Exercise 8

Exercise to the Lecture

Superconductivity and Low Temperature Physics I
WS 2022/2023

4 Microscopic Theory

4.5 The BCS Ground State Energy

Exercise:

Calculate the zero temperature condensation energy of a superconductor by comparing the BCS ground state energy to that of a normal metal.

Solution:

In order to determine the zero temperature condensation energy of a superconductor we calculate the reduction of the total energy of the electron system in the superconducting state compared to that in the normal conducting state. We start with the BCS Hamilton operator

$$\mathcal{H}_{\text{BCS}} = \sum_{k} \left(\tilde{\epsilon}_{k} - E_{k} + g_{k}^{\dagger} \Delta_{k}\right) + \sum_{k} E_{k} \left[\alpha_{k}^{\dagger} \alpha_{k} + \beta_{k}^{\dagger} \beta_{k}\right] \quad (1)$$

and make use of the fact that the term $$\sum_{k} E_{k} \left[\alpha_{k}^{\dagger} \alpha_{k} + \beta_{k}^{\dagger} \beta_{k}\right]$$ representing the Bogoliubov quasiparticles does not contribute at $$T = 0$$, since no quasiparticles are excited. This term also vanishes in the limit $$\Delta_{k} \to 0$$, i.e. for a normal metal. For the superconducting state at $$T = 0$$ we therefore obtain the expectation value

$$\langle \mathcal{H}_{\text{BCS}} \rangle = \sum_{k} \left(\tilde{\epsilon}_{k} - E_{k} + g_{k}^{\dagger} \Delta_{k}\right). \quad (2)$$

In the limit $$\Delta_{k} \to 0$$, we obtain with $$E_{k} = \sqrt{\tilde{\epsilon}_{k}^{2} + \Delta_{k}^{2}} \simeq |\tilde{\epsilon}_{k}|$$ for the normal state the expression

$$\langle \mathcal{H}_{n} \rangle = \lim_{\Delta \to 0} \langle \mathcal{H}_{\text{BCS}} \rangle = \sum_{k} \tilde{\epsilon}_{k} - |\tilde{\epsilon}_{k}| = \sum_{|k| < k_{F}} \tilde{\epsilon}_{k} - |\tilde{\epsilon}_{k}| + \sum_{|k| \geq k_{F}} \tilde{\epsilon}_{k} - |\tilde{\epsilon}_{k}| = 2 \sum_{|k| < k_{F}} \tilde{\epsilon}_{k}. \quad (3)$$
Here we made use of $|\xi_k| = -\xi_k$ für $|k| \leq k_F$ (particle-hole symmetry, see Fig. 1). For the reduction of the ground state energy in the superconducting state for $T = 0$ we then obtain

$$\Delta E = \langle H_{BCS} \rangle - \langle H_n \rangle = \sum_{|k|<k_F} (\xi_k - E_k + g_k^+\Delta_k) - 2\xi_k + \sum_{|k|\geq k_F} (\xi_k - E_k + g_k^+\Delta_k).$$

(4)

Again making us of the particle-hole symmetry, $|\xi_k| = -\xi_k$ für $|k| \leq k_F$, and $E_k = \sqrt{\xi_k^2 + |\Delta_k|^2}$, results in

$$\Delta E = 2 \sum_{|k|>k_F} \left(\xi_k - \sqrt{\xi_k^2 + |\Delta_k|^2} + g_k^+\Delta_k\right).$$

(5)

The last term in the round brackets can be rewritten by using $g_k^+ = u_kv_k^*$ and $\frac{\Delta_k u_k}{v_k} = \xi_k + E_k$. We obtain

$$g_k^+\Delta_k = \frac{\Delta_k u_k v_k^*}{v_k} = (\xi_k - E_k) \left(\frac{1}{2} - \frac{\xi_k}{2E_k}\right) = \frac{|\Delta_k|^2}{2E_k}$$

(6)

and by insertion into (5) finally

$$\Delta E = 2 \sum_{|k|>k_F} \left[\xi_k - \sqrt{\xi_k^2 + |\Delta_k|^2} + \frac{|\Delta_k|^2}{2\sqrt{\xi_k^2 + |\Delta_k|^2}}\right].$$

(7)

In order to keep our discussion simple, we use $|\Delta_k| = \Delta$ in the following. By using the single spin density of states $D(0)/2 = D(E_F)/2$ (note that we are not summing up over the two spin projections) we can convert the summation into an integration. With the substitution $x = \frac{\xi_k}{\Delta}$ we obtain

$$\Delta E = D(E_F)\Delta^2 \int_0^\infty dx \left[ x - \sqrt{x^2 + 1} + \frac{1}{2\sqrt{x^2 + 1}} \right].$$

(8)
Here, \( z = \hbar \omega_D / \Delta \) is the upper integration limit which is determined by the Debye energy. With \( \int dx \sqrt{x^2 + 1} = \frac{1}{2} (x \sqrt{x^2 + 1} + \sinh^{-1} x) \) sowie \( \int dx (2 \sqrt{x^2 + 1})^{-1} = \frac{1}{2} \sinh^{-1} x \) we obtain
\[
\Delta E = D(E_F) \Delta^2 \left[ \frac{1}{2} z^2 - \frac{1}{2} \left( z \sqrt{z^2 + 1} - \sinh^{-1} z \right) + \frac{1}{2} \sinh^{-1} z \right]. \tag{9}
\]
Since \( z = \hbar \omega_D / \Delta \gg 1 \), we can use the approximation \( \sqrt{1 + 1/z^2} \simeq 1 + 1/2z^2 \) and obtain
\[
\Delta E = \frac{1}{2} D(E_F) \Delta^2 \left[ z^2 - z^2 \left( 1 + \frac{1}{2z^2} \right) \right] = -\frac{1}{4} D(E_F) \Delta^2. \tag{10}
\]
With this result we obtain the condensation energy at \( T = 0 \) to
\[
E_{\text{cond}}(0) = \langle H_{\text{BCS}} \rangle - \langle H_n \rangle = -\frac{1}{4} D(E_F) \Delta^2(0). \tag{11}
\]
With \( N_F = D_F / V = 3n / 2E_F \) and \( \Delta(0) / k_B T_c = \pi / e^2 = 1.76387699 \) we can rewrite this expression into
\[
\frac{E_{\text{cond}}}{V} = -\frac{3}{8} n E_F^2 = -\frac{3\pi^2}{8 e^2} n (k_B T_c)^2 = -1.167 n (k_B T_c)^2 E_F. \tag{12}
\]
We see that the condensation energy density is proportional to the electron density \( n \) and is of the order of \( (k_B T_c)^2 / E_F \) per electron. Obviously, the condensation energy density is independent of the Debye energy \( \hbar \omega_D \) in the weak coupling limit. The proportionality to \( (k_B T_c)^2 / E_F \) can be understood easily. Only a small fraction \( k_B T_c / E_F \) of all electrons is participating in the pairing process and the energy gain of these electrons is \( k_B T_c \) in average.

### 4.6 The Bogoliubov Quasiparticles

Exercise:

The operators for the Bogoliubov quasiparticles are obtained from the electron creation and annihilation operators by the Bogoliubov-Valatin transformation
\[
\begin{pmatrix}
\alpha_{k,\uparrow}^\dagger & \beta_{k,\uparrow}^\dagger \\
\alpha_{k,\downarrow} & \beta_{k,\downarrow}
\end{pmatrix} =
\begin{pmatrix}
u_k^* & -v_k^* \\
u_k & u_k
\end{pmatrix}
\begin{pmatrix}
c_{k,\uparrow}^\dagger \\
c_{k,\downarrow}
\end{pmatrix} \quad \text{or} \quad
\begin{pmatrix}
\alpha_{k,\uparrow}^\dagger & \beta_{k,\uparrow}^\dagger \\
\alpha_{k,\downarrow} & \beta_{k,\downarrow}
\end{pmatrix} =
\begin{pmatrix}
u_k & u_k^* \\
v_k^* & -u_k
\end{pmatrix}
\begin{pmatrix}
c_{k,\uparrow} \\
c_{k,\downarrow}
\end{pmatrix}.
\]

The inverse transformations are obtained by inverting the unitarian matrices and read as
\[
\begin{pmatrix}
c_{k,\uparrow} & c_{-k,\downarrow}
\end{pmatrix} =
\begin{pmatrix}
u_k & u_k^* \\
v_k^* & -u_k
\end{pmatrix}
\begin{pmatrix}
\alpha_{k,\uparrow} & \beta_{k,\uparrow} \\
\alpha_{k,\downarrow} & \beta_{k,\downarrow}
\end{pmatrix} \quad \text{or} \quad
\begin{pmatrix}
c_{k,\uparrow} & c_{-k,\downarrow}
\end{pmatrix} =
\begin{pmatrix}
u_k^* & -v_k \\
v_k & u_k
\end{pmatrix}
\begin{pmatrix}
\alpha_{k,\uparrow}^\dagger & \beta_{k,\uparrow}^\dagger \\
\alpha_{k,\downarrow}^\dagger & \beta_{k,\downarrow}^\dagger
\end{pmatrix}.
\]

(a) Derive the anti-commutation relations for the Bogoliubov operators.

(b) Use the Bogoliubov operators to derive the pairing (Gorkov) amplitude \( \langle c_{-k,\downarrow} c_{k,\uparrow}^\dagger \rangle \).
Solution:

(a) Before deriving the anti-commutation relations for the Bogoliubov operators, we briefly repeat how the Bogoliubov quasiparticles are obtained from the electron creation and annihilation operators by the Bogoliubov-Valatin transformation. We start with the mean field BCS Hamiltonian in matrix representation as introduced by Nambu

\[ H_{\text{BCS}} = \sum_k \begin{pmatrix} \xi_k + g_k^\dagger \Delta_k + (c_{k\uparrow}^\dagger c_{-k\downarrow}) & c_{k\uparrow}^\dagger \\ c_{-k\downarrow} & -\xi_k - \Delta_k \end{pmatrix} \begin{pmatrix} \xi_k \Delta_k \\ -\xi_k \end{pmatrix} \]

\[ = \sum_k \begin{pmatrix} \xi_k + g_k^\dagger \Delta_k + C_k^\dagger (U_k U_k^\dagger) E_k (U_k U_k^\dagger) C_k \\ C_k \end{pmatrix} \]

Here, we have introduced the spinors \( C_k^\dagger \) and \( C_k \), the energy matrix \( E_k \) and the unitary matrix \( U_k \) with \( U_k U_k^\dagger = 1 \) and \( U_k^\dagger = (U_k^\dagger)^T \). With \( |u_k|^2 + |v_k|^2 = 1 \), we can express the unitary transformation in terms of \( u_k \) and \( v_k \) as

\[ U_k = \begin{pmatrix} u_k & v_k^* \\ -v_k & u_k^* \end{pmatrix} \]

\[ U_k^\dagger = \begin{pmatrix} u_k^* & -v_k^* \\ v_k & u_k \end{pmatrix} \]

resulting in the diagonalized energy matrix

\[ U_k^\dagger E_k U_k = \begin{pmatrix} -E_k & 0 \\ 0 & +E_k \end{pmatrix} \]

with the new quasiparticle eigenenergies \( \pm E_k = \pm \sqrt{\xi_k^2 + \Delta_k^2} \).

With the spinors \( B_k^\dagger = (\alpha_k^\dagger, \beta_k) = C_k^\dagger U_k \) and \( B_k = (\alpha_k, \beta_k^\dagger) = U_k^\dagger C_k \), we can express the operators for the Bogoliubov quasiparticles as

\[ \alpha_k = u_k c_{k\uparrow} + v_k c_{-k\downarrow} \]

\[ \beta_k = v_k c_{k\uparrow} - u_k c_{-k\downarrow} \]

\[ \alpha_k^\dagger = u_k c_{k\uparrow}^\dagger - v_k c_{-k\downarrow}^\dagger \]

\[ \beta_k^\dagger = v_k c_{k\uparrow}^\dagger + u_k c_{-k\downarrow}^\dagger \]

Note that the operator \( \alpha_k^\dagger \) creates an electron with \( k \uparrow \) with the probability amplitude \( u_k \) and destroys an electron with \( k \downarrow \) with the probability amplitude \( v_k \). The same is true for \( \beta_k \), but with different probability amplitudes. In total, \( \alpha_k^\dagger \) and \( \beta_k \) both increase the total momentum by \( k \) and the total spin by \( \hbar/2 \). On the other hand, the operator \( \alpha_k \) creates an electron with \( k \downarrow \) with the probability amplitude \( v_k \) and destroys an electron with \( k \uparrow \) with the probability amplitude \( u_k \). Again, the same is true for \( \beta_k^\dagger \), but with different probability amplitudes. In total, \( \alpha_k \) and \( \beta_k^\dagger \) decrease the total momentum by \( k \) and the total spin by \( \hbar/2 \).
With these expression (5)–(8) the anti-commutator \( \{a_k, a_{k'}^\dagger\} \) reads as

\[
\{a_k, a_{k'}^\dagger\} = (u_k^* c_{k'} + v_{k'}^* c_{-k'}^\dagger)(u_k^* c_{k'} + v_{k'}^* c_{-k'}^\dagger) \\
+ (u_k^* c_{k'} + v_{k'}^* c_{-k'}^\dagger)(u_k^* c_{k'} + v_{k'}^* c_{-k'}^\dagger)
\]

\[
= u_k^* u_k^* (c_{k'} + c_{k'}^\dagger) + u_k^* v_{k'}^* (c_{k'}^\dagger + c_{-k'}^\dagger c_{k'}^\dagger)
\]

\[
\{c_{k'} c_{k'}^\dagger\} = \delta_{k,k'}
\]

\[
+ v_k^* v_k^* (c_{k'}^\dagger + c_{-k'}^\dagger) + v_k^* v_k^* (c_{k'}^\dagger + c_{-k'}^\dagger)
\]

\[
= \delta_{k,k'}.
\] (9)

In the same way as above we can show

\[
\{\beta_k, \beta_{k'}^\dagger\} = \delta_{k,k'}.
\] (10)

For the anti-commutator \( \{a_k, a_{k'}\} \) we obtain

\[
\{a_k, a_{k'}\} = (u_k^* c_{k'} - v_{k'}^* c_{-k'}^\dagger)(u_k^* c_{k'} - v_{k'}^* c_{-k'}^\dagger)
\]

\[
+ (u_k^* c_{k'} - v_{k'}^* c_{-k'}^\dagger)(u_k^* c_{k'} - v_{k'}^* c_{-k'}^\dagger)
\]

\[
= u_k^* u_k^* (c_{k'} + c_{k'}^\dagger) - u_k^* v_{k'}^* (c_{k'}^\dagger + c_{-k'} c_{k'}^\dagger)
\]

\[
\{c_{k'} c_{k'}^\dagger\} = \delta_{k,k'}
\]

\[
- v_k^* v_k^* (c_{k'}^\dagger + c_{-k'} c_{k'}^\dagger) + v_k^* v_k^* (c_{k'}^\dagger + c_{-k'} c_{k'}^\dagger)
\]

\[
= 0.
\] (11)

In the same way we can show that

\[
\{\beta_k, \beta_{k'}\} = \{\beta_k^\dagger, \beta_{k'}^\dagger\} = \{a_k, a_{k'}\} = 0.
\] (12)

In summary, we obtain the following anti-commutators for the Bogoliubov quasiparticle operators

\[
\{a_k, a_{k'}^\dagger\} = \{\beta_k, \beta_{k'}^\dagger\} = \delta_{k,k'}
\] (13)

\[
\{a_k, a_{k'}\} = \{\beta_k, \beta_{k'}\} = \delta_{k,k'}
\] (14)

\[
\{a_k^\dagger, a_{k'}^\dagger\} = \{\beta_k^\dagger, \beta_{k'}^\dagger\} = 0.
\] (15)

This shows that the Bogoliubov quasiparticles are fermions.

(b) We can use the inverse transformations

\[
(c_{k'}^\dagger, c_{-k'}) = \begin{pmatrix} u_k & v_k \\ -v_k & u_k \end{pmatrix} \begin{pmatrix} a_k^\dagger \\ \beta_k \end{pmatrix}
\] (16)

\[
(c_{k'}^\dagger, c_{-k'}) = \begin{pmatrix} u_k & v_k \\ -v_k & u_k \end{pmatrix} \begin{pmatrix} a_k \\ \beta_k \end{pmatrix}
\] (17)
to derive the expectation value of the pairing (Gorkov) amplitude \( \langle c_{-k\downarrow}c_{k\uparrow} \rangle \). With (16) and (17) we obtain

\begin{align*}
    c_{k\uparrow}^\dagger &= u_k a_k^\dagger + v_k \beta_k^\dagger \quad (18) \\
    c_{-k\downarrow} &= -v_k^* a_k^\dagger + u_k \beta_k \\
    c_{k\uparrow} &= u_k a_k + v_k^* \beta_k^\dagger \quad (20) \\
    c_{-k\downarrow}^\dagger &= -v_k a_k + u_k \beta_k^\dagger \quad (21)
\end{align*}

and we can express the pairing amplitude as

\[
    \langle c_{-k\downarrow}c_{k\uparrow} \rangle = \langle (-v_k^* a_k^\dagger + u_k \beta_k)(u_k a_k + v_k^* \beta_k^\dagger) \rangle
    = u_k^2 \langle \beta_k a_k \rangle - u_k v_k^* \langle a_k^\dagger a_k \rangle + u_k v_k^* \langle \beta_k \beta_k^\dagger \rangle + (v_k^*)^2 \langle a_k^\dagger \beta_k^\dagger \rangle
    = 0 = n_{qp}(E_k) = 1 - n_{qp}(E_k) = 0
\]

\begin{equation}
    \langle c_{-k\downarrow}c_{k\uparrow} \rangle = u_k v_k^* [1 - 2n_{qp}(E_k)] . \quad (22)
\end{equation}

Here, \( n_{qp}(E_k) \) is the expectation value of the quasiparticle number operator and we have used the fact that the expectation value for Bogoliubov quasiparticle pairs vanishes. Since the Bogoliubov quasiparticles are fermions, the expectation value of the particle number operator is given by the Fermi-Dirac distribution and we obtain

\[
    \langle c_{-k\downarrow}c_{k\uparrow} \rangle = u_k v_k^* \left[ 1 - \frac{2}{\exp(E_k/k_B T) + 1} \right]
    = u_k v_k^* \frac{\exp(E_k/k_B T) - 1}{\exp(E_k/k_B T) + 1}
    = u_k v_k^* \tanh \left( \frac{E_k}{2k_B T} \right). \quad (23)
\]

For \( T \to 0 \), the hyperbolic tangent approaches 1 and we obtain the ground state expectation value \( \langle c_{-k\downarrow}c_{k\uparrow} \rangle = u_k v_k^* \).