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Exercise 7

Exercise to the Lecture

Superconductivity and Low Temperature Physics I
WS 2022/2023

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 ($\hat{c}^\dagger_{\mathbf{k}\sigma}$) and annihilation operator ($\hat{c}_{\mathbf{k}\sigma}$)

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

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

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

$$\hat{\Psi}^\dagger_\sigma(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\sigma} \mathrm{e}^{-\imath\mathbf{k}\cdot\mathbf{r}} \qquad \hat{c}^\dagger_{\mathbf{k}\sigma} = \frac{1}{\sqrt{V}}\int \hat{\Psi}^\dagger_\sigma(\mathbf{r})\mathrm{e}^{\imath\mathbf{k}\cdot\mathbf{r}} d^3\mathbf{r}\,. \tag{2}$$

(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 $\hat{\Psi}^\dagger_\sigma(\mathbf{r})$ as Fourier expansions in terms of plane waves, forming a complete basis of eigenfunctions for the Hamilton operator of the electron system:

$$\hat{\Psi}_\sigma(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma} e^{\imath\mathbf{k}\cdot\mathbf{r}} \qquad \hat{c}_{\mathbf{k}\sigma} = \frac{1}{\sqrt{V}} \int \hat{\Psi}_\sigma(\mathbf{r}) e^{-\imath\mathbf{k}\cdot\mathbf{r}} d3\mathbf{r} \tag{3}$$

$$\hat{\Psi}^\dagger_\sigma(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\sigma} e^{-\imath\mathbf{k}\cdot\mathbf{r}} \qquad \hat{c}^\dagger_{\mathbf{k}\sigma} = \frac{1}{\sqrt{V}} \int \hat{\Psi}^\dagger_\sigma(\mathbf{r}) e^{\imath\mathbf{k}\cdot\mathbf{r}} d^3\mathbf{r}\,. \tag{4}$$

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

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

(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

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

For the potential energy we obtain

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

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

$$V_\sigma(\mathbf{r}) = \sum_{\mathbf{q}} V_\sigma(\mathbf{q})\, e^{\imath\mathbf{q}\cdot\mathbf{r}} \tag{7}$$

we obtain

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

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

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

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

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

Using the field operators, the interaction energy then reads as

$$
\begin{aligned}
\mathcal{U} &= \frac{1}{2V^2}\sum_{\sigma_1,\sigma_2}\sum_{\mathbf{k_1},\mathbf{k_1}',\mathbf{k_2},\mathbf{k_2}',\mathbf{q}}\iint \hat{c}^{\dagger}_{\mathbf{k}_1'\sigma_1}\hat{c}^{\dagger}_{\mathbf{k}_2'\sigma_2}\mathrm{e}^{-\imath\mathbf{k}_1'\cdot\mathbf{r}_i}\mathrm{e}^{-\imath\mathbf{k}_2'\cdot\mathbf{r}_j}\; V_{\sigma_1\sigma_2}(\mathbf{q})\;\mathrm{e}^{\imath\mathbf{q}\cdot(\mathbf{r}_j-\mathbf{r}_i)} \\
&\qquad \hat{c}_{\mathbf{k}_2\sigma_2}\hat{c}_{\mathbf{k}_1\sigma_1}\mathrm{e}^{\imath\mathbf{k}_2\cdot\mathbf{r}_j}\mathrm{e}^{\imath\mathbf{k}_1\cdot\mathbf{r}_i}\; d^3\mathbf{r}_i d^3\mathbf{r}_j \\
&= \frac{1}{2}\sum_{\sigma_1,\sigma_2}\sum_{\mathbf{k_1},\mathbf{k_1}',\mathbf{k_2},\mathbf{k_2}',\mathbf{q}} V_{\sigma_1\sigma_2}(\mathbf{q})\;\hat{c}^{\dagger}_{\mathbf{k}_1'\sigma_1}\hat{c}^{\dagger}_{\mathbf{k}_2'\sigma_2}\hat{c}_{\mathbf{k}_2\sigma_2}\hat{c}_{\mathbf{k}_1\sigma_1} \\
&\qquad \underbrace{\frac{1}{V}\int \mathrm{e}^{\imath(\mathbf{k}_1-\mathbf{k}_1'+\mathbf{q})\cdot\mathbf{r}_i}\; d^3\mathbf{r}_i}_{\delta^3(\mathbf{k}_1+\mathbf{q}-\mathbf{k}_1')}\;\underbrace{\frac{1}{V}\int \mathrm{e}^{\imath(\mathbf{k}_2-\mathbf{k}_2'-\mathbf{q})\cdot\mathbf{r}_j}\; d^3\mathbf{r}_j}_{\delta^3(\mathbf{k}_2-\mathbf{q}-\mathbf{k}_2')} \\
&= \frac{1}{2}\sum_{\sigma_1,\sigma_2}\sum_{\mathbf{k_1},\mathbf{k_2},\mathbf{q}} V_{\sigma_1\sigma_2}(\mathbf{q})\;c^{\dagger}_{\mathbf{k_1}+\mathbf{q},\sigma_1}c^{\dagger}_{\mathbf{k_2}-\mathbf{q},\sigma_2}c_{\mathbf{k}_2,\sigma_2}c_{\mathbf{k}_1,\sigma_1}\,.
\end{aligned}
\tag{13}
$$

In total we then obtain

$$\mathcal{H}_{\mathrm{BCS}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + \frac{1}{2} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q},\sigma_1,\sigma_2} V_{\sigma_1\sigma_2}(\mathbf{q}) c^\dagger_{\mathbf{k_1+q},\sigma_1} c^\dagger_{\mathbf{k_2-q},\sigma_2} c_{\mathbf{k}_2,\sigma_2} c_{\mathbf{k}_1,\sigma_1} . \tag{14}$$

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 $\sigma_2 = \downarrow$:

$$\mathcal{H}_{\mathrm{BCS}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} . \tag{15}$$

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 μ. In this case we have to use

$$\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu \tag{16}$$

in expressions (14) and (15).

4.4 Expectation Values

Exercise:

Use the BCS many particle wave function

$$|\Psi_{\mathrm{BCS}}\rangle = \prod_{\mathbf{k}=\mathbf{k}_1,\ldots,\mathbf{k}_M} (u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})|0\rangle$$

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 ΔN 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 $\langle \mathcal{H}_{\mathrm{BCS}}\rangle$.

Solution:

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

$$\langle \mathcal{O}\phi|\psi\rangle = \langle \phi|\mathcal{O}^\dagger\psi\rangle \tag{1}$$
$$\langle \phi|(\mathcal{A}\mathcal{B})^\dagger|\psi\rangle = \langle \phi|\mathcal{B}^\dagger\mathcal{A}^\dagger|\psi\rangle . \tag{2}$$

For the single spin particle number operator we obtain

$$\begin{aligned} \langle n_{\mathbf{k}\uparrow}\rangle &= \langle \Psi^*_{\mathrm{BCS}}|c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow}|\Psi_{\mathrm{BCS}}\rangle \\ &= \langle 0|(u^*_{\mathbf{k}} + v^*_{\mathbf{k}} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}) c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} (u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}) \\ &\quad \times \prod_{\mathbf{l}\neq\mathbf{k}} (u^*_{\mathbf{l}} + v^*_{\mathbf{l}} c_{-\mathbf{l}\downarrow} c_{\mathbf{l}\uparrow})(u_{\mathbf{l}} + v_{\mathbf{l}} c^\dagger_{\mathbf{l}\uparrow} c^\dagger_{-\mathbf{l}\downarrow})|0\rangle . \end{aligned} \tag{3}$$

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

$$\begin{aligned}
\langle n_{\mathbf{k}\uparrow} \rangle = {} & |u_\mathbf{k}|^2 \underbrace{\langle 0| c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} |0\rangle}_{=0} + u^*_\mathbf{k} v_\mathbf{k} \underbrace{\langle 0| c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} |0\rangle}_{=0} \\
& + v^*_\mathbf{k} u_\mathbf{k} \underbrace{\langle 0| c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} |0\rangle}_{=0} + |v_\mathbf{k}|^2 \underbrace{\langle 0| c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} |0\rangle}_{=1} \\
= {} & |v_\mathbf{k}|^2 .
\end{aligned} \tag{4}$$

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 $\ldots c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} |0\rangle = n_{\mathbf{k}\uparrow} |0\rangle = 0|0\rangle$ and thus vanish. The term with the prefactor $|v_\mathbf{k}|^2$ can be rewritten using the anti-commutator $\{c_{\mathbf{k},\sigma}, c^\dagger_{\mathbf{k}',\sigma'}\} = c_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}',\sigma'} + c^\dagger_{\mathbf{k}',\sigma'} c_{\mathbf{k},\sigma} = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'}$ as

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

Only the first term on the r.h.s. gives 1 since $\langle 0| c_{-\mathbf{k}\downarrow} c^\dagger_{-\mathbf{k}\downarrow} |0\rangle = \langle 0| 1 - n_{-\mathbf{k}\downarrow} |0\rangle = 1 - 0 = 1$. All the other terms again can be rearranged by an even number of permutations into $\ldots c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} |0\rangle = 0$. 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

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

The statistical fluctuation of the particle number is given by

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

With (6) we can rewrite this into

$$(\Delta N)^2 = \left\langle \left(\sum_{\mathbf{k},\sigma} n_{\mathbf{k}\sigma} \right)^2 \right\rangle - \left(\left\langle \sum_{\mathbf{k},\sigma} n_{\mathbf{k}\sigma} \right\rangle \right)^2 = 2 \sum_{\mathbf{k},\mathbf{k}'} \langle n_\mathbf{k} n_{\mathbf{k}'} \rangle - 2 \sum_{\mathbf{k},\mathbf{k}'} \langle n_\mathbf{k} \rangle \langle n_{\mathbf{k}'} \rangle . \tag{8}$$

In order to evaluate this expression we distinguish between the two case $\mathbf{k} \neq \mathbf{k}'$ and $\mathbf{k} = \mathbf{k}'$.

(i) $\mathbf{k} \neq \mathbf{k}'$:

Since there is no correlation between the calculation of $\sum_\mathbf{k}$ and $\sum_{\mathbf{k}'}$, we obtain $\langle n_\mathbf{k} n_{\mathbf{k}'} \rangle = \langle n_\mathbf{k} \rangle \langle n_{\mathbf{k}'} \rangle$ and therefore the contributions of $\langle n_\mathbf{k} n_{\mathbf{k}'} \rangle$ and $\langle n_\mathbf{k} \rangle \langle n_{\mathbf{k}'} \rangle$ in (8) just cancel each other due to the minus sign.

(ii) $\mathbf{k} = \mathbf{k}'$:

In oder to discuss this case, we first determine the expectation value $\langle n^2_{\mathbf{k}\sigma}\rangle$. We obtain

$$
\begin{aligned}
\langle \Psi^*_{\rm BCS}|n^2_{\mathbf{k}\sigma}|\Psi_{\rm BCS}\rangle &= \langle \Psi^*_{\rm BCS}|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}|\Psi_{\rm BCS}\rangle \\
&= \langle \Psi^*_{\rm BCS}|c^\dagger_{\mathbf{k}\sigma}(1-c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma})c_{\mathbf{k}\sigma}|\Psi_{\rm BCS}\rangle \\
&= \langle \Psi^*_{\rm BCS}|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}-c^\dagger_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}|\Psi_{\rm BCS}\rangle \\
&= \langle \Psi^*_{\rm BCS}|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}|\Psi_{\rm BCS}\rangle \\
&= |v_{\mathbf{k}}|^2+|v_{\mathbf{k}}|^4\,. \qquad (9)
\end{aligned}
$$

Here, we have again used the anti-commutator relation and the fact that an odd permutation of the operators changes sign. Plugging in this result in (8) we obtain

$$
(\Delta N)^2 \;=\; 2\sum_{\mathbf{k}}\langle n_{\mathbf{k}}n_{\mathbf{k}}\rangle - 2\sum_{\mathbf{k}}\langle n_{\mathbf{k}}\rangle\langle n_{\mathbf{k}}\rangle = 2\sum_{\mathbf{k}}|v_{\mathbf{k}}|^2+|v_{\mathbf{k}}|^4-2\sum_{\mathbf{k}}|v_{\mathbf{k}}|^4 = 2\sum_{\mathbf{k}}|v_{\mathbf{k}}|^2\,. \qquad (10)
$$

With (6) we then obtain

$$
\Delta N \;=\; \sqrt{2\sum_{\mathbf{k}}|v_{\mathbf{k}}|^2} \;=\; \sqrt{\overline{N}}\,. \qquad (11)
$$

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

For the pairing amplitude

$$
\begin{aligned}
g_{\mathbf{k}} &\equiv \langle c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\rangle \qquad (12)\\
g^\dagger_{\mathbf{k}} &\equiv \langle c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}\rangle \qquad (13)
\end{aligned}
$$

we obtain

$$
\begin{aligned}
g_{\mathbf{k}} &= \langle \Psi^*_{\rm BCS}|c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}|\Psi_{\rm BCS}\rangle \\
&= \langle 0|(u^*_{\mathbf{k}}+v^*_{\mathbf{k}}c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow})c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}(u_{\mathbf{k}}+v_{\mathbf{k}}c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}) \\
&\quad\times\prod_{\mathbf{l}\neq\mathbf{k}}(u^*_{\mathbf{l}}+v^*_{\mathbf{l}}c_{-\mathbf{l}\downarrow}c_{\mathbf{l}\uparrow})(u_{\mathbf{l}}+v_{\mathbf{l}}c^\dagger_{\mathbf{l}\uparrow}c^\dagger_{-\mathbf{l}\downarrow})|0\rangle\,.
\end{aligned} \qquad (14)
$$

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

$$
\begin{aligned}
g_{\mathbf{k}} &= |u_{\mathbf{k}}|^2\underbrace{\langle 0|c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}|0\rangle}_{=0}+u^*_{\mathbf{k}}v_{\mathbf{k}}\underbrace{\langle 0|c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}|0\rangle}_{=1} \\
&\quad+v^*_{\mathbf{k}}u_{\mathbf{k}}\underbrace{\langle 0|c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}|0\rangle}_{=0}+|v_{\mathbf{k}}|^2\underbrace{\langle 0|c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}|0\rangle}_{=0} \\
&= u^*_{\mathbf{k}}v_{\mathbf{k}}\,.
\end{aligned} \qquad (15)
$$

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

$$
\begin{aligned}
\langle 0|c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}|0\rangle &= \langle 0|c_{-\mathbf{k}\downarrow}(c_{\mathbf{k},\uparrow}c^\dagger_{\mathbf{k},\uparrow}+c^\dagger_{\mathbf{k},\uparrow}c_{\mathbf{k},\uparrow})c_{\mathbf{k}\uparrow}|0\rangle \\
&= \langle 0|c_{-\mathbf{k}\downarrow}c_{\mathbf{k},\uparrow}c^\dagger_{\mathbf{k},\uparrow}c_{\mathbf{k}\uparrow}+c_{-\mathbf{k}\downarrow}c^\dagger_{\mathbf{k},\uparrow}c_{\mathbf{k},\uparrow}c_{\mathbf{k}\uparrow}|0\rangle \\
&= \langle 0|c_{-\mathbf{k}\downarrow}c_{\mathbf{k},\uparrow}c^\dagger_{\mathbf{k},\uparrow}c_{\mathbf{k}\uparrow}+c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}c^\dagger_{\mathbf{k},\uparrow}c_{\mathbf{k},\uparrow}|0\rangle \\
&= 0\,. \qquad (16)
\end{aligned}
$$

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

Equivalently, we obtain

$$g^\dagger_{\mathbf{k}} \;\equiv\; \langle c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}\rangle = u_{\mathbf{k}} v^*_{\mathbf{k}}\,. \tag{17}$$

Using the same procedure we further can show that

$$\langle \Psi^*_{\mathrm{BCS}} | c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} | \Psi_{\mathrm{BCS}}\rangle = v_{\mathbf{k}} v^*_{\mathbf{k}'} u_{\mathbf{k}'} u^*_{\mathbf{k}}\,. \tag{18}$$

For the BCS Hamilton operator

$$\mathcal{H}_{\mathrm{BCS}} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} n_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \tag{19}$$

we obtain we obtain with the results (4) and (18)

$$E \;=\; \langle \Psi^*_{\mathrm{BCS}} | \mathcal{H}_{\mathrm{BCS}} | \Psi_{\mathrm{BCS}}\rangle \;=\; \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} |v_{\mathbf{k}}|^2 + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} v_{\mathbf{k}} v^*_{\mathbf{k}'} u_{\mathbf{k}'} u^*_{\mathbf{k}}\,. \tag{20}$$