Karlsruher Institut für Technologie

Institut für Theorie der Kondensierten Materie

Exercises for "Superconductivity, Josephson ..." WS 2023/2024

Prof. Dr. A. Shnirman

Dr. K. Piasotski

Exercise 2: Solution

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1. **Expectation value of operators in the BCS ground state: (30 Points)**

   Following the dream team of Bardeen, Cooper, and Schrieffer, in the class we considered the following family of states as our variational ansatz for the ground state of the BCS Hamiltonian:

$$|\mathbf{BCS}\rangle = \prod_k \left(u_k + v_k c^\dagger_{k,\,\uparrow} c^\dagger_{-k,\,\downarrow} \right) |0\rangle \,. \tag{1}$$

   Here $|0\rangle$ is the Fermionic vacuum state $c_{k,\sigma}|0\rangle = 0$, $c^\dagger_{k,\sigma}$ and $c_{k,\sigma}$ are the Fermionic creation and annihilation operators obeying the standard canonical commutation relations

$$\{c_{k,\sigma},\ c_{k',\sigma'}\} = \{c^\dagger_{k,\sigma},\ c^\dagger_{k',\sigma'}\} = 0, \quad \{c_{k,\sigma},\ c^\dagger_{k',\sigma'}\} = \delta_{k,k'}\delta_{\sigma,\sigma'}. \tag{2}$$

   Prove the following result

$$\left\langle \mathbf{BCS} \middle| c^\dagger_{k',\uparrow} c^\dagger_{-k',\downarrow} c_{-k,\downarrow} c_{k,\uparrow} \middle| \mathbf{BCS} \right\rangle = u_k v_k u_{k'} v_{k'}. \tag{3}$$

One has

$$
\begin{aligned}
&\left\langle \mathrm{BCS} \middle| c^\dagger_{k',\uparrow} c^\dagger_{-k',\downarrow} c_{-k,\downarrow} c_{k,\uparrow} \middle| \mathrm{BCS} \right\rangle \\
=& \langle 0| \prod_{k_2 \neq k} \left(u_{k_2} + v_{k_2} c_{k_2,\,\uparrow} c_{-k_2,\,\downarrow} \right) \\
&\times \left(u_k + v_k c_{k,\,\uparrow} c_{-k,\,\downarrow} \right) c^\dagger_{k',\uparrow} c^\dagger_{-k',\downarrow} c_{-k,\downarrow} c_{k,\uparrow} \left(u_k + v_k c^\dagger_{k,\,\uparrow} c^\dagger_{-k,\,\downarrow} \right) \\
&\times \prod_{k_1 \neq k} \left(u_{k_1} + v_{k_1} c^\dagger_{k_1,\,\uparrow} c^\dagger_{-k_1,\,\downarrow} \right) |0\rangle \\
=& v_k \langle 0| \prod_{k_2 \neq k} \left(u_{k_2} + v_{k_2} c_{k_2,\,\uparrow} c_{-k_2,\,\downarrow} \right) \left(u_k c^\dagger_{k',\uparrow} c^\dagger_{-k',\downarrow} + v_k c_{k,\,\uparrow} c_{-k,\,\downarrow} c^\dagger_{k',\uparrow} c^\dagger_{-k',\downarrow} \right) \\
&\times \prod_{k_1 \neq k} \left(u_{k_1} + v_{k_1} c^\dagger_{k_1,\,\uparrow} c^\dagger_{-k_1,\,\downarrow} \right) |0\rangle \\
=& v_k u_k \langle 0| \prod_{k_2 \neq k,k'} \left(u_{k_2} + v_{k_2} c_{k_2,\,\uparrow} c_{-k_2,\,\downarrow} \right) \left(u_{k'} + v_{k'} c_{k',\,\uparrow} c_{-k',\,\downarrow} \right) c^\dagger_{k',\uparrow} c^\dagger_{-k',\downarrow} \\
&\times \left(u_{k'} + v_{k'} c^\dagger_{k',\,\uparrow} c^\dagger_{-k',\,\downarrow} \right) \prod_{k_1 \neq k} \left(u_{k_1} + v_{k_1} c^\dagger_{k_1,\,\uparrow} c^\dagger_{-k_1,\,\downarrow} \right) |0\rangle
\end{aligned}
$$

$$
\begin{aligned}
=&v_k u_k u_{k'} v_{k'} \langle 0| \prod_{k_2 \neq k,k'} (u_{k_2} + v_{k_2} c_{k_2,\uparrow} c_{-k_2,\downarrow})\, c_{k',\uparrow} c_{-k',\downarrow} c^\dagger_{k',\uparrow} c^\dagger_{-k',\downarrow} \\
&\times \prod_{k_1 \neq k,k'} \left(u_{k_1} + v_{k_1} c^\dagger_{k_1,\uparrow} c^\dagger_{-k_1,\downarrow} \right) |0\rangle \\
=&v_k u_k u_{k'} v_{k'} \langle 0| \prod_{k_2 \neq k,k'} (u_{k_2} + v_{k_2} c_{k_2,\uparrow} c_{-k_2,\downarrow}) \prod_{k_1 \neq k,k'} \left(u_{k_1} + v_{k_1} c^\dagger_{k_1,\uparrow} c^\dagger_{-k_1,\downarrow} \right) |0\rangle \\
=&v_k u_k u_{k'} v_{k'} \langle 0| \prod_{k_1 \neq k,k'} (u^2_{k_1} + v^2_{k_1})\, |0\rangle = v_k u_k u_{k'} v_{k'} . \qquad (4)
\end{aligned}
$$

2. **Generalized Cooper problem: (35 Points)**

In the lecture we have considered the Cooper problem, in which two electrons are created on top of the full Fermi sea. Consider now a generalized Cooper problem. In this case the excited state is assumed to be a superposition of either of two electrons slightly above the Fermi level or of two holes slightly below the Fermi level (the total number of particles is, thus, not sharply defined). Note that in the grand-canonical description the energies of both electrons and holes are positive. Find the bound state wave function and the binding energy per particle Δ. Compare with Δ of the Cooper problem and with Δ of the BCS theory.

Analogously to script we assume the following Ansatz for the wave function

$$
|\Psi\rangle = \sum_{-\hbar\omega_D < \xi_k < 0} \alpha(k) \chi(\sigma_1, \sigma_2) c_{-k,\sigma_2} c_{k,\sigma_1} |\Psi_0\rangle + \sum_{0 < \xi_k < \hbar\omega_D} \alpha(k) \chi(\sigma_1, \sigma_2) c^\dagger_{k,\sigma_1} c^\dagger_{-k,\sigma_2} |\Psi_0\rangle , \qquad (5)
$$

where $|\Psi_0\rangle = \prod_{k \le k_F} c^\dagger_{k,\sigma} |0\rangle$ stands for the fully occupied Fermi sea, and $\xi_k \equiv \epsilon_k - \mu$. In contrast to the script the wave function (5) includes the hole-like ($\xi_k < 0$) excitation as well as the electron-like ($\xi_k > 0$) ones.

The (BCS) Hamiltonian reads

$$
H_{\text{BCS}} = \sum_{k,\sigma} \epsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} - \frac{1}{2} \frac{g}{V} \sum_{k,k',\sigma} c^\dagger_{k',\sigma} c^\dagger_{-k',-\sigma} c_{-k,-\sigma} c_{k,\sigma} . \qquad (6)
$$

Substituting the Ansatz (5) into the Schrödinger equation $(E + E_{\text{FS}}) |\Psi\rangle = H_{\text{BCS}} |\Psi\rangle$[1] we obtain:

$$
(2\text{sign}(\xi_k)\epsilon_k - E)\, \alpha(k) = \frac{g}{V} \sum_{-\hbar\omega_D < \xi_{k_1} < \hbar\omega_D} \alpha(k_1) . \qquad (7)
$$

Here $\alpha(k)$ for $\xi_k < 0$ describes hole-like excitations und for $\xi_k > 0$ it describes the particle-like excitations. We introduce again

$$
C = \frac{1}{V} \sum_{-\hbar\omega_D < \xi_{k_1} < \hbar\omega_D} \alpha(k) , \qquad (8)
$$

[1]The energy of particles is measured relative to the filled Fermi sphere $E_{\text{FS}} = 2 \sum_{k \le k_F} \epsilon_k$.

substitute it self-consistently and obtain the equation for E

$$1 = \frac{g}{2}\int_{E_F}^{E_F+\hbar\omega_D} d\omega \frac{\rho(\omega)}{\omega - E/2} - \frac{g}{2}\int_{E_F-\hbar\omega_D}^{E_F} d\omega \frac{\rho(\omega)}{\omega + E/2}$$
$$= \frac{g\rho_F}{2}\log\left(\frac{E_F + (\hbar\omega_D - E/2)}{E_F - E/2}\right) + \frac{g\rho_F}{2}\log\left(\frac{E_F - (\hbar\omega_D - E/2)}{E_F + E/2}\right). \tag{9}$$

Here we have used $1/V\sum_k \to \int \rho(\omega)d\omega$. The density of states in the vicinity of the Fermi surface can be replaced by a constant one $\rho(\omega) \approx \rho_F$.

it follows that

$$\frac{2}{g\rho_F} = \log\left(\frac{E_F^2 - (\hbar\omega_D - E/2)^2}{E_F^2 - E^2/4}\right) \tag{10}$$

Thus for weak coupling $g\rho_F \ll 1$, under the usual condition $E_F \gg \hbar\omega_D$, we obtain

$$E \simeq 2E_F - 2\hbar\omega_D e^{-\frac{1}{g\rho_F}} \tag{11}$$

The binding energy per electron is then found from $E = 2E_F - 2\Delta$

$$\Delta = \hbar\omega_D e^{-\frac{1}{g\rho_F}} \tag{12}$$

(In the script is was $\Delta = \hbar\omega_D e^{-\frac{2}{g\rho_F}}$)

3. **Better intuition behind the Bogulubov buisness: (35 Points)**

Part1: Constructive transformation of the field operators

Consider the following toy Hamiltonian

$$H = \epsilon(c_\uparrow^\dagger c_\uparrow + c_\downarrow^\dagger c_\downarrow) + V(c_\uparrow^\dagger c_\downarrow^\dagger + c_\downarrow c_\uparrow), \tag{13}$$

with the single mode Fermionic field operators

$$\{c_\sigma,\ c_{\sigma'}\} = \{c_\sigma^\dagger,\ c_{\sigma'}^\dagger\} = 0, \quad \{c_\sigma,\ c_{\sigma'}^\dagger\} = \delta_{\sigma,\sigma'}. \tag{14}$$

Defining the following objects

$$J_+ = c_\uparrow^\dagger c_\downarrow^\dagger, \quad J_- = c_\downarrow c_\uparrow, \quad J_z = \frac{1}{2}(N-1), \quad N = n_\uparrow + n_\downarrow, \quad n_\sigma = c_\sigma^\dagger c_\sigma, \tag{15}$$

demonstrate the following relations hold:

$$[J_+,\ J_-] = 2J_z, \quad [J_\pm,\ J_z] = \mp J_\pm. \tag{16}$$

One has

$$\begin{aligned}[J_+,\ J_-] =& c_\uparrow^\dagger c_\downarrow^\dagger c_\downarrow c_\uparrow - c_\downarrow c_\uparrow c_\uparrow^\dagger c_\downarrow^\dagger \\ =& n_\uparrow n_\downarrow - (1-n_\uparrow)(1-n_\downarrow) \\ =& n_\uparrow + n_\downarrow - 1 = N - 1 \equiv 2J_z.\end{aligned} \tag{17}$$

Next

$$[J_+,\ J_z] = \frac{1}{2} c^\dagger_\uparrow c^\dagger_\downarrow (c^\dagger_\uparrow c_\uparrow + c^\dagger_\downarrow c_\downarrow) - \frac{1}{2}(c^\dagger_\uparrow c_\uparrow + c^\dagger_\downarrow c_\downarrow) c^\dagger_\uparrow c^\dagger_\downarrow$$
$$= -\frac{1}{2}(c^\dagger_\uparrow c^\dagger_\downarrow + c^\dagger_\uparrow c^\dagger_\downarrow) = -J_+. \tag{18}$$

Using $J_+ = J_-^\dagger$ we naturally obtain

$$[J_-,\ J_z] = J_-.$$

In other words, we may assert that the operators $J_x = \frac{1}{2}(J_+ + J_-)$, $J_y = \frac{1}{2i}(J_+ - J_-)$, and J_z form a representation of the $\mathfrak{su}(2)$ Lie algebra (note that the representation is reducible since the parity operator $e^{i\pi N}$ is conserved).

Using our definitions (15) we write the Hamiltonian in the language of Js:

$$H = 2(\epsilon J_z + V J_x) + \epsilon = 2\sqrt{\epsilon^2 + V^2}(\cos\vartheta J_z + \sin\vartheta J_x) + \epsilon, \tag{19}$$
$$\cos\vartheta = \frac{\epsilon}{\sqrt{\epsilon^2 + V^2}}, \quad \sin\vartheta = \frac{V}{\sqrt{\epsilon^2 + V^2}}. \tag{20}$$

Show that the Hamiltonian (19) is diagonalised by the following unitary transformation $U = e^{i\vartheta J_y}$, that is

$$H_d = UHU^\dagger = 2\sqrt{\epsilon^2 + V^2} J_z + \epsilon. \tag{21}$$

Let us check the inverse transformation

$$U^\dagger J_z U = \cos\vartheta J_z + \sin\vartheta J_x \tag{22}$$

with the help of Baker-Campbell-Hausdor (BCH) formula

$$e^{-i\vartheta J_y} J_z e^{i\vartheta J_y} = \sum_{n=0}^{\infty} (-i\vartheta)^n \frac{[(J_y)^n,\ J_z]}{n!} \tag{23}$$

where the notation is such that

$$[(J_y)^n,\ J_z] = \big[J_y,\ [(J_y)^{n-1},\ J_z]\big] \tag{24}$$

and evaluate

$$\big[(J_y)^{2m},\ J_z\big] = \big[J_y,\ \big[(J_y)^{2m-1},\ J_z\big]\big] = J_z, \tag{25}$$
$$\big[(J_y)^{2m+1},\ J_z\big] = \big[J_y,\ \big[(J_y)^{2m},\ J_z\big]\big] = iJ_x. \tag{26}$$

So that:

$$e^{-i\vartheta J_y} J_z e^{i\vartheta J_y} = J_z \sum_{n=0}^{\infty} \frac{(-1)^n \vartheta^{2n}}{(2n)!} + J_x \sum_{n=0}^{\infty} \frac{(-1)^n \vartheta^{2n+1}}{(2n+1)!} = \cos\vartheta J_z + \sin\vartheta J_x. \tag{27}$$

Next we define the Bogolubov operators

$$\gamma_\sigma = U^\dagger c_\sigma U, \quad \gamma^\dagger_\sigma = U^\dagger c^\dagger_\sigma U \equiv (\gamma_\sigma)^\dagger. \tag{28}$$

These guys are helpful since by virtue of Eq. (21) **we have**

$$H = U^\dagger H_d U = 2\sqrt{\epsilon^2 + V^2}U^\dagger J_z U + \epsilon = \sqrt{\epsilon^2 + V^2}(\gamma_\uparrow^\dagger \gamma_\uparrow + \gamma_\downarrow^\dagger \gamma_\downarrow) + \epsilon - \sqrt{\epsilon^2 + V^2}. \quad (29)$$

Using BCH formula, or otherwise, show that

$$\gamma_\uparrow = \cos\frac{\vartheta}{2}c_\uparrow + \sin\frac{\vartheta}{2}c_\downarrow^\dagger, \quad \gamma_\downarrow = \cos\frac{\vartheta}{2}c_\downarrow - \sin\frac{\vartheta}{2}c_\uparrow^\dagger. \quad (30)$$

In the same notations as before we have

$$\gamma_\sigma = U^\dagger c_\sigma U = \sum_{n=0}^{\infty} \left(-\frac{\theta}{2}\right)^n \frac{[(2iJ_y)^n,\ c_\sigma]}{n!}. \quad (31)$$

First we establish

$$[2iJ_y,\ c_\uparrow] = -\,c_\downarrow^\dagger, \quad [2iJ_y,\ c_\downarrow] = c_\uparrow^\dagger, \quad (32)$$

$$\left[2iJ_y,\ c_\uparrow^\dagger\right] = -\,c_\downarrow, \quad \left[2iJ_y,\ c_\downarrow^\dagger\right] = c_\uparrow. \quad (33)$$

Or, introducing the secular notation, $\sigma = \uparrow \equiv +$ and $\sigma = \downarrow \equiv -$, we compactly write

$$[2iJ_y,\ c_\sigma] = -\,\sigma c_{-\sigma}^\dagger, \quad \left[2iJ_y,\ c_\sigma^\dagger\right] = -\sigma c_{-\sigma}. \quad (34)$$

It follows that

$$\left[(2iJ_y)^{2m},\ c_\sigma\right] = \left[2iJ_y, \left[(2iJ_y)^{2m-1},\ c_\sigma\right]\right] = (-1)^m c_\sigma, \quad (35)$$

$$\left[(2iJ_y)^{2m+1},\ c_\sigma\right] = \left[2iJ_y, \left[(2iJ_y)^{2m},\ c_\sigma\right]\right] = -(-1)^m \sigma c_{-\sigma}^\dagger, \quad (36)$$

and hence

$$\gamma_\sigma = c_\sigma \sum_{m=0}^{\infty} \left(\frac{\vartheta}{2}\right)^{2m} \frac{(-1)^m}{(2m)!} + \sigma c_{-\sigma}^\dagger \sum_{m=0}^{\infty} \left(\frac{\vartheta}{2}\right)^{2m+1} \frac{(-1)^m}{(2m+1)!} \quad (37)$$

$$= c_\sigma \cos\frac{\vartheta}{2} + \sigma c_{-\sigma}^\dagger \cos\frac{\vartheta}{2}, \quad (38)$$

exactly what we wanted to show.

Part2: BCS ground state

The ground state is defined via the following condition

$$\gamma_\sigma \left|0\right\rangle_\gamma = 0. \quad (39)$$

Show that this implies the following relation

$$U \left|0\right\rangle_\gamma = \left|0\right\rangle, \quad (40)$$

where

$$c_\sigma \left|0\right\rangle = 0, \quad (41)$$

is the vacuum state of original Fermions.

Consider the following representation

$$U^\dagger = e^{-i\vartheta J_y} = e^{a_+ J_+} e^{a_z J_z} e^{a_- J_-}, \tag{42}$$

where $a_\pm,\ a_z$ **are functions of the angle** ϑ**. By differentiating the Eq.** (42) **with respect to** ϑ**, establish the following system of non-linear differential equations**

$$\frac{d}{d\vartheta}a_+ = -\frac{1}{2}e^{a_z}, \quad \frac{d}{d\vartheta}a_z = a_-, \quad \frac{d}{d\vartheta}a_- = \frac{1}{2}(1+a_-^2), \tag{43}$$

$$a_+(0) = a_-(0) = a_z(0) = 0. \tag{44}$$

Applying the derivative we find

$$\begin{aligned}\frac{d}{d\vartheta}U^\dagger =& -iU^\dagger J_y = e^{a_+J_+}e^{a_zJ_z}e^{a_-J_-}\dot{a}_-J_- + e^{a_+J_+}e^{a_zJ_z}\dot{a}_zJ_ze^{a_-J_-} + e^{a_+J_+}\dot{a}_+J_+e^{a_zJ_z}e^{a_-J_-}\\ =& U^\dagger J_-\dot{a}_- + U^\dagger e^{-a_-J_-}J_ze^{a_-J_-}\dot{a}_z + U^\dagger e^{-a_-J_-}e^{-a_zJ_z}J_+e^{a_zJ_z}e^{a_-J_-}\dot{a}_+.\end{aligned} \tag{45}$$

It follows that

$$-iJ_y = J_-\dot{a}_- + e^{-a_-J_-}J_ze^{a_-J_-}\dot{a}_z + e^{-a_-J_-}e^{-a_zJ_z}J_+e^{a_zJ_z}e^{a_-J_-}\dot{a}_+. \tag{46}$$

Now we consider

$$e^{-a_-J_-}J_ze^{a_-J_-} = J_z - a_-[J_-, J_z] = J_z - a_-J_-, \tag{47}$$

$$e^{-a_zJ_z}J_+e^{a_zJ_z} = J_+e^{-a_z}, \tag{48}$$

$$e^{-a_-J_-}J_+e^{a_-J_-} = J_+ + 2a_-J_z - a_-^2J_-. \tag{49}$$

The equality (46) is now

$$-\frac{1}{2}[J_+ - J_-] = J_-\dot{a}_- + (J_z - a_-J_-)\dot{a}_z + (J_+ + 2a_-J_z - a_-^2J_-)e^{-a_z}\dot{a}_+. \tag{50}$$

Which yields the following system of ODEs

$$\frac{d}{d\vartheta}a_+ = -\frac{1}{2}e^{a_z}, \quad \frac{d}{d\vartheta}a_z = a_-, \quad \frac{d}{d\vartheta}a_- = \frac{1}{2}(1+a_-^2), \tag{51}$$

$$a_+(0) = a_-(0) = a_z(0) = 0, \tag{52}$$

with the initial conditions deduced from the requirement

$$U^\dagger\Big|_{\vartheta=0} = 1. \tag{53}$$

Show that these are solved by

$$a_\pm(\vartheta) = \mp\tan\frac{\vartheta}{2}, \quad a_z(\vartheta) = -2\log\cos\frac{\vartheta}{2}. \tag{54}$$

Equation (49) is solved by direct integration

$$\frac{da_-}{d\vartheta} = \frac{1}{2}(1+a_-^2) \implies \int^{a_-}\frac{dy}{1+y^2} = \frac{1}{2}(\vartheta-\vartheta_0) \tag{55}$$

$$\implies \arctan(a_-) = \frac{1}{2}(\vartheta-\vartheta_0) \implies a_-(\vartheta) = \tan\left(\frac{\vartheta}{2}\right), \tag{56}$$

where the integration constant is fixed by the initial conditions. Other equations yield

$$a_z(\vartheta) = \int_0^{\vartheta} d\vartheta' \tan\left(\frac{\vartheta'}{2}\right) = -2\ln\left(\cos\frac{\vartheta}{2}\right), \tag{57}$$

$$a_+(\vartheta) = -\frac{1}{2}\int_0^{\vartheta} d\vartheta' e^{-2\ln\left(\cos\frac{\vartheta'}{2}\right)} = -\tan\left(\frac{\vartheta}{2}\right). \tag{58}$$

Using the equation (40) **along with the decomposition** (42) **and the result** (54)**, prove that**

$$|0\rangle_{\gamma} = (1 + a_+ J_+) e^{-\frac{1}{2}a_z} |0\rangle \equiv \left(\cos\frac{\vartheta}{2} - \sin\frac{\vartheta}{2} c_{\uparrow}^{\dagger} c_{\downarrow}^{\dagger}\right) |0\rangle . \tag{59}$$

To see this we consider

$$\begin{aligned} U^{\dagger} |0\rangle =& e^{a_+ J_+} e^{a_z J_z} e^{a_- J_-} |0\rangle = e^{a_+ J_+} e^{a_z J_z} |0\rangle = e^{a_+ J_+} e^{\frac{1}{2}a_z (N-1)} |0\rangle = e^{-\frac{a_z}{2}} e^{a_+ J_+} |0\rangle \\ =& e^{-\frac{a_z}{2}} (1 + a_+ J_+) |0\rangle , \end{aligned} \tag{60}$$

where we used that $J_+^2 |0\rangle = 0$. Now substituting the results of our previous consideration we find that

$$|0\rangle_{\gamma} = \left(\cos\frac{\vartheta}{2} - \sin\frac{\vartheta}{2} c_{\uparrow}^{\dagger} c_{\downarrow}^{\dagger}\right) |0\rangle . \tag{61}$$