Karlsruhe Institute of Technology | Institute for Theoretical Condensed Matter physics

Condensed Matter Theory I WS 2022/2023

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Sheet 14
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Category A

1. Properties of the BCS ground state $(5 + 15 + 10 + 5 = 35$ points)

The BCS ground state $|\Phi_{\rm BCS}\rangle$ was derived in the lecture.

(a) Show that the ground state is properly normalized, $\langle \Phi_{\rm BCS} |\Phi_{\rm BCS}\rangle = 1$.

Solution: The BCS ground state is given by

$$|\Phi_{\rm BCS}\rangle = \prod_{\boldsymbol{k}} \left(u_{\boldsymbol{k}} + v_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow} \right) |0\rangle \, .$$

Here, $|0\rangle$ is the vacuum and therefore $c_{\boldsymbol{k}\sigma} |0\rangle = \langle 0| c^\dagger_{\boldsymbol{k}\sigma} = 0$. Therefore,

$$\begin{aligned}
\langle \Phi_{\rm BCS} | \Phi_{\rm BCS}\rangle &= \langle 0| \prod_{\boldsymbol{k},\boldsymbol{k}'} \left(u^*_{\boldsymbol{k}'} + v^*_{\boldsymbol{k}'} c_{-\boldsymbol{k}'\downarrow} c_{\boldsymbol{k}'\uparrow} \right) \left(u_{\boldsymbol{k}} + v_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow} \right) |0\rangle \\
&= \prod_{\boldsymbol{k}} \left[u^*_{\boldsymbol{k}} u_{\boldsymbol{k}} + v^*_{\boldsymbol{k}} v_{\boldsymbol{k}} \langle 0| c_{-\boldsymbol{k}\downarrow} c_{\boldsymbol{k}\uparrow} c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow} |0\rangle \right] \\
&= \prod_{\boldsymbol{k}} \left(|u_{\boldsymbol{k}}|^2 + |v_{\boldsymbol{k}}|^2 \right)
\end{aligned}$$

where we have used that

$$\prod_{\boldsymbol{k},\boldsymbol{k}'} u^*_{\boldsymbol{k}'} u_{\boldsymbol{k}} = u^*_{\boldsymbol{k}_1} u^*_{\boldsymbol{k}_2} \cdots u^*_{\boldsymbol{k}_N} u_{\boldsymbol{k}_1} u_{\boldsymbol{k}_2} \cdots u_{\boldsymbol{k}_N} = \prod_{\boldsymbol{k}} |u_{\boldsymbol{k}}|^2 \, .$$

As you know from the lecture, $|u_{\boldsymbol{k}}|^2 + |v_{\boldsymbol{k}}|^2 = 1$. Hence $\Phi_{\rm BCS}$ is normalized.

(b) Calculate the expectation value of the electron number operator $N = \sum_{\boldsymbol{k}\sigma} c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}$ and its standard deviation in the ground state.

Solution: Let us evaluate the expectation values of $N_\uparrow = \sum_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\uparrow} c_{\boldsymbol{k}\uparrow}$ and $N_\downarrow = \sum_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\downarrow} c_{\boldsymbol{k}\downarrow}$ separately. It is convenient to express the electron operators in terms of the Bogoliubov operators,

$$c_{\boldsymbol{k}\sigma} = u_{\boldsymbol{k}} b_{\boldsymbol{k}\sigma} + \sigma v_k b^\dagger_{-\boldsymbol{k}-\sigma}; \quad c^\dagger_{\boldsymbol{k}\sigma} = u^*_{\boldsymbol{k}} b^\dagger_{\boldsymbol{k}\sigma} + \sigma v^*_k b_{-\boldsymbol{k}-\sigma};$$

such that we can use that $b_{\boldsymbol{k}\sigma} |\Phi_{\rm BCS}\rangle = 0$. It follows for the expectation values that

$$\begin{aligned}
\langle\Phi_{\rm BCS}| \hat{N}_\uparrow |\Phi_{\rm BCS}\rangle &= \sum_{\boldsymbol{k}} \langle\Phi_{\rm BCS}| \left(u^*_{\boldsymbol{k}} b^\dagger_{\boldsymbol{k}\uparrow} + v^*_{\boldsymbol{k}} b_{-\boldsymbol{k}\downarrow}\right) \left(u_{\boldsymbol{k}} b_{\boldsymbol{k}\uparrow} + v_{\boldsymbol{k}} b^\dagger_{-\boldsymbol{k}\downarrow}\right) |\Phi_{\rm BCS}\rangle \\
&= \sum_{\boldsymbol{k}} |v_{\boldsymbol{k}}|^2 \langle\Phi_{\rm BCS}| b_{-\boldsymbol{k}\downarrow} b^\dagger_{-\boldsymbol{k}\downarrow} |\Phi_{\rm BCS}\rangle = \sum_{\boldsymbol{k}} |v_{\boldsymbol{k}}|^2 , \\
\langle\Phi_{\rm BCS}| \hat{N}_\downarrow |\Phi_{\rm BCS}\rangle &= \sum_{\boldsymbol{k}} \langle\Phi_{\rm BCS}| \left(u^*_{\boldsymbol{k}} b^\dagger_{\boldsymbol{k}\downarrow} - v^*_{\boldsymbol{k}} b_{-\boldsymbol{k}\uparrow}\right) \left(u_{\boldsymbol{k}} b_{\boldsymbol{k}\downarrow} - v_{\boldsymbol{k}} b^\dagger_{-\boldsymbol{k}\uparrow}\right) |\Phi_{\rm BCS}\rangle \\
&= \sum_{\boldsymbol{k}} |v_{\boldsymbol{k}}|^2 \langle\Phi_{\rm BCS}| b_{-\boldsymbol{k}\downarrow} b^\dagger_{-\boldsymbol{k}\downarrow} |\Phi_{\rm BCS}\rangle = \sum_{\boldsymbol{k}} |v_{\boldsymbol{k}}|^2 .
\end{aligned}$$

Consequently, $\langle N\rangle = \langle N_\uparrow + N_\downarrow\rangle = 2\sum_{\boldsymbol{k}} |v_{\boldsymbol{k}}|^2$. Now let us calculate the expectation value of $N^2 = N_\uparrow^2 + N_\downarrow^2 + 2N_\uparrow N_\downarrow$:

$$\begin{aligned}
\langle\Phi_{\rm BCS}| N_\uparrow^2 |\Phi_{\rm BCS}\rangle &= \sum_{\boldsymbol{k},\boldsymbol{k}'} \Big\{ v^*_{\boldsymbol{k}} u^*_{\boldsymbol{k}} u_{\boldsymbol{k}'} v_{\boldsymbol{k}'} \langle\Phi_{\rm BCS}| b_{-\boldsymbol{k}\downarrow} b_{\boldsymbol{k}\uparrow} b^\dagger_{\boldsymbol{k}'\uparrow} b^\dagger_{-\boldsymbol{k}'\downarrow} |\Phi_{\rm BCS}\rangle \\
&\qquad + |v_{\boldsymbol{k}}|^2 |v_{\boldsymbol{k}'}|^2 \langle\Phi_{\rm BCS}| b_{-\boldsymbol{k}\downarrow} b^\dagger_{-\boldsymbol{k}\downarrow} b_{-\boldsymbol{k}'\downarrow} b^\dagger_{-\boldsymbol{k}'\downarrow} |\Phi_{\rm BCS}\rangle \Big\} \\
&= \sum_{\boldsymbol{k}} |u_{\boldsymbol{k}}|^2 |v_{\boldsymbol{k}}|^2 + \sum_{\boldsymbol{k},\boldsymbol{k}'} |v_{\boldsymbol{k}}|^2 |v_{\boldsymbol{k}'}|^2 \\
\langle\Phi_{\rm BCS}| N_\downarrow^2 |\Phi_{\rm BCS}\rangle &= \langle\Phi_{\rm BCS}| N_\uparrow^2 |\Phi_{\rm BCS}\rangle , \\
\langle\Phi_{\rm BCS}| N_\uparrow N_\downarrow |\Phi_{\rm BCS}\rangle &= \sum_{\boldsymbol{k},\boldsymbol{k}'} \Big\{ - v^*_{\boldsymbol{k}} u^*_{\boldsymbol{k}} u_{\boldsymbol{k}'} v_{\boldsymbol{k}'} \langle\Phi_{\rm BCS}| b_{-\boldsymbol{k}\downarrow} b_{\boldsymbol{k}\uparrow} b^\dagger_{\boldsymbol{k}'\downarrow} b^\dagger_{-\boldsymbol{k}'\uparrow} |\Phi_{\rm BCS}\rangle \\
&\qquad + |v_{\boldsymbol{k}}|^2 |v_{\boldsymbol{k}'}|^2 \langle\Phi_{\rm BCS}| b_{-\boldsymbol{k}\downarrow} b^\dagger_{-\boldsymbol{k}\downarrow} b_{-\boldsymbol{k}'\uparrow} b^\dagger_{-\boldsymbol{k}'\uparrow} |\Phi_{\rm BCS}\rangle \Big\} \\
&= \sum_{\boldsymbol{k}} |u_{\boldsymbol{k}}|^2 |v_{\boldsymbol{k}}|^2 + \sum_{\boldsymbol{k},\boldsymbol{k}'} |v_{\boldsymbol{k}}|^2 |v_{\boldsymbol{k}'}|^2 .
\end{aligned}$$

In total,

$$\langle\Phi_{\rm BCS}| \hat{N}^2 |\Phi_{\rm BCS}\rangle = 4\sum_{\boldsymbol{k},\boldsymbol{k}'} |v_{\boldsymbol{k}}|^2 |v_{\boldsymbol{k}'}|^2 + 4\sum_{\boldsymbol{k}} |u_{\boldsymbol{k}}|^2 |v_{\boldsymbol{k}}|^2$$

and the standard deviation is

$$\delta N = \sqrt{\langle N^2\rangle - \langle N\rangle^2} = 2\sqrt{\sum_{\boldsymbol{k}} |u_{\boldsymbol{k}}|^2 |v_{\boldsymbol{k}}|^2} .$$

(c) Let us define the operator of Cooper-pair creation, $B^\dagger_{\boldsymbol{k}} = c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow}$ (Not to be confused with the Bogoliubov operator $b_{\boldsymbol{k}}$!). Calculate the expectation value $< B^\dagger_{\boldsymbol{k}} >$ in the BCS ground state. Show that $< B^\dagger_{\boldsymbol{k}} >$ as a function of k has a maximum at the Fermi momentum ($\Delta(\boldsymbol{k}) \equiv \Delta \in \mathbb{R}$ for simplicity).

Solution:

$$\begin{aligned}
\langle\Phi_{\rm BCS}| c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow} |\Phi_{\rm BCS}\rangle &= \langle\Phi_{\rm BCS}| (u^*_{\boldsymbol{k}} b^\dagger_{\boldsymbol{k}\uparrow} + v^*_{\boldsymbol{k}} b_{-\boldsymbol{k}\downarrow})(u^*_{\boldsymbol{k}} b^\dagger_{-\boldsymbol{k}\downarrow} - v^*_{\boldsymbol{k}} b_{\boldsymbol{k}\uparrow}) |\Phi_{\rm BCS}\rangle \\
&= u^*_{\boldsymbol{k}} v^*_{\boldsymbol{k}} .
\end{aligned}$$

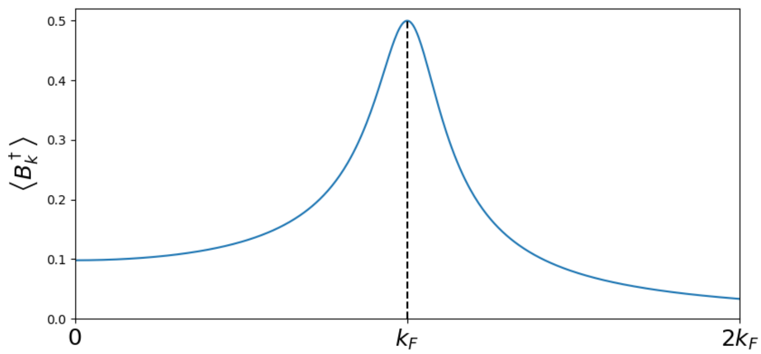

Figure 1: The expectation value of Cooper pair creation $\left\langle B_{\boldsymbol{k}}^\dagger \right\rangle$ in the BCS ground state for momentum-independent gap Δ.

You know from the lecture that

$$u_{\boldsymbol{k}} = \sqrt{\frac{1}{2}\left(1 + \frac{\xi_{\boldsymbol{k}}}{\sqrt{\xi_{\boldsymbol{k}}^2 + \Delta_{\boldsymbol{k}}^2}}\right)}, \qquad v_{\boldsymbol{k}} = \sqrt{\frac{1}{2}\left(1 - \frac{\xi_{\boldsymbol{k}}}{\sqrt{\xi_{\boldsymbol{k}}^2 + \Delta_{\boldsymbol{k}}^2}}\right)},$$

such that

$$\left\langle B_{\boldsymbol{k}}^\dagger \right\rangle = \frac{1}{2}\frac{|\Delta|}{\sqrt{\xi_{\boldsymbol{k}}^2 + \Delta^2}} = \frac{1}{2}\frac{|\Delta|}{\sqrt{\left(\hbar^2 k^2/(2m) - \mu\right)^2 + \Delta^2}}$$

The Fermi momentum is related to μ by $k_F = \sqrt{2m\mu}/\hbar$ and $\xi_{|\boldsymbol{k}|=k_F} = 0$. We find that

$$\frac{\partial}{\partial k}\left\langle B_{\boldsymbol{k}}^\dagger \right\rangle = \frac{\hbar^2 k}{2m}\frac{\partial}{\partial \xi}\frac{|\Delta|}{\sqrt{\xi^2 + \Delta^2}} = -\frac{\hbar^2 k}{2m}|\Delta|\frac{\xi}{(\xi^2 + \Delta^2)^{3/2}}$$

and therefore

$$\frac{\partial}{\partial k}\left\langle B_{\boldsymbol{k}}^\dagger \right\rangle\bigg|_{|\boldsymbol{k}|=k_F} = -\frac{\hbar^2 k_F}{2m}|\Delta|\frac{\xi}{(\xi^2 + \Delta^2)^{3/2}}\bigg|_{\xi=0} = 0.$$

There is only one other local extremum ($k = 0$). On the one hand,

$$\left\langle B_{\boldsymbol{k}}^\dagger \right\rangle_{k=0} = \frac{1}{2}\frac{|\Delta|}{\sqrt{\mu^2 + \Delta^2}} < \left\langle B_{\boldsymbol{k}}^\dagger \right\rangle_{k=k_F} = \frac{1}{2}$$

and on the other hand $\left\langle B_{\boldsymbol{k}}^\dagger \right\rangle \to 0$ as $k \to \infty$. Therefore, $k = k_F$ must be a local maximum and also the global maximum of the function (cf. Fig. 1). Pair creation therefore happens mostly at k_F. Note that the same behavior is found in the standard deviation of the particle number (previous subtask), which is of course related to the Cooper pair formation.

(d) Calculate the commutators $[B_{\boldsymbol{k}}, B_{\boldsymbol{k}'}^\dagger]$, $[B_{\boldsymbol{k}}, B_{\boldsymbol{k}'}]$, and $[B_{\boldsymbol{k}}^\dagger, B_{\boldsymbol{k}'}^\dagger]$ and their ground-state expectation values. Decide whether Cooper pairs are bosons.

Solution: It is easy to see that

$$[B_{\boldsymbol{k}}, B_{\boldsymbol{k}'}] = \left[B^\dagger_{\boldsymbol{k}}, B^\dagger_{\boldsymbol{k}'}\right] = 0$$

because all involved electron operators anticommute with each other. This agrees with the bosonic commutation relations $[a_k, a_{k'}] = [a^\dagger_k, a^\dagger_{k'}] = 0$. For the remaining commutator, we find

$$\left[B_{\boldsymbol{k}}, B^\dagger_{\boldsymbol{k}'}\right] = \left[c_{-\boldsymbol{k}\downarrow}c_{\boldsymbol{k}\uparrow},\, c^\dagger_{\boldsymbol{k}\uparrow}c^\dagger_{-\boldsymbol{k}\downarrow}\right] = \delta_{\boldsymbol{k}\boldsymbol{k}'}\left(1 - c^\dagger_{-\boldsymbol{k}\downarrow}c_{-\boldsymbol{k}\downarrow} - c^\dagger_{\boldsymbol{k}\uparrow}c_{\boldsymbol{k}\uparrow}\right) = \delta_{\boldsymbol{k}\boldsymbol{k}'}\left(1 - N_{\boldsymbol{k}}\right)$$

with the expectation value [see part (b) for $\langle N\rangle$]

$$\left\langle\left[B_{\boldsymbol{k}}, B^\dagger_{\boldsymbol{k}'}\right]\right\rangle = \delta_{\boldsymbol{k}\boldsymbol{k}'}\left(1 - |v_{\boldsymbol{k}}|^2 - |v_{-\boldsymbol{k}}|^2\right).$$

If $\boldsymbol{k} = \boldsymbol{k}'$, we obtain $\left\langle\left[B_{\boldsymbol{k}}, B^\dagger_{\boldsymbol{k}'}\right]\right\rangle < 1$ whenever $|v|^2 \neq 0$, i.e., whenever $\Delta \neq 0$ (always in the superconducting phase). Thus, Cooper pairs are not bosons.

Category B

2. 4-component Nambu spinor with spin-orbit coupling (15 bonus points)

Let us generalize the 2×2 Nambu matrix formalism (see lecture notes) to explicitly spin-dependent cases, where $\xi_{\boldsymbol{k}}$ in the mean-field Hamiltonian is replaced by $h_0(\boldsymbol{k}) = \xi_{\boldsymbol{k}} + \mathbf{b}_{\boldsymbol{k}} \cdot \boldsymbol{\sigma}$ with a vector $\mathbf{b}_{\boldsymbol{k}}$. Thus, h_0 is a 2×2 matrix in spin space. Let us define the 4-Nambu spinor $\left(c^\dagger_{k,\uparrow}, c^\dagger_{k,\downarrow}, c_{-k,\downarrow}, -c_{-k,\uparrow}\right)$. Find the corresponding 4×4 Hamiltonian.
Remark: Note that this Hamiltonian is redundant. If terms can be expressed through more than one matrix element, distribute them evenly between these elements.

Solution:

The standard mean-field Hamiltonian reads in the 2×2 basis (see lecture notes)

$$H = \sum_{\mathbf{k}} \begin{pmatrix} c^\dagger_{\mathbf{k},\uparrow} & c_{-\mathbf{k},\downarrow}\end{pmatrix} \begin{pmatrix} \xi_k & -\Delta \\ -\Delta^* & -\xi_k \end{pmatrix} \begin{pmatrix} c_{\mathbf{k},\uparrow} \\ c^\dagger_{-\mathbf{k},\downarrow}\end{pmatrix}.$$

making the dispersion relation spin dependent, as specified in the task we obtain

$$H \to \sum_{\mathbf{k}} \begin{pmatrix} c^\dagger_{\mathbf{k},\uparrow} & c_{-\mathbf{k},\downarrow}\end{pmatrix} \begin{pmatrix} \xi_k & -\Delta \\ -\Delta^* & -\xi_k \end{pmatrix} \begin{pmatrix} c_{\mathbf{k},\uparrow} \\ c^\dagger_{-\mathbf{k},\downarrow}\end{pmatrix} + \sum_{\mathbf{k}} \begin{pmatrix} c^\dagger_{\mathbf{k},\uparrow} & c^\dagger_{\mathbf{k},\downarrow}\end{pmatrix} \boldsymbol{\sigma}\mathbf{b}_{\mathbf{k}} \begin{pmatrix} c_{\mathbf{k},\uparrow} \\ c_{\mathbf{k},\downarrow}\end{pmatrix}.$$

With

$$\boldsymbol{\sigma}\mathbf{b}_{\mathbf{k}} = \begin{pmatrix} b_{3,\mathbf{k}} & b_{1,\mathbf{k}} - \mathrm{i}b_{2,\mathbf{k}} \\ b_{1,\mathbf{k}} + \mathrm{i}b_{2,\mathbf{k}} & -b_{3,\mathbf{k}} \end{pmatrix}$$

and a new spinor basis for the Hamiltonian

$$\begin{pmatrix} c^\dagger_{\mathbf{k},\uparrow} & c^\dagger_{\mathbf{k},\downarrow} & c_{-\mathbf{k},\downarrow} & -c_{-\mathbf{k},\uparrow}\end{pmatrix}$$

we find

$$H = \sum_{\mathbf{k}} \begin{pmatrix} c^\dagger_{\mathbf{k},\uparrow} & c^\dagger_{\mathbf{k},\downarrow} & c_{-\mathbf{k},\downarrow} & -c_{-\mathbf{k},\uparrow}\end{pmatrix} \begin{pmatrix} \xi_k + b_{3,\mathbf{k}} & b_{1,\mathbf{k}} - \mathrm{i}b_{2,\mathbf{k}} & -\Delta & 0 \\ b_{1,\mathbf{k}} + \mathrm{i}b_{2,\mathbf{k}} & \xi_k - b_{3,\mathbf{k}} & 0 & 0 \\ -\Delta^* & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} c_{\mathbf{k},\uparrow} \\ c_{\mathbf{k},\downarrow} \\ c^\dagger_{-\mathbf{k},\downarrow} \\ -c^\dagger_{-\mathbf{k},\uparrow}\end{pmatrix}.$$

Distributing everything evenly, as demanded in the task:

$$H = \sum_{\mathbf{k}} \begin{pmatrix} c^\dagger_{\mathbf{k},\uparrow} & c^\dagger_{\mathbf{k},\downarrow} & c_{-\mathbf{k},\downarrow} & -c_{-\mathbf{k},\uparrow} \end{pmatrix} \tilde{\mathcal{H}}(\boldsymbol{k}) \begin{pmatrix} c_{\mathbf{k},\uparrow} \\ c_{\mathbf{k},\downarrow} \\ c^\dagger_{-\mathbf{k},\downarrow} \\ -c^\dagger_{-\mathbf{k},\uparrow} \end{pmatrix} + \frac{1}{2}\sum_k \xi_k$$

$$\tilde{\mathcal{H}}(\boldsymbol{k}) = \frac{1}{2}\begin{pmatrix} \xi_k + b_{3,\mathbf{k}} & b_{1,\mathbf{k}} - \mathrm{i}b_{2,\mathbf{k}} & -\Delta & 0 \\ b_{1,\mathbf{k}} + \mathrm{i}b_{2,\mathbf{k}} & \xi_k - b_{3,\mathbf{k}} & 0 & -\Delta \\ -\Delta^* & 0 & -\xi_{-k} + b_{3,-\mathbf{k}} & b_{1,-\mathbf{k}} - \mathrm{i}b_{2,-\mathbf{k}} \\ 0 & -\Delta^* & b_{1,-\mathbf{k}} + \mathrm{i}b_{2,-\mathbf{k}} & -\xi_{-k} - b_{3,-\mathbf{k}} \end{pmatrix}.$$