

## Exercise to the Lecture

## Superconductivity and Low Temperature Physics I

### WS 2021/2022

#### 4 Microscopic Theory

##### 4.3 The BCS Hamilton Operator in Second Quantization

###### Exercise:

We can use the second quantization formalism to express the BCS Hamiltonian in terms of creation and annihilation operators.

- (a) Use the anti-commutator relation for the fermionic creation ( $\hat{c}_{\mathbf{k}\sigma}^\dagger$ ) and annihilation operator ( $\hat{c}_{\mathbf{k}\sigma}$ )

$$\{\hat{c}_{\mathbf{k}\sigma}, \hat{c}_{\mathbf{k}'\sigma'}^\dagger\} = \delta_{\sigma,\sigma'} \delta^3(\mathbf{k} - \mathbf{k}')$$

to derive the corresponding commutator relation for the field operators  $\hat{\Psi}_\sigma(\mathbf{r})$  and  $\hat{\Psi}_\sigma^\dagger(\mathbf{r})$  defined as

$$\hat{\Psi}_\sigma(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r}} \quad \hat{c}_{\mathbf{k}\sigma} = \frac{1}{\sqrt{V}} \int \hat{\Psi}_\sigma(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} d^3\mathbf{r} \quad (1)$$

$$\hat{\Psi}_\sigma^\dagger(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger e^{-i\mathbf{k}\cdot\mathbf{r}} \quad \hat{c}_{\mathbf{k}\sigma}^\dagger = \frac{1}{\sqrt{V}} \int \hat{\Psi}_\sigma^\dagger(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} d^3\mathbf{r}. \quad (2)$$

- (b) Derive the operator for the total kinetic energy and the potential energy of a non-interacting electron system.
- (c) Derive the BCS Hamilton operator for an electron system with pairing interaction.

**Solution:**

- (a) The position dependent wave functions of the conduction electrons can be described by wave packets which can be constructed from plane waves. We therefore introduce the field operators  $\hat{\Psi}_\sigma(\mathbf{r})$  and  $\hat{\Psi}_\sigma^\dagger(\mathbf{r})$  as Fourier expansions in terms of plane waves, forming a complete basis of eigenfunctions for the Hamilton operator of the electron system:

$$\hat{\Psi}_\sigma(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r}} \quad \hat{c}_{\mathbf{k}\sigma} = \frac{1}{\sqrt{V}} \int \hat{\Psi}_\sigma(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} d^3\mathbf{r} \quad (3)$$

$$\hat{\Psi}_\sigma^\dagger(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger e^{-i\mathbf{k}\cdot\mathbf{r}} \quad \hat{c}_{\mathbf{k}\sigma}^\dagger = \frac{1}{\sqrt{V}} \int \hat{\Psi}_\sigma^\dagger(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} d^3\mathbf{r}. \quad (4)$$

This formalism turns out to be very helpful in describing many-body systems. The expressions on the r.h.s. represent the respective  $\mathbf{k}$ -space representations of the field operators obtained by Fourier transformation.

With these definitions the anti-commutator of the field operators reads as

$$\begin{aligned} \left\{ \hat{\Psi}_\sigma(\mathbf{r}), \hat{\Psi}_{\sigma'}^\dagger(\mathbf{r}') \right\} &= \frac{1}{V} \sum_{\mathbf{k}\mathbf{k}'} \underbrace{\left\{ \hat{c}_{\mathbf{k}\sigma}, \hat{c}_{\mathbf{k}'\sigma'}^\dagger \right\}}_{\delta_{\sigma,\sigma'} \delta^3(\mathbf{k}-\mathbf{k}')} e^{i\mathbf{k}\cdot\mathbf{r} - i\mathbf{k}'\cdot\mathbf{r}'} \\ &= \delta_{\sigma,\sigma'} \underbrace{\frac{1}{V} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}_{\delta^3(\mathbf{r}-\mathbf{r}')} \\ &= \delta_{\sigma,\sigma'} \delta^3(\mathbf{r} - \mathbf{r}') \end{aligned}$$

- (b) In real space, the Hamilton operator of a non-interacting electron systems can be expressed as the sum of the kinetic and potential energy of  $N$  independent electrons. We start with the kinetic energy

$$\begin{aligned} \mathcal{T} &= \int \hat{\Psi}_\sigma^\dagger(\mathbf{r}) \left( -\frac{\hbar^2}{2m} \nabla_i^2 \right) \hat{\Psi}_\sigma(\mathbf{r}) d^3\mathbf{r} \\ &= \frac{1}{V} \sum_{\sigma} \sum_{\mathbf{k}, \mathbf{k}'} \int \hat{c}_{\mathbf{k}'\sigma}^\dagger e^{-i\mathbf{k}'\cdot\mathbf{r}} \frac{\hbar^2 k^2}{2m} \hat{c}_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r}} d^3\mathbf{r} \\ &= \sum_{\sigma} \sum_{\mathbf{k}, \mathbf{k}'} \frac{\hbar^2 k^2}{2m} \hat{c}_{\mathbf{k}'\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} \underbrace{\frac{1}{V} \int e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} d^3\mathbf{r}}_{\delta^3(\mathbf{k}-\mathbf{k}')} \\ &= \sum_{\sigma} \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma}. \end{aligned} \quad (5)$$

For the potential energy we obtain

$$\mathcal{U} = \int \hat{\Psi}_\sigma^\dagger(\mathbf{r}) V_\sigma(\mathbf{r}) \hat{\Psi}_\sigma(\mathbf{r}) d^3\mathbf{r}. \quad (6)$$

Expressing the potential  $V_\sigma(\mathbf{r})$  by a Fourier series

$$V_\sigma(\mathbf{r}) = \sum_{\mathbf{q}} V_\sigma(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}} \quad (7)$$

we obtain

$$\begin{aligned}
\mathcal{U} &= \frac{1}{V} \sum_{\sigma} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} \int \hat{c}_{\mathbf{k}'\sigma}^{\dagger} e^{-i\mathbf{k}'\cdot\mathbf{r}} V_{\sigma}(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}} \hat{c}_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r}} d^3\mathbf{r} \\
&= \sum_{\sigma} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} V_{\sigma}(\mathbf{q}) \hat{c}_{\mathbf{k}'\sigma}^{\dagger} \hat{c}_{\mathbf{k}\sigma} \underbrace{\frac{1}{V} \int e^{i(\mathbf{k}-\mathbf{k}'+\mathbf{q})\cdot\mathbf{r}} d^3\mathbf{r}}_{\delta^3(\mathbf{k}+\mathbf{q}-\mathbf{k}')} \\
&= \sum_{\sigma} \sum_{\mathbf{k}, \mathbf{q}} V_{\sigma}(\mathbf{q}) \hat{c}_{\mathbf{k}+\mathbf{q},\sigma}^{\dagger} \hat{c}_{\mathbf{k}\sigma}. \tag{8}
\end{aligned}$$

With (5) and (8) the total Hamilton operator of the non-interacting electron system reads as

$$\mathcal{H} = \sum_{\sigma} \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} \hat{c}_{\mathbf{k}\sigma}^{\dagger} \hat{c}_{\mathbf{k}\sigma} + \sum_{\sigma} \sum_{\mathbf{k}, \mathbf{q}} V_{\sigma}(\mathbf{q}) \hat{c}_{\mathbf{k}+\mathbf{q},\sigma}^{\dagger} \hat{c}_{\mathbf{k}\sigma}. \tag{9}$$

When we consider a non-interacting electron system in the external electromagnetic potentials  $\phi(\mathbf{r})$  and  $\mathbf{A}(\mathbf{r})$ , the potential  $V_{\sigma}(\mathbf{q})$  has to be replaced by the electromagnetic potentials  $\phi(\mathbf{r})$  and  $\mathbf{A}(\mathbf{r})$ . It can be shown that the total Hamilton operator is obtained by replacing

$$V_{\sigma}(\mathbf{q}) \rightarrow e\phi(\mathbf{q}) - e\mathbf{v}_{\mathbf{k}} \cdot \mathbf{A}(\mathbf{q}) + \mathcal{O}(\mathbf{A})^2. \tag{10}$$

in expression (9).

- (c) Discussing the BCS Hamilton operator, we first can state that the expression for the kinetic energy stays the same. In order to discuss the contribution of the pair interaction energy

$$\mathcal{U} = \frac{1}{2} \sum_{\sigma_1, \sigma_2} \sum_{i, j=1}^N V(\mathbf{r}_j - \mathbf{r}_i) \tag{11}$$

in an  $N$  electron system (the factor  $1/2$  appears to avoid double counting) we express the interaction potential in terms of a Fourier series

$$V_{\sigma_1\sigma_2}(\mathbf{r}_j - \mathbf{r}_i) = \sum_{\mathbf{q}} V_{\sigma_1\sigma_2}(\mathbf{q}) e^{i\mathbf{q}\cdot(\mathbf{r}_j - \mathbf{r}_i)}. \tag{12}$$

Using the field operators, the interaction energy then reads as

$$\begin{aligned}
\mathcal{U} &= \frac{1}{2V^2} \sum_{\sigma_1, \sigma_2} \sum_{\mathbf{k}_1, \mathbf{k}_1', \mathbf{k}_2, \mathbf{k}_2', \mathbf{q}} \iint \hat{c}_{\mathbf{k}_1'\sigma_1}^{\dagger} \hat{c}_{\mathbf{k}_2'\sigma_2}^{\dagger} e^{-i\mathbf{k}_1'\cdot\mathbf{r}_i} e^{-i\mathbf{k}_2'\cdot\mathbf{r}_j} V_{\sigma_1\sigma_2}(\mathbf{q}) e^{i\mathbf{q}\cdot(\mathbf{r}_j - \mathbf{r}_i)} \\
&\quad \hat{c}_{\mathbf{k}_2\sigma_2} \hat{c}_{\mathbf{k}_1\sigma_1} e^{i\mathbf{k}_2\cdot\mathbf{r}_j} e^{i\mathbf{k}_1\cdot\mathbf{r}_i} d^3\mathbf{r}_i d^3\mathbf{r}_j \\
&= \frac{1}{2} \sum_{\sigma_1, \sigma_2} \sum_{\mathbf{k}_1, \mathbf{k}_1', \mathbf{k}_2, \mathbf{k}_2', \mathbf{q}} V_{\sigma_1\sigma_2}(\mathbf{q}) \hat{c}_{\mathbf{k}_1'\sigma_1}^{\dagger} \hat{c}_{\mathbf{k}_2'\sigma_2}^{\dagger} \hat{c}_{\mathbf{k}_2\sigma_2} \hat{c}_{\mathbf{k}_1\sigma_1} \\
&\quad \underbrace{\frac{1}{V} \int e^{i(\mathbf{k}_1 - \mathbf{k}_1' + \mathbf{q})\cdot\mathbf{r}_i} d^3\mathbf{r}_i}_{\delta^3(\mathbf{k}_1 + \mathbf{q} - \mathbf{k}_1')} \underbrace{\frac{1}{V} \int e^{i(\mathbf{k}_2 - \mathbf{k}_2' - \mathbf{q})\cdot\mathbf{r}_j} d^3\mathbf{r}_j}_{\delta^3(\mathbf{k}_2 - \mathbf{q} - \mathbf{k}_2')} \\
&= \frac{1}{2} \sum_{\sigma_1, \sigma_2} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{q}} V_{\sigma_1\sigma_2}(\mathbf{q}) c_{\mathbf{k}_1 + \mathbf{q}, \sigma_1}^{\dagger} c_{\mathbf{k}_2 - \mathbf{q}, \sigma_2}^{\dagger} c_{\mathbf{k}_2, \sigma_2} c_{\mathbf{k}_1, \sigma_1}. \tag{13}
\end{aligned}$$

In total we then obtain

$$\mathcal{H}_{\text{BCS}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} + \frac{1}{2} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{q}, \sigma_1, \sigma_2} V_{\sigma_1 \sigma_2}(\mathbf{q}) c_{\mathbf{k}_1 + \mathbf{q}, \sigma_1}^\dagger c_{\mathbf{k}_2 - \mathbf{q}, \sigma_2}^\dagger c_{\mathbf{k}_2, \sigma_2} c_{\mathbf{k}_1, \sigma_1}. \quad (14)$$

The interaction term can be simplified by assuming spin singlet Cooper pairs with opposite momentum, i.e.,  $\mathbf{k}_1 = -\mathbf{k}_2 = \mathbf{k}$  as well as  $\sigma_1 = \uparrow$  and  $\sigma_2 = \downarrow$ :

$$\mathcal{H}_{\text{BCS}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{k}, \mathbf{k}'} V_{\mathbf{k}, \mathbf{k}'} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}. \quad (15)$$

Here we used  $V_{\mathbf{k}, \mathbf{k}'}$  for  $V(\mathbf{k} - \mathbf{k}') = V(\mathbf{q})$  with  $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ . The kinetic energy usually is taken relativ to the chemical potential  $\mu$ . In this case we have to use

$$\tilde{\zeta}_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu \quad (16)$$

in expressions (14) and (15).

#### 4.4 Expectation Values

##### Exercise:

Use the BCS many particle wave function

$$|\Psi_{\text{BCS}}\rangle = \prod_{\mathbf{k}=\mathbf{k}_1, \dots, \mathbf{k}_M} (u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger) |0\rangle$$

to calculate the expectation values for the single spin particle number operator  $\langle n_{\mathbf{k}\uparrow} \rangle$ , the average particle number  $\langle N \rangle = \langle \sum_{\mathbf{k}\sigma} n_{\mathbf{k}\sigma} \rangle$ , the statistical fluctuation  $\Delta N$  of the average particle number, the pairing (Gorkov) amplitude  $g_{\mathbf{k}} \equiv \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle$ , and the BCS Hamilton operator  $\langle \mathcal{H}_{\text{BCS}} \rangle$ .

##### Solution:

For the calculation of the expectation values we use the following identities:

$$\langle \mathcal{O} \phi | \psi \rangle = \langle \phi | \mathcal{O}^\dagger | \psi \rangle \quad (1)$$

$$\langle \phi | (\mathcal{A}\mathcal{B})^\dagger | \psi \rangle = \langle \phi | \mathcal{B}^\dagger \mathcal{A}^\dagger | \psi \rangle. \quad (2)$$

For the single spin particle number operator we obtain

$$\begin{aligned} \langle n_{\mathbf{k}\uparrow} \rangle &= \langle \Psi_{\text{BCS}}^* | c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} | \Psi_{\text{BCS}} \rangle \\ &= \langle 0 | (u_{\mathbf{k}}^* + v_{\mathbf{k}}^* c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}) c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} (u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger) \\ &\quad \times \prod_{\mathbf{l} \neq \mathbf{k}} (u_{\mathbf{l}}^* + v_{\mathbf{l}}^* c_{-\mathbf{l}\downarrow} c_{\mathbf{l}\uparrow}) (u_{\mathbf{l}} + v_{\mathbf{l}} c_{\mathbf{l}\uparrow}^\dagger c_{-\mathbf{l}\downarrow}^\dagger) |0\rangle. \end{aligned} \quad (3)$$

The factors for  $\mathbf{l} \neq \mathbf{k}$  yield  $|u_{\mathbf{l}}|^2 + |v_{\mathbf{l}}|^2 = 1$ , resulting in

$$\begin{aligned} \langle n_{\mathbf{k}\uparrow} \rangle &= |u_{\mathbf{k}}|^2 \underbrace{\langle 0 | c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} | 0 \rangle}_{=0} + u_{\mathbf{k}}^* v_{\mathbf{k}} \underbrace{\langle 0 | c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger | 0 \rangle}_{=0} \\ &\quad + v_{\mathbf{k}}^* u_{\mathbf{k}} \underbrace{\langle 0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} | 0 \rangle}_{=0} + |v_{\mathbf{k}}|^2 \underbrace{\langle 0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger | 0 \rangle}_{=1} \\ &= |v_{\mathbf{k}}|^2. \end{aligned} \quad (4)$$

The terms with the prefactors  $|u_{\mathbf{k}}|^2$ ,  $u_{\mathbf{k}}^* v_{\mathbf{k}}$  and  $v_{\mathbf{k}}^* u_{\mathbf{k}}$  can be rearranged by an even number of permutations into  $\dots c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} | 0 \rangle = n_{\mathbf{k}\uparrow} | 0 \rangle = 0 | 0 \rangle$  and thus vanish. The term with the prefactor  $|v_{\mathbf{k}}|^2$  can be rewritten using the anti-commutator  $\{c_{\mathbf{k},\sigma}, c_{\mathbf{k}',\sigma'}^\dagger\} = c_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma'}^\dagger + c_{\mathbf{k}',\sigma'}^\dagger c_{\mathbf{k},\sigma} = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'}$  as

$$\begin{aligned} \langle 0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger | 0 \rangle &= \langle 0 | c_{-\mathbf{k}\downarrow} (1 - c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow}) (1 - c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow}) c_{-\mathbf{k}\downarrow}^\dagger | 0 \rangle \\ &= \langle 0 | c_{-\mathbf{k}\downarrow} c_{-\mathbf{k}\downarrow}^\dagger | 0 \rangle \\ &\quad - \langle 0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}^\dagger | 0 \rangle \\ &\quad - \langle 0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}^\dagger | 0 \rangle \\ &\quad + \langle 0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}^\dagger | 0 \rangle \\ &= 1. \end{aligned} \quad (5)$$

Only the first term on the r.h.s. gives 1 since  $\langle 0 | c_{-\mathbf{k}\downarrow} c_{-\mathbf{k}\downarrow}^\dagger | 0 \rangle = \langle 0 | 1 - n_{-\mathbf{k}\downarrow} | 0 \rangle = 1 - 0 = 1$ . All the other terms again can be rearranged by an even number of permutations into  $\dots c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} | 0 \rangle = 0$ . We see that the expectation value of the single spin particle number operator is given by the probability  $|v_{\mathbf{k}}|^2$  that the pair state  $(\mathbf{k} \uparrow, -\mathbf{k} \downarrow)$  is occupied.

With the result (4) we obtain for the average particle number

$$N = \langle \mathcal{N} \rangle = \left\langle \sum_{\mathbf{k},\sigma} n_{\mathbf{k}\sigma} \right\rangle = \sum_{\mathbf{k},\sigma} |v_{\mathbf{k}}|^2 = 2 \sum_{\mathbf{k}} |v_{\mathbf{k}}|^2. \quad (6)$$

The statistical fluctuation of the average particle number is given by

$$\Delta N = \sqrt{\langle \mathcal{N}^2 \rangle - \langle \mathcal{N} \rangle^2}. \quad (7)$$

To determine  $\Delta N$  we first calculate

$$\begin{aligned} \langle \Psi_{\text{BCS}}^* | n_{\mathbf{k}\sigma}^2 | \Psi_{\text{BCS}} \rangle &= \langle \Psi_{\text{BCS}}^* | c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} | \Psi_{\text{BCS}} \rangle \\ &= \langle \Psi_{\text{BCS}}^* | c_{\mathbf{k}\sigma}^\dagger (1 - c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}) c_{\mathbf{k}\sigma} | \Psi_{\text{BCS}} \rangle \\ &= \langle \Psi_{\text{BCS}}^* | c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} - c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} | \Psi_{\text{BCS}} \rangle \\ &= \langle \Psi_{\text{BCS}}^* | c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} | \Psi_{\text{BCS}} \rangle \\ &= |v_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^4. \end{aligned} \quad (8)$$

Here we have again used the anti-commutator relation and the fact that an odd permutation of the operators changes sign. With (6) and (8) we obtain

$$\begin{aligned} \Delta N &= \sqrt{2 \sum_{\mathbf{k}} (\langle n_{\mathbf{k}}^2 \rangle - \langle n_{\mathbf{k}} \rangle^2)} \\ &= \sqrt{2 \sum_{\mathbf{k}} |v_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^4 - |v_{\mathbf{k}}|^4} = \sqrt{2 \sum_{\mathbf{k}} |v_{\mathbf{k}}|^2} = \sqrt{N}. \end{aligned} \quad (9)$$

We see that the fluctuation  $\Delta N = \sqrt{N}$  is very large for large particle number. However, the relative fluctuation  $\Delta N/N = 1/\sqrt{N}$  is very small and vanishes for  $N \rightarrow \infty$ . Obviously, the particle number has the statistical properties of a coherent state (Poisson statistics).

For the pairing amplitude

$$g_{\mathbf{k}} \equiv \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle \quad (10)$$

$$g_{\mathbf{k}}^{\dagger} \equiv \langle c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} \rangle \quad (11)$$

we obtain

$$\begin{aligned} g_{\mathbf{k}} &= \langle \Psi_{\text{BCS}}^* | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} | \Psi_{\text{BCS}} \rangle \\ &= \langle 0 | (u_{\mathbf{k}}^* + v_{\mathbf{k}}^* c_{-\mathbf{k}\downarrow}^{\dagger} c_{\mathbf{k}\uparrow}^{\dagger}) c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} (u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger}) \\ &\quad \times \prod_{\mathbf{l} \neq \mathbf{k}} (u_{\mathbf{l}}^* + v_{\mathbf{l}}^* c_{-\mathbf{l}\downarrow}^{\dagger} c_{\mathbf{l}\uparrow}^{\dagger}) (u_{\mathbf{l}} + v_{\mathbf{l}} c_{\mathbf{l}\uparrow}^{\dagger} c_{-\mathbf{l}\downarrow}^{\dagger}) | 0 \rangle. \end{aligned} \quad (12)$$

As already discussed above, the factors for  $\mathbf{l} \neq \mathbf{k}$  yield  $|u_{\mathbf{l}}|^2 + |v_{\mathbf{l}}|^2 = 1$ , resulting in

$$\begin{aligned} g_{\mathbf{k}} &= |u_{\mathbf{k}}|^2 \underbrace{\langle 0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} | 0 \rangle}_{=0} + u_{\mathbf{k}}^* v_{\mathbf{k}} \underbrace{\langle 0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} | 0 \rangle}_{=1} \\ &\quad + v_{\mathbf{k}}^* u_{\mathbf{k}} \underbrace{\langle 0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} | 0 \rangle}_{=0} + |v_{\mathbf{k}}|^2 \underbrace{\langle 0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} | 0 \rangle}_{=0} \\ &= u_{\mathbf{k}}^* v_{\mathbf{k}}. \end{aligned} \quad (13)$$

We easily can prove that the different term give zero by using the anti-commutator  $\{c_{\mathbf{k},\sigma}, c_{\mathbf{k}',\sigma'}^{\dagger}\} = c_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma'}^{\dagger} + c_{\mathbf{k}',\sigma'}^{\dagger} c_{\mathbf{k},\sigma} = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'}$ . For example, for the first term we obtain

$$\begin{aligned} \langle 0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} | 0 \rangle &= \langle 0 | c_{-\mathbf{k}\downarrow} (c_{\mathbf{k},\uparrow} c_{\mathbf{k},\uparrow}^{\dagger} + c_{\mathbf{k},\uparrow}^{\dagger} c_{\mathbf{k},\uparrow}) c_{\mathbf{k}\uparrow} | 0 \rangle \\ &= \langle 0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k},\uparrow} c_{\mathbf{k},\uparrow}^{\dagger} c_{\mathbf{k}\uparrow} + c_{-\mathbf{k}\downarrow} c_{\mathbf{k},\uparrow}^{\dagger} c_{\mathbf{k},\uparrow} c_{\mathbf{k}\uparrow} | 0 \rangle \\ &= \langle 0 | c_{-\mathbf{k}\downarrow} c_{\mathbf{k},\uparrow} c_{\mathbf{k},\uparrow}^{\dagger} c_{\mathbf{k}\uparrow} + c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} c_{\mathbf{k},\uparrow}^{\dagger} c_{\mathbf{k}\uparrow} | 0 \rangle \\ &= 0. \end{aligned} \quad (14)$$

Here, we again have used an even number of permutations to obtain expressions  $\dots c_{\mathbf{k}\uparrow}^{\dagger} c_{\mathbf{k}\uparrow} | 0 \rangle = 0$ .

Equivalently, we obtain

$$g_{\mathbf{k}}^{\dagger} \equiv \langle c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} \rangle = u_{\mathbf{k}} v_{\mathbf{k}}^*. \quad (15)$$

Using the same procedure we further can show that

$$\langle \Psi_{\text{BCS}}^* | c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} | \Psi_{\text{BCS}} \rangle = v_{\mathbf{k}} v_{\mathbf{k}'}^* u_{\mathbf{k}} u_{\mathbf{k}'}^*. \quad (16)$$

For the BCS Hamilton operator

$$\mathcal{H}_{\text{BCS}} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} n_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \quad (17)$$

we obtain we obtain with the results (4) and (16)

$$E = \langle \Psi_{\text{BCS}}^* | \mathcal{H}_{\text{BCS}} | \Psi_{\text{BCS}} \rangle = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} |v_{\mathbf{k}}|^2 + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} v_{\mathbf{k}} v_{\mathbf{k}'}^* u_{\mathbf{k}} u_{\mathbf{k}'}^*. \quad (18)$$