_{k\downarrow}^\dagger \quad \text{pair creation operator} \quad p_k = \hat{c}_{-k\downarrow} \hat{c}_{k\uparrow} \quad \text{pair annihilation operator}
\]

\[
[p_k,p_{k'}^\dagger] = \hat{c}_{-k\downarrow} \hat{c}_{k\uparrow} \hat{c}_{k'\uparrow} - \hat{c}_{k'\uparrow} \hat{c}_{k\uparrow} \hat{c}_{-k\downarrow} = 0
\]

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*

\[
[p_k^\dagger,p_{k'}^\dagger] = \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\downarrow}^\dagger \hat{c}_{k'\uparrow} - \hat{c}_{k'\uparrow}^\dagger \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\downarrow}^\dagger = 0
\]

\[
[p_k,p_{k'}^\dagger] = \delta_{kk'} (1 - n_{k\uparrow} - n_{-k\downarrow}) \quad \text{see next slide}
\]

**powers of pair operators**

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

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
The BCS Ground State

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

pair creation and annihilation operators:

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

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

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

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

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

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

spin \hspace{2cm} kinetic energy \hspace{2cm} potential energy \hspace{2cm} interaction energy

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

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

$$\mathcal{H}_{\text{BCS}} = \sum_{\sigma} \sum_{k} \varepsilon_k \hat{c}_k^\dagger \hat{c}_{k\sigma} + \frac{1}{2} \sum_{\sigma_1, \sigma_2} \sum_{k_1, k_2, q} V_q \hat{c}_{k_1+q, \sigma_1}^\dagger \hat{c}_{k_2-q, \sigma_2} \hat{c}_{k_2, \sigma_2} \hat{c}_{k_1, \sigma_1}$$

energy of non-interacting free electron gas \hspace{2cm} 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 $\mathbf{q}$

$$\varepsilon_k = \frac{\hbar^2 \mathbf{k}^2}{2m^*}, V_{\text{ext}}(\mathbf{r}) = 0$$

$$V_q = \frac{1}{\Omega} \int V(\mathbf{r}) e^{i \mathbf{q} \cdot \mathbf{r}} dV$$

factor $\frac{1}{2}$ avoids double counting
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 $q = k - k'$

$$\frac{1}{2} \sum_{\sigma_1,\sigma_2} \sum_{k_1,k_2,q} N V_q \hat{c}^{\dagger}_{k_1+q,\sigma_1} \hat{c}^{\dagger}_{k_2-q,\sigma_2} \hat{c}_{k_2,\sigma_2} \hat{c}_{k_1,\sigma_1} \Rightarrow \sum_{k,k'} N V_{k,k'} \hat{c}^{\dagger}_{k_1,k} \hat{c}^{\dagger}_{k_2,k} \hat{c}_{k_2,k'} \hat{c}_{k_1,k'}$$

summation over spin yields factor 2

two-particle interaction potential

pair creation and annihilation operators

$$H_{BCS} = \sum_{\sigma} \sum_k \varepsilon_k \hat{c}^{\dagger}_{k\sigma} \hat{c}_{k\sigma} + \sum_{k,k'} V_{k,k'} \hat{c}^{\dagger}_{k_1,k} \hat{c}^{\dagger}_{k_2,k} \hat{c}_{k_2,k'} \hat{c}_{k_1,k'}$$

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:
   \[ V_{k,k'} = \begin{cases} 
   -V_0 & \text{for } |\xi_k|, |\xi_{k'}| < \hbar \omega_D \\
   0 & \text{else} 
   \end{cases} \]
   \[ V_0D(E_F) \ll 1 \]

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

**calculation of the ground state energy**

- **Hamilton operator:**

\[
H_{\text{BCS}} = \sum_{\sigma} \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^+ \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{k}, \mathbf{k}'} V_{\mathbf{k}, \mathbf{k}'} \hat{c}_{\mathbf{k}\uparrow}^+ \hat{c}_{-\mathbf{k}\downarrow}^+ \hat{c}_{-\mathbf{k}'\downarrow} \hat{c}_{\mathbf{k}'\uparrow}
\]

\[n_{\mathbf{k}\sigma} = \text{particle number operator}\]

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

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

\[|\Psi_N\rangle = \sum g(\mathbf{k}_i, \ldots, \mathbf{k}_l) \hat{c}_{\mathbf{k}_i\uparrow}^+ \hat{c}_{-\mathbf{k}_i\downarrow}^+ \ldots \hat{c}_{\mathbf{k}_l\uparrow}^+ \hat{c}_{-\mathbf{k}_l\downarrow}^+ |0\rangle\]

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

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

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

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

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

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

\[|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1\]
4.2 The BCS Ground State

How to guess the BCS many particle wavefunction?

\[ |\Psi_{\text{BCS}}\rangle = \prod_{k=k_1,\ldots,k_M} (\alpha_k + \beta_k \hat{c}^+_k \hat{c}^-_{-k}) |0\rangle \]

wave function assumed by Bardeen, Cooper and Schrieffer

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

• coherent state of bosons

discussed first by 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 Roy J. Glauber to Fock state representation


Nobel Prize in Physics 2005 "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

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

- boson creation operator
- 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

$$\alpha = |\alpha| e^{i\varphi}$$ is complex number

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

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

$\langle n \rangle = |\alpha|^2 = \bar{N}$

- expectation value of number operator:
- relative standard deviation:
- uncertainty relation

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

- **Poisson distribution**

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

\[
\bar{N} = |\alpha|^2 = \begin{cases} 
5 \\
10 \\
20 
\end{cases}
\]

![Graph showing Poisson distribution](image)
4.2 The BCS Ground State

- **Poisson and normal distribution**

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

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

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

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

starting point: coherent bosonic state

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

in analogy: coherent fermionic state

\(|\Psi_{BCS}\rangle = c_1 \exp(\sum_k \alpha_k P_k^\dagger) |0\rangle\)

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

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

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

**Normalization:**

\[ \langle \Psi_{BCS}^* | \Psi_{BCS} \rangle = c_1^2 \langle 0 | \prod_k (1 + \alpha_k^* P_k) (1 + \alpha_k P_k^\dagger) |0\rangle = 1 \]

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**

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

\[
|\Psi_{\text{BCS}}\rangle = \prod_k \left( u_k \hat{c}_k + \alpha_k \hat{c}_k^\dagger \hat{c}_{-k}^\dagger \right) |0\rangle
\]

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

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

**coherence factors**

**coherent superposition of pair states → only average pair number is fixed**

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

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

\( u_k \) and \( v_k \) are complex probability amplitudes:

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

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

\( |u_k|^2 + |v_k|^2 = 1 \)
4.2 The BCS Ground State

- some expectation values \((1)\):

single spin particle number

\[
\langle n_{k\uparrow} \rangle = \langle \psi_{BCS} | \hat{c}_{k\uparrow}^\dagger \hat{c}_{k\uparrow} | \psi_{BCS} \rangle
\]

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

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

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

\[
\bar{N} = \langle N \rangle = \sum_{k\sigma} \langle n_{k\sigma} \rangle = \sum_{k\sigma} |v_k|^2 = 2 \sum_k |v_k|^2 = \sum_k |v_k|^2 - |u_k|^2 + 1
\]

we use the identities:

- \(\langle \phi | \psi \rangle = \langle \phi | 0^+ \psi \rangle\)
- \(\langle \phi | (AB)^+ | \psi \rangle = \langle \phi | B^+ A^+ | \psi \rangle\)

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

- **some expectation values (2a):**

  statistical fluctuation of average particle number

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

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

  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 $\langle n_{k\sigma}^2 \rangle = \langle c_{k\sigma}^\dagger c_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} \rangle = \langle c_{k\sigma}^\dagger (1 - c_{k\sigma}^\dagger c_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma}) \rangle = \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle - \langle c_{k\sigma}^\dagger c_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} \rangle = |v_k|^2 + |v_k|^4$

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

  (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

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

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

BCS Hamiltonian

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

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

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

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

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

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

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

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

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

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

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)

$$
u_k = \sin \theta_k, \quad v_k = \cos \theta_k, \quad \text{and} \quad 2 \sin \theta_k \cos \theta_k = \sin 2 \theta_k$$

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

minimization

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

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

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

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

- we switch back to old summation \((I \rightarrow k)\) 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 \(\Delta_k \equiv -\sum_{k'} V_{k,k'} u_{k'} v_{k'}\):

\[
\tan 2\theta_k = -\frac{\Delta_k}{\xi_k}
\]

- with \(\tan 2\theta_k = \frac{\sin 2\theta_k}{\cos 2\theta_k} = \frac{2 \sin \theta_k \cos \theta_k}{\cos^2 \theta_k - \sin^2 \theta_k} = \frac{2u_k v_k}{u_k^2 - v_k^2}\) we obtain

\[
\frac{2u_k v_k}{u_k^2 - v_k^2} = -\frac{\Delta_k}{\xi_k}
\]

- 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

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

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

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

pairing amplitude \quad self-consistent gap equation
4.2 The BCS Ground State

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

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

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

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

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

\[ \Rightarrow \text{smearing is required to allow for pairing interaction: reduction of potential energy} > \text{increase of kinetic energy} \]

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

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

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

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

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

- 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:

\[
\begin{align*}
(\epsilon_k - \lambda_1) u_k + \Delta_k v_k - \lambda_2 u_k &= 0 \\
\Delta_k^+ u_k - (\epsilon_k - \lambda_1) v_k - \lambda_2 v_k &= 0
\end{align*}
\]

- physical meaning of the Lagrangian multipliers
  i. \( \lambda_1 \) shifts the energy and corresponds the 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 \( E_k \equiv \sqrt{\xi_k^2 + \Delta_k^2} \)
  \[ |u_k|^2 = \frac{1}{2} \left[ 1 + \frac{\xi_k}{E_k} \right], \quad |v_k|^2 = \frac{1}{2} \left[ 1 - \frac{\xi_k}{E_k} \right], \quad u_k v_k^* = g_k = \frac{\Delta_k}{2E_k} \]
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

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

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

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

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

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

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

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

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

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

energy relative to chemical potential

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

(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 $\Delta_k = \Delta$

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

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

$$\langle \Psi_{\text{BCS}} | H_n - N\mu | \Psi_{\text{BCS}} \rangle = \lim_{\Delta \to 0} \langle \Psi_{\text{BCS}} | H_{\text{BCS}} - N\mu | \Psi_{\text{BCS}} \rangle = \sum_k \xi_k - |\xi_k| = 2 \sum_{|k| < k_F} \xi_k$$

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

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

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

$$\Delta g_k^* = \frac{\Delta^2}{2\sqrt{\xi_k^2 + |\Delta|^2}}$$
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 \( \frac{\Delta(0)}{k_B T_c} = \frac{\pi}{e^\gamma} = 1.7638 \) ... 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**:

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

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

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

- **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

- **expectation values**:

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

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

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

(kinetic energy)

(interaction energy)

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

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

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

determination of \(u_{\mathbf{k}}, v_{\mathbf{k}}\) by minimization of expectation value
Summary of Lecture No. 8 (2)

- **minimization of expectation value**

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

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

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

  Pairing amplitude

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

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

  Self-consistent gap equation

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

  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

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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
Chapter 4 - Superconductivity and Low Temperature Physics

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)

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

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

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 $\delta g_k, \delta g_k^*$

$g_k \equiv \langle c_{-k\downarrow} c_{k\uparrow} \rangle \neq 0$

$g_k^* \equiv \langle c_{-k\downarrow}^\dagger c_{k\uparrow}^\dagger \rangle \neq 0$
4.2.3 The Bogoliubov-Valatin Transformation

- Rewriting of pair creation and annihilation operators in
  \[ 
  \hat{c}_{-\mathbf{k} l} \hat{c}^{\dagger}_{\mathbf{k} l} = \frac{\langle \hat{c}_{-\mathbf{k} l} \hat{c}^{\dagger}_{\mathbf{k} l} \rangle}{g_{\mathbf{k}}} + \frac{\langle \hat{c}_{-\mathbf{k} l} \hat{c}^{\dagger}_{\mathbf{k} l} \rangle}{\delta g_{\mathbf{k}}} - \langle \hat{c}_{-\mathbf{k} l} \hat{c}^{\dagger}_{\mathbf{k} l} \rangle 
  \]

- Insert into Hamiltonian and consider only terms linear in \( \delta g_{\mathbf{k}}^{(*)} \) (and after some math)

\[
\mathcal{H}_{\text{BCS}} = \sum_{\sigma} \sum_{\mathbf{k}} \xi_{\mathbf{k}} n_{\mathbf{k} \sigma} + \sum_{\mathbf{k}, \mathbf{k}'}^{N} V_{\mathbf{k}, \mathbf{k}'} \left[ g_{\mathbf{k}}^{*} \hat{c}_{-\mathbf{k} l} \hat{c}^{\dagger}_{\mathbf{k} l} + g_{\mathbf{k}'} \hat{c}_{\mathbf{k} l}^{\dagger} \hat{c}^{\dagger}_{-\mathbf{k} l} - g_{\mathbf{k}} g_{\mathbf{k}'} \right] 
\]

- Make use of pair potential

\[
\Delta_{\mathbf{k}} \equiv - \sum_{\mathbf{k}'} V_{\mathbf{k}, \mathbf{k}'} g_{\mathbf{k}'} \\
\Delta_{\mathbf{k}}^{*} \equiv - \sum_{\mathbf{k}'} V_{\mathbf{k}, \mathbf{k}'} g_{\mathbf{k}'}^{*} 
\]

\[
\mathcal{H}_{\text{BCS}} - N \mu = \sum_{\mathbf{k}, \sigma} \xi_{\mathbf{k}} n_{\mathbf{k} \sigma} - \sum_{\mathbf{k}} \left[ \Delta_{\mathbf{k}}^{*} \hat{c}_{-\mathbf{k} l} \hat{c}^{\dagger}_{\mathbf{k} l} + \Delta_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k} l} \hat{c}^{\dagger}_{-\mathbf{k} l} - \Delta_{\mathbf{k}} g_{\mathbf{k}}^{*} \right] 
\]
4.2.3 The Bogoliubov-Valatin Transformation

- we use

\[ \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} n_{\mathbf{k}\sigma} = \sum_{\mathbf{k}} \xi_{\mathbf{k}} (\hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{\mathbf{k}\uparrow} + \hat{c}_{\mathbf{k}\downarrow}^\dagger \hat{c}_{\mathbf{k}\downarrow}) \]

\[ = 1 \hat{c}_{-\mathbf{k}\downarrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger \]

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

\[ \mathcal{H}_{\text{BCS}} - \mathcal{N}\mu = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} n_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} [\Delta_{\mathbf{k}} \hat{c}_{-\mathbf{k}\downarrow}^\dagger \hat{c}_{\mathbf{k}\uparrow} + \Delta_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger - \Delta_{\mathbf{k}} g_{\mathbf{k}}] \]

\[ \mathcal{H}_{\text{BCS}} - \mathcal{N}\mu = \sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} + \Delta_{\mathbf{k}} g_{\mathbf{k}}^* \right\} + \left( \hat{c}_{\mathbf{k}\uparrow}^\dagger, \hat{c}_{-\mathbf{k}\downarrow}^\dagger \right) \begin{pmatrix} \xi_{\mathbf{k}} & -\Delta_{\mathbf{k}} \\ -\Delta_{\mathbf{k}}^* & -\xi_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}\uparrow}^\dagger \\ \hat{c}_{-\mathbf{k}\downarrow}^\dagger \end{pmatrix} \]

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

- derive excitation energies by diagonalization of Hamiltonian

\[ \rightarrow \text{Bogoliubov-Valatin transformation} \]

\[ \rightarrow \text{define new fermionic operators } \alpha_{\mathbf{k}}, \beta_{\mathbf{k}}^\dagger \text{ and } \alpha_{\mathbf{k}}^\dagger, \beta_{\mathbf{k}} \text{ by unitary transformation (rotation)} \]
4.2.3 The Bogoliubov-Valatin Transformation

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

\[
\mathcal{H}_{BCS} - N\mu = \sum_{k} \left\{ \xi_k + \Delta_k g_k^* + \left( \frac{\hat{c}_{k\uparrow}^\dagger}{\xi_k + \Delta_k} , \frac{\hat{c}_{k\downarrow}^\dagger}{-\xi_k + \Delta_k} \right) \begin{pmatrix} \xi_k & -\Delta_k \\ -\Delta_k & -\xi_k \end{pmatrix} \left( \frac{\hat{c}_{k\uparrow}}{\epsilon_k} , \frac{\hat{c}_{k\downarrow}}{-\epsilon_k} \right) \right\}
\]

spinors

\[
\mathcal{H}_{BCS} - N\mu = \sum_{k} \left\{ \xi_k + \Delta_k g_k^* + \frac{c_k^\dagger u_k}{b_k^\dagger} u_k^\dagger \mathcal{E}_k \right\} = \sum_{k} \left\{ \xi_k + \Delta_k g_k^* + B_k^\dagger \bar{\mathcal{E}}_k B_k \right\} \quad u_k u_k^\dagger = 1
\]

spinors of Bogoliubov quasiparticle operators:

\[
B_k^\dagger = (\alpha_k^+, \beta_{-k}^-) = c_k^\dagger u_k \\
B_k = (\alpha_k, \beta_{-k}^+) = u_k c_k
\]

appropriate unitary matrix to make transformed energy matrix \( \bar{\mathcal{E}}_k = u_k^\dagger \mathcal{E}_k u_k \) diagonal:

\[
u_k = \begin{pmatrix} u_k \\ v_k \end{pmatrix}, \quad u_k^\dagger = \begin{pmatrix} u_k^* \\ -v_k^* \end{pmatrix} \quad \Rightarrow \quad u_k^\dagger \mathcal{E}_k u_k = \bar{\mathcal{E}}_k = \begin{pmatrix} \alpha_k & D_k \\ -D_k & -\alpha_k \end{pmatrix}
\]

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

\[
\mathcal{H}_{BCS} - N\mu = \sum_{k} \left\{ \xi_k + \Delta_k g_k^* + (\alpha_{k\uparrow}^+, \beta_{-k\downarrow}^-) \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} \right\}
\]

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

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

\[ \Rightarrow (\alpha_k^\dagger, \beta_{-k}) = \begin{pmatrix} u_k & -v_k \\ v_k^* & u_k^* \end{pmatrix} \begin{pmatrix} \hat{c}_{k\uparrow}^\dagger \\ \hat{c}_{-k\downarrow} \end{pmatrix} \]

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

\[ \Rightarrow (\alpha_k, \beta_{-k}^\dagger) = \begin{pmatrix} u_k & -v_k \\ v_k^* & u_k^* \end{pmatrix} \begin{pmatrix} \hat{c}_{k\uparrow}^\dagger \\ \hat{c}_{-k\downarrow} \end{pmatrix} \]

- 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: \( \{\alpha_k, \beta_{-k}\} = \delta_{kk'} \) and \( \{\alpha_k, \alpha_{k'}\} = \{\alpha^\dagger, \alpha^\dagger\} = 0 \)

**Inverse Transformation**

\[ \mathcal{B}_k^\dagger \mathbf{u}_k^\dagger = \mathcal{C}_k^\dagger \mathbf{u}_k \Rightarrow \mathcal{C}_k^\dagger = (\mathbf{u}_k^\dagger)^T \mathcal{B}_k^\dagger \]

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

\[ \mathbf{u}_k \mathcal{B}_k = \mathbf{u}_k \mathcal{C}_k^\dagger \Rightarrow \mathcal{C}_k = \mathbf{u}_k \mathcal{B}_k \]

\[ \Rightarrow \begin{pmatrix} \hat{c}_{k\uparrow}^\dagger \\ \hat{c}_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} u_k & v_k^* \\ -v_k & u_k^* \end{pmatrix} \begin{pmatrix} \alpha_k \\ \beta_{-k} \end{pmatrix} \]
### The Bogoliubov-Valatin Transformation

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

- \( \alpha_k = u_k^* \hat{c}_{k\uparrow} - v_k^* \hat{c}_{-k\downarrow} \)
- \( \beta_{-k}^+ = v_k \hat{c}_{k\uparrow} + u_k \hat{c}_{-k\downarrow} \)
- \( \alpha_{-k}^+ = u_k^* \hat{c}_{k\uparrow} - v_k^* \hat{c}_{-k\downarrow} \)
- \( \beta_{-k} = v_k^* \hat{c}_{k\uparrow} + u_k^* \hat{c}_{-k\downarrow} \)

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

- \( \xi_k = 0 \)

**Symmetry:**

- \( \alpha_k = 1/\sqrt{2} (\hat{c}_{k\uparrow} - \hat{c}_{-k\downarrow}) \)
- \( \beta_{-k}^+ = 1/\sqrt{2} (\hat{c}_{k\uparrow} + \hat{c}_{-k\downarrow}) \)
- \( \alpha_{-k}^+ = 1/\sqrt{2} (\hat{c}_{k\uparrow} - \hat{c}_{-k\downarrow}) \)
- \( \beta_{-k} = 1/\sqrt{2} (\hat{c}_{k\uparrow} + \hat{c}_{-k\downarrow}) \)

- **Hole-like excitation**

- **Particle-like excitation**

**Key Points:**

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

- **Reduces** the total momentum by \( \mathbf{k} \) and the total spin by \( \hbar/2 \)

- **Increases** the total momentum by \( \mathbf{k} \) and the total spin by \( \hbar/2 \)

\( \mathcal{T} \mathbf{k} = 0 \rightarrow u \mathbf{k}^2 \)

\[ \mathbf{u} \mathbf{k}^2 = \text{hole fraction}, \quad \mathbf{v} \mathbf{k}^2 = \text{electron fraction} \]

- \( \mathbf{u} \mathbf{k}^2 \) reduces the total momentum by \( \mathbf{k} \) and the total spin by \( \hbar/2 \)

- \( \mathbf{v} \mathbf{k}^2 \) increases the total momentum by \( \mathbf{k} \) and the total spin by \( \hbar/2 \)
4.2.3 The Bogoliubov-Valatin Transformation

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

BCS Hamiltonian

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

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

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

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

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

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

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

$$\left[ \ldots \right] = 0$$

- 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
4.2.3 The Bogoliubov-Valatin Transformation

\[ 2 \xi_k u_k v_k + \Delta_k^* v_k^2 - \Delta_k u_k^2 = 0 \quad \text{and} \quad 2 \xi_k u_k^* v_k^* + \Delta_k v_k^* - \Delta_k^* u_k^2 = 0 \]

- multiply by \( \Delta_k^*/u_k^2 (\Delta_k^*/u_k^2) \), solve the resulting quadratic eqn. for \( \Delta_k^* v_k/u_k \) (\( \Delta_k v_k^*/u_k^* \))

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

\[
\left( \Delta_k^* \frac{v_k}{u_k} \right)_{1,2} = \left( \Delta_k \frac{v_k^*}{u_k^*} \right)_{1,2} = -\xi_k \pm \sqrt{\xi_k^2 + |\Delta_k|^2} = -\xi_k + E_k
\]

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

negative sign is unphysical
\[ \rightarrow \] corresponds to solution with maximum energy

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

\[ \rightarrow \] the relative phase of \( u_k \) and \( v_k \) must be fixed and must be the phase of \( \Delta_k^* \)

\[ \rightarrow \] we can choose \( u_k \) real and use \( v_k = |v_k|e^{i\phi} \), the phase of \( v_k \) corresponds to that of \( \Delta_k^* \)

\[
\left| \frac{v_k}{u_k} \right| = \frac{E_k - \xi_k}{|\Delta_k|}
\]
4.2.3 The Bogoliubov-Valatin Transformation

- 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

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

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

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

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

\[
\Delta_k^* \equiv - \sum_{k'} V_{k,k'} g_{k'}^* = - \sum_{k'} V_{k,k'} \frac{\Delta_{k'}^*}{2E_{k'}}
\]
4.2.3 The Bogoliubov-Valatin Transformation

Excitation spectrum of Bogoliubov quasiparticles and energy gap

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

**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.
4.2.3 The Bogoliubov-Valatin Transformation

\begin{equation}
\frac{E_k}{E_F}, \xi_k / E_F, (k-k_F)/k_F
\end{equation}

\begin{itemize}
  \item \textbf{quasiparticles}
  \item \textbf{electrons}
  \item \textbf{holes}
\end{itemize}

\begin{itemize}
  \item \( +E_k \)
  \item \( -E_k \)
\end{itemize}

\( \xi_{k,h} \)

\( \xi_{k,e} \)
4.2.3 The Bogoliubov-Valatin Transformation

**reformulation of the BCS Hamilton operator**

- we start from the Hamiltonian $\mathcal{H}_{BCS} - N\mu = \sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} + \Delta_{\mathbf{k}} g_{\mathbf{k}}^* \right\} + \left( \begin{array}{c} \alpha_{\mathbf{k}}^+ \beta_{\mathbf{-k}}^+ \\ \alpha_{\mathbf{k}} \beta_{\mathbf{-k}} \end{array} \right) \left( \begin{array}{cc} E_{\mathbf{k}} & 0 \\ 0 & -E_{\mathbf{k}} \end{array} \right) \left( \begin{array}{c} \alpha_{\mathbf{k}} \\ \beta_{\mathbf{-k}}^+ \end{array} \right)$

\[
\mathcal{H}_{BCS} - N\mu = \sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} + \Delta_{\mathbf{k}} g_{\mathbf{k}}^* \right\} + \sum_{\mathbf{k}} \left\{ E_{\mathbf{k}} \alpha_{\mathbf{k}}^+ \alpha_{\mathbf{k}} - E_{\mathbf{k}} \beta_{\mathbf{-k}}^+ \beta_{\mathbf{-k}} \right\} = \sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} + \Delta_{\mathbf{k}} g_{\mathbf{k}}^* \right\} + \sum_{\mathbf{k}} \left\{ E_{\mathbf{k}} \alpha_{\mathbf{k}}^+ \alpha_{\mathbf{k}} - E_{\mathbf{k}} + E_{\mathbf{k}} \beta_{\mathbf{-k}}^+ \beta_{\mathbf{-k}} \right\}
\]

\[
\mathcal{H}_{BCS} - N\mu = \sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} - E_{\mathbf{k}} + \Delta_{\mathbf{k}} g_{\mathbf{k}}^* \right\} + \sum_{\mathbf{k}} \left\{ E_{\mathbf{k}} \alpha_{\mathbf{k}}^+ \alpha_{\mathbf{k}} + E_{\mathbf{k}} \beta_{\mathbf{-k}}^+ \beta_{\mathbf{-k}} \right\}
\]

Minimization of free energy yields BCS gap equation for finite $T$

**mean-field contribution ($T = 0$)**

differs from the normal state value by the condensation energy

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

spinless quasiparticles since they consist of superposition of spin-$\uparrow$ and spin-$\downarrow$ 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
  \[ \langle \alpha_k^\dagger \alpha_k \rangle = \langle \beta_{-k}^\dagger \beta_{-k} \rangle = f(E_k) = \frac{1}{\exp(E_k/k_B T) + 1} \]
4.2.3 The BCS Gap Equation and QP Excitations

determination of temperature dependence of $\Delta$ by minimization of free energy

- Hamiltonian has two terms:
  $\mathcal{H}_{BCS} = \mathcal{H}_0 + \mathcal{N} \mu = \sum_k \{ \xi_k - E_k + \Delta_k g_k^* \} + \sum_k \{ E_k \alpha_k^+ \alpha_k + E_k \beta_k^+ \beta_k \}$

  - constant term $\mathcal{H}_0$
  - term of free Fermi gas composed of two kind of fermions with energy $E_k$

- Grand canonical partition function:
  $$Z = e^{-\mathcal{H}_0/k_B T} \prod_k \left( 1 + e^{-E_k/k_B T} \right) \left( 1 + e^{E_k/k_B T} \right) = e^{-\mathcal{F}/Nk_B T}$$

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

- 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

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

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

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

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

\[
g_k^* = \frac{\Delta_k^*}{2 E_k} \tanh \left( \frac{E_k}{2 k_B T} \right) = u_k v_k^* \tanh \left( \frac{E_k}{2 k_B T} \right)
\]

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:

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

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 $T \rightarrow 0$: (already discussed above for $V_{k,k'} = -V_0$ and $\Delta_k = \Delta$)

$$1 = V_0 \sum_{k'} \frac{1}{2E_{k'}} \tanh \left( \frac{E_{k'}}{2k_BT} \right)$$ transforming sum into integration

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

with $D(E) \approx D(E_F)/2$

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

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

• solve for $\Delta$:

• 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 $\Delta_k \to 0$

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

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

with $x = \xi_k / 2k_B T_c$

• integral gives $2 \ln(p \hbar \omega_D / 2k_B T_c)$ with $p = \frac{2e^\gamma}{\pi} \approx 1.13$ and $\gamma = 0.577 \ldots$ (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 $\omega_D \propto 1/\sqrt{M}$

⇒ explains isotope effect!!
4.2.3 The BCS Gap Equation and QP Excitations

relation between energy gap at zero temperature and critical temperature

\[ \Delta(0) \approx 2\hbar \omega_D \, e^{-2/V_0 D(E_F)} \]

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

\[ \frac{\Delta(0)}{k_B T_c} = \frac{\pi}{e^\gamma} = 1.764 \]

key prediction of BCS theory

<table>
<thead>
<tr>
<th>Tc (K)</th>
<th>2\Delta(0) (meV)</th>
<th>2\Delta(0) / k_B Tc</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>1.19</td>
<td>0.36</td>
</tr>
<tr>
<td>Nb</td>
<td>9.2</td>
<td>2.90</td>
</tr>
<tr>
<td>Pb</td>
<td>7.2</td>
<td>2.70</td>
</tr>
<tr>
<td>Ta</td>
<td>4.29</td>
<td>1.30</td>
</tr>
<tr>
<td>NbN</td>
<td>15</td>
<td>4.65</td>
</tr>
<tr>
<td>NbSe2</td>
<td>7</td>
<td>2.2</td>
</tr>
<tr>
<td>In</td>
<td>3.4</td>
<td>1.05</td>
</tr>
<tr>
<td>Hg</td>
<td>4.15</td>
<td>1.65</td>
</tr>
<tr>
<td>Sn</td>
<td>3.72</td>
<td>1.15</td>
</tr>
<tr>
<td>Tl</td>
<td>2.39</td>
<td>0.75</td>
</tr>
<tr>
<td>Nb3Sn</td>
<td>18</td>
<td>6.55</td>
</tr>
<tr>
<td>MgB2</td>
<td>40</td>
<td>3.6-15</td>
</tr>
</tbody>
</table>

considerable deviations for „strong-coupling“ superconductors:

\[ V_0 D(E_F) \ll 1 \] is no longer a good approximation
The BCS Gap Equation and QP Excitations

solution for $0 < T < T_c$ (numerical solution of integral)

$$1 = V_0 \sum_{k'} \frac{1}{2E_{k'}} \tanh \left( \frac{E_{k'}}{2k_B T} \right) \quad \text{sum} \Rightarrow \text{integral}$$

$$1 = \frac{V_0 D(E_F)}{2} \int_{-\hbar \omega_D}^{\hbar \omega_D} \frac{1}{2E_k} \tanh \left( \frac{E_k}{2k_B T} \right) d\xi_k$$

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)

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

  $$\lambda(\omega) = 2 \int_0^\infty \frac{\alpha^2(\omega) F(\omega)}{\omega} \, d\omega$$

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


- **McMillan approximation**
  - several attempts have been made to improve prediction for $T_c$ using strong coupling theory, e.g. by McMillan:

  $$T_c = \frac{\hbar \omega_D}{1.45} \exp \left( \frac{1.04(1 + \lambda)}{\lambda - \mu^*(1 + 0.62 \lambda)} \right)$$

  $\mu^*$: matrix element of the short-range screened Coulomb repulsion

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)

- break up of Cooper pair requires energy \( 2E_k \)
- \( \Delta \) represents energy gap for quasiparticle excitation from ground state
  ⇒ minimum excitation energy
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 \( E_F \): \( D_n(\xi_k) \approx D_n(E_F) = \text{const.} \)

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

- measurement by tunneling spectroscopy

\[ \Delta = 1.34 \text{ meV} \]
\[ T = 0.33 \text{ K} \]

I. Giaever, 
Phys. Rev. 126, 941 (1962)
4.3 Thermodynamic Quantities

- occupation probability of qp-excitations is given by \( f(E_k) = \left[ \exp(E_k/k_B T) + 1 \right]^{-1} \)

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

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

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

\[
\text{hole like} \\
\text{electron like}
\]

\[ S = -k_B \sum_n \rho_n \ln \rho_n \]

- \textit{heat capacity}: \( C_s = T \left( \frac{\partial S_s}{\partial T} \right)_{p,B} \)

after some math:

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

results from redistribution of qp on available energy levels

results from \( T \)-dependence of energy gap

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

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

discussion of limiting cases

i. $T \ll T_c$:

- 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

(we use $\Delta^2 + \xi_k^2 = \Delta^2 (1 + \xi_k^2/\Delta^2) \approx \Delta^2$ and $\sqrt{\Delta^2 + \xi_k^2} = \Delta \sqrt{1 + \xi_k^2/\Delta^2} \approx \Delta + \xi_k^2/2\Delta$, as $\partial f(E_k)/\partial E_k$ has significant weight only for small values of $\xi_k/\Delta$)

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

$$C_s \approx \frac{D(E_F)}{k_B T^2} \Delta^2(0) e^{-\Delta(0)/k_B T} \int_0^{\infty} e^{-\xi_k^2/2\Delta(0)k_B T} d\xi_k$$

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

exponential decrease of heat capacity at low $T$
4.3 Thermodynamic Quantities

specific heat of superconductors at $T \ll T_c$:

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

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

4.3 Thermodynamic Quantities

ii. \(0.5 < T/T_c < 1:\)

\[ \Delta(T) \text{ decreases with increasing } T \rightarrow \text{ there is a rapid increase of the number of thermally excited quasiparticles} \]

\[ \Rightarrow \frac{\partial S_s}{\partial T} > \frac{\partial S_n}{\partial T} \Rightarrow C_s \text{ is getting larger than } C_n \]
4.3 Thermodynamic Quantities

iii. $T \approx T_c$:

$\Delta(T) \to 0 \Rightarrow$ 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 $T > T_c$

\{jump of specific heat\}

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

Vanadium

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

Vanadium ($B_{ext} = 0$)

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

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 \( |\xi_k| \))

\[
\Delta C = (C_S - C_n)_{T=T_c} = \frac{2}{T} \sum_k - \frac{\partial f(\xi_k)}{\partial \xi_k} \left( -\frac{1}{2} T \frac{d\Delta^2(T)}{dT} \right)_{T=T_c}
\]

\[
\Delta C = D(E_F) \left( -\frac{d\Delta^2(T)}{dT} \right)_{T=T_c} - \int_{-\infty}^{\infty} - \frac{\partial f(\xi_k)}{\partial \xi_k} d\xi_k
\]

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{cth}}(T)}{\partial T} \right)^2 = \frac{1}{C_n T_c} \frac{B_{\text{cth}}^2(0)}{2 \mu_0} = \frac{8}{\gamma T_c^2} \frac{B_{\text{cth}}^2(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
\]

(\text{Rutgers formula})

further key prediction of BCS theory
\( \text{(in good agreement with experiment)} \)

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

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

M. A. Biondi et al.,
Rev. Mod. Phys. 30, 1109-1136 (1958)
Summary of Lecture No. 9 (1)

- **Bogoliubov-Valatin transformation → BCS Gap Equation and Excitation Spectrum**

\[
\mathcal{H}_{\text{BCS}} - N\mu = \sum_k \left\{ \xi_k + \Delta_k g^+_k + \left( \hat{c}^+_k \cdot \hat{c}^-_{-k} \right) u_k u^+_k \left( \frac{\xi_k}{\Delta_k} \right) u_k u^+_k \left( \frac{\hat{c}^+_k}{\hat{c}^-_{-k}} \right) \right\} = \sum_k \left\{ \xi_k + \Delta_k g^+_k + B^+_k u_k \xi_k u_k B_k \right\}
\]

\[
B^+_k = (\alpha^+_k, \beta^-_{-k}) = \left( \hat{c}^+_k, \hat{c}^-_{-k} \right) u_k \quad \quad B_k = (\alpha_k, \beta^+_{-k}) = u_k^+ \left( \hat{c}^+_k \hat{c}^-_{-k} \right)
\]

**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 \( \xi_k = u^+_k \xi_k u_k \) diagonal:

\[
u_k \begin{pmatrix} u_k & v_k^* \\ -v_k^* & u_k^* \end{pmatrix} \quad \quad u_k^+ \begin{pmatrix} u_k^* & -v_k^* \\ v_k & u_k \end{pmatrix} \quad \quad \Rightarrow \quad u_k^+ \xi_k u_k = \begin{pmatrix} E_k & D_k \\ -D_k & -E_k \end{pmatrix}
\]

\( \Rightarrow D_k = 0 \)

- **reformulation of the BCS Hamilton operator**

\[
\mathcal{H}_{\text{BCS}} - N\mu = \sum_k \{ \xi_k - E_k + \Delta_k g^+_k \} + \sum_k \{ E_k \alpha^+_k \alpha_k + E_k \beta^+_k \beta^-_{-k} \}
\]

- mean-field contribution differs from the normal state value by the condensation energy (see below)

- contribution of spinless Fermion system with two kinds of quasiparticles described by operators \( \hat{c}^+_k, \alpha_k \) and \( \beta^+_k, \beta^-_{-k} \) and excitation energies \( \pm E_k \)

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

\[ \Rightarrow \text{minimization of free energy yields BCS gap equation for finite } T \]
Summary of Lecture No. 9 (2)

- minimization of free energy yields BCS gap equation:

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

\textbf{BCS gap equation}

- analytical solution with simplifications: \( \Delta_0 \approx 2\hbar \omega_D e^{-2V_0D(E_F)} \)

\[ \Delta_0 \approx 2\hbar \omega_D e^{-2V_0D(E_F)} \]

\[ k_B T_c = 1.13 \hbar \omega_D e^{-2V_0D(E_F)} \]

\[ \Delta_0 = \frac{\pi}{e^r} = 1.764 \]

- condensation energy at \( T = 0 \)

\[ E_{\text{kond}}(0) = \langle \mathcal{H}_{\text{BCS}} \rangle - \langle \mathcal{H}_n \rangle = -D(E_F)\Delta^2(0)/4 \]

comparison to \( E_{\text{cond}}(0) = -B_{\text{c1h}}^2(0) / 2\mu_0 \) (thermodynamics) yields

\[ B_{\text{c1h}}(0) = \sqrt{\frac{\mu_0 D(E_F)\Delta^2(0)}{2V}} \]
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**

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

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

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

\[
\text{SC 1} \quad I \quad \text{SC 2}
\]

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

- sketch:

  ![Diagram](image-url)

  **top view:**
  - oxide (2nm)
  - substrate
  - \(0.1\ \mu\text{m} \ldots 1\text{mm}\)
4.4.2 Tunneling Spectroscopy

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

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

- 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 \( \xi_{k'} = -\xi_k \)

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

\[ \propto \left| \frac{|v_{k}|^2}{|u(-\xi_{k})|} \right| |T_{k'q}|^2 \]

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

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

elastic tunneling between two metals (NIN):

\[
I_{1\to2} = C \int_{-\infty}^{\infty} |T|^2 \frac{D_1(E)f(E)}{\text{occupied states in } N_1} \frac{D_2(E + eV) [1 - f(E + eV)]}{\text{empty states in } N_2} \, dE
\]

- 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 \( D_n(E + eV) \approx D_n(E_F) = \text{const.} \)

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

\[
I_{nn}(V) = C |T|^2 D_{n1}(E_F)D_{n2}(E_F) eV = G_{nn} V
\]
elastic tunneling between N and S (NIS junction):

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

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

- 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

\[ \frac{I_{ns}}{(G_{nn}/e)\Delta(0)} \]

\[ T > T_c \]

\[ T = 0 \]

\[ N/S \]

\[ \delta N - S \]

\[ E \]

\[ eV / \Delta(0) \]

\[ D_{1n} \]

\[ D_{2s} \]

\[ \mu_1 \]

\[ \mu_2 \]

\[ 2\Delta \]

\[ D_{1n} \]

\[ D_{2s} \]

\[ 1 \]

\[ 2 \]

\[ 3 \]

\[ 4 \]
4.4.2 Tunneling Spectroscopy

Differential tunneling conductance of NIS junction

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

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

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

\[
G_{ns}(V) = G_{nn} \frac{D_{s2}(eV)}{D_{n2}(E_F)} @ T = 0
\]

\( G_{ns}(V) \) 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

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

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

**BCS Theorie**

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

**interpretation of tunneling in SIS junction at \( T = 0 \)**

- **single electron tunnels from left to right:**

  - **before tunneling**
  
  ![before_tunneling_diagram](image)

  - **occupied and empty pair state**

  - **after tunneling**
  
  ![after_tunneling_diagram](image)

  - **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:**

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

current-voltage characteristics of SIS junction at finite temperatures

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

\[ 2\Delta(T) \] 2\(\Delta_0 \)

\[ eV \] (≈ few meV)

\[ T = 0 \]

Increasing I
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

\[ H_1 = \sum_{k\sigma, k'\sigma'} P_{k'\sigma', k\sigma} c_{k'\sigma'}^+ c_{k\sigma} \]

interaction hamiltonian

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

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

\[ \hat{c}_{k\uparrow} = \hat{c}_{-k\downarrow} = \sum_{\sigma} \left( u_k^{\sigma} a_k^{\sigma} + v_k^{\sigma} \beta_{-k}^{\sigma} \right) \]

\[ \hat{c}_{k\downarrow} = \hat{c}_{-k\uparrow} = \sum_{\sigma} \left( u_k^{\sigma} a_k^{\sigma} + v_k^{\sigma} \beta^*_{-k}^{\sigma} \right) \]

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

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

\[ \hat{c}_{k\uparrow} = \hat{c}_{-k\downarrow} = \sum_{\sigma} \left( u_k^{\sigma} a_k^{\sigma} + v_k^{\sigma} \beta_{-k}^{\sigma} \right) \]

\[ \hat{c}_{-k\downarrow} = \hat{c}_{k\uparrow} = \sum_{\sigma} \left( u_k^{\sigma} a_k^{\sigma} + v_k^{\sigma} \beta_{-k}^{\sigma} \right) \]

\[ P_{k'\sigma', k\sigma} \]

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

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

connect the same qp states

\[ \hat{c}_{k\uparrow} = \hat{c}_{-k\downarrow} = \sum_{\sigma} \left( u_k^{\sigma} a_k^{\sigma} + v_k^{\sigma} \beta_{-k}^{\sigma} \right) \]

\[ \hat{c}_{-k\downarrow} = \hat{c}_{k\uparrow} = \sum_{\sigma} \left( u_k^{\sigma} a_k^{\sigma} + v_k^{\sigma} \beta_{-k}^{\sigma} \right) \]

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

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

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

\[ u_k, v_k \] are assumed real

see e.g.

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Introduction to Superconductivity
4.5 Coherence Effects

temperature dependence of low-frequency absorption processes in superconductors

- **case I coherence factor**: 
  - $$\Rightarrow \text{nuclear relaxation, electromagnetic absorption}$$
  - (for perturbation which are odd under time reversal)

- **case II coherence factor**: 
  - $$\Rightarrow \text{ultrasound attenuation}$$
  - (for perturbation which are even under time reversal)

BCS theory makes prediction for coherence factors
4.5 Coherence Effects

**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
