Condensed Matter - HW 11 :: BCS theory

PHSX 545

Problem 1

The Cooper pair wave function for a triplet state is given by rank-2 spinor

$$\psi(\mathbf{k}) = \mathbf{\Delta}(\mathbf{k}) \cdot [i\boldsymbol{\sigma}\sigma_y]\,,$$

where $\mathbf{\Delta}(\mathbf{k})$ is the vector gap function in momentum space, and $\sigma_{x,y,z}$ are Pauli matrices. Show that the expectation value for the spin of the pair is:

$$\mathbf{S} = \langle \hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2 \rangle = i\hbar \int \frac{d^3k}{(2\pi)^3} \;\cdots \times \mathbf{\Delta}(\mathbf{k})$$

and determine the missing piece to go in place of the $\ldots$.

Problem 2

The mean-field Hamiltonian in the BCS theory can be written as:

$$\mathcal{H} = E_0^{mf} + \sum_{\mathbf{k}} h_{\mathbf{k}} \qquad\qquad h_{\mathbf{k}} = \xi_{\mathbf{k}}(a^\dagger_{\mathbf{k}\uparrow}a_{\mathbf{k}\uparrow} + a^\dagger_{-\mathbf{k}\downarrow}a_{-\mathbf{k}\downarrow}) - (\Delta_{\mathbf{k}}a^\dagger_{\mathbf{k}\uparrow}a^\dagger_{-\mathbf{k}\downarrow} + \Delta^*_{\mathbf{k}}a_{-\mathbf{k}\downarrow}a_{\mathbf{k}\uparrow})$$

with $E_0^{mf} = \sum_{\mathbf{k}} \Delta^*_{\mathbf{k}}\langle a_{-\mathbf{k}\downarrow}a_{\mathbf{k}\uparrow}\rangle$.

For each pair $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ consider a basis in Fock space made up of 4 states: $|\, n_{\mathbf{k}\uparrow}, n_{-\mathbf{k}\downarrow}\,\rangle = (|\,0,0\,\rangle, |\,1,0\,\rangle, |\,0,1\,\rangle, |\,1,1\,\rangle)$.

(a) By acting with $h_{\mathbf{k}}$ on $|\, n_{\mathbf{k}\uparrow}, n_{-\mathbf{k}\downarrow}\,\rangle$ show that this is a complete set of states (no new states appear). Find the eigenstates of $h_{\mathbf{k}}$ in terms of $|\, n_{\mathbf{k}\uparrow}, n_{-\mathbf{k}\downarrow}\,\rangle$ and their energies. Properly normalize them.

(b) Write the state with the lowest energy in the form $|\,BCS\,\rangle = u_{\mathbf{k}}|\,0,0\,\rangle + v_{\mathbf{k}}|\,1,1\,\rangle$. Determine $u_{\mathbf{k}}, v_{\mathbf{k}}$. Show that operator $b_{\mathbf{k}\uparrow} = u_{\mathbf{k}}a_{\mathbf{k}\uparrow} - v_{\mathbf{k}}a^\dagger_{-\mathbf{k}\downarrow}$ annihilates this state. Construct $b_{\mathbf{k}\downarrow}$ in a similar fashion.

(c) Express the other 3 eigenstates of $h_{\mathbf{k}}$ in terms of $b^\dagger$-operators acting on $|\,BCS\,\rangle$ ground state. Find the excitation energies of these states compared to the BCS ground state.

Answer of exercise 1

According to the usual rules of finding an expectation value of an operator, for a single spin in a state α described by spinor ('spin wave function') $\chi_\alpha(s)$ we have

$$\langle \hat{\mathbf{S}} \rangle = \sum_{s,s'} \chi^*_\alpha(s)\ \frac{\hbar}{2}\boldsymbol{\sigma}_{ss'}\ \chi_\alpha(s')$$

with summation over coordinate values for the spin $s = 1, 2$ (or $s = -1, +1$). If we have a two-particle state $\chi_{\alpha\beta}(s_1, s_2)$ we need to sum over spin coordinates of both particles. To find the expectation value of say spin 1, we write:

$$\langle \hat{\mathbf{S}}_1 \rangle = \sum_{s_2,s_2'} \sum_{s_1,s_1'} \chi^*_{\alpha\beta}(s_1, s_2)\ \delta_{s_2 s_2'} \frac{\hbar}{2}\boldsymbol{\sigma}_{s_1 s_1'}\ \chi_{\alpha\beta}(s_1', s_2')$$

and bring it to a more compact form, that will allow us to use the trace and multiplication properties of the Pauli matrices:

$$\langle \hat{\mathbf{S}}_1 \rangle = \sum_{s_2} \sum_{s_1,s_1'} \chi^*_{\alpha\beta}(s_1, s_2)\ \frac{\hbar}{2}\boldsymbol{\sigma}_{s_1 s_1'}\ \chi_{\alpha\beta}(s_1', s_2) = \sum_{s_2} \sum_{s_1,s_1'} \chi^\dagger_{\alpha\beta}(s_2, s_1)\ \frac{\hbar}{2}\boldsymbol{\sigma}_{s_1 s_1'}\ \chi_{\alpha\beta}(s_1', s_2) = \frac{\hbar}{2}\mathrm{Tr}\left\{\chi^\dagger_{\alpha\beta}\ \boldsymbol{\sigma}\ \chi_{\alpha\beta}\right\}$$

where the $\dagger$ operation means taking complex conjugate and exchange of coordinates $s_1 \leftrightarrow s_2$. Similarly, for spin 2 one can show:

$$\langle \hat{\mathbf{S}}_2 \rangle = \frac{\hbar}{2}\mathrm{Tr}\left\{\chi_{\alpha\beta}\ \boldsymbol{\sigma}^*\ \chi^\dagger_{\alpha\beta}\right\}^* = \frac{\hbar}{2}\mathrm{Tr}\left\{\chi^{\dagger T}_{\alpha\beta}\ \boldsymbol{\sigma}\ \chi^T_{\alpha\beta}\right\} = \frac{\hbar}{2}\mathrm{Tr}\left\{\chi^\dagger_{\alpha\beta}\ \boldsymbol{\sigma}\ \chi_{\alpha\beta}\right\}$$

where T is the tranpose operation. Triplet states are symmetric in spin coordinates and the transposition leaves the state the same.

The given two-particle wave function is written using Pauli matrices, with the rows and columns being the coordinates of spin 1 and spin 2 respectively:

$$\psi(\mathbf{k}; s_1, s_2) = \boldsymbol{\Delta}(\mathbf{k}) \cdot [i\boldsymbol{\sigma}\sigma_y]_{s_1 s_2}\ ,$$

and we write for the spin expectation value,

$$\mathbf{S} = \langle \hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2 \rangle = \sum_{s_1,s_1'} \sum_{s_2,s_2'} \int \frac{d^3k}{(2\pi)^3}\ \psi^*(\mathbf{k}; s_1, s_2) \left(\frac{\hbar}{2}\boldsymbol{\sigma}_{s_1 s_1'}\ \delta_{s_2 s_2'} + \delta_{s_1 s_1'} \frac{\hbar}{2}\boldsymbol{\sigma}_{s_2 s_2'}\right) \psi(\mathbf{k}; s_1', s_2')$$

$$= \hbar \int \frac{d^3k}{(2\pi)^3}\ \mathrm{Tr}\left\{\psi^\dagger(\mathbf{k})\, \boldsymbol{\sigma}\, \psi(\mathbf{k})\right\}$$

where in the last step we used the symmetric property of the triplet states. Calculation of the spin trace is done using the properties of the Pauli matrices:

$$\mathrm{Tr}\left\{\psi^\dagger(\mathbf{k})\, \boldsymbol{\sigma}\, \psi(\mathbf{k})\right\} = \mathrm{Tr}\left\{[-i\sigma_y \boldsymbol{\sigma} \cdot \boldsymbol{\Delta}^*(\mathbf{k})]\boldsymbol{\sigma}[i\boldsymbol{\sigma} \cdot \boldsymbol{\Delta}(\mathbf{k})\sigma_y]\right\} = \mathrm{Tr}\left\{[\boldsymbol{\sigma} \cdot \boldsymbol{\Delta}^*(\mathbf{k})]\boldsymbol{\sigma}[\boldsymbol{\sigma} \cdot \boldsymbol{\Delta}(\mathbf{k})]\right\}$$

$$= \mathrm{Tr}\left\{\boldsymbol{\sigma}[\boldsymbol{\sigma} \cdot \boldsymbol{\Delta}(\mathbf{k})][\boldsymbol{\sigma} \cdot \boldsymbol{\Delta}^*(\mathbf{k})]\right\} = \mathrm{Tr}\left\{\boldsymbol{\sigma}[\boldsymbol{\Delta}(\mathbf{k}) \cdot \boldsymbol{\Delta}^*(\mathbf{k}) + i\boldsymbol{\sigma} \cdot (\boldsymbol{\Delta}(\mathbf{k}) \times \boldsymbol{\Delta}^*(\mathbf{k}))]\right\}$$

$$= 2i\boldsymbol{\Delta}(\mathbf{k}) \times \boldsymbol{\Delta}^*(\mathbf{k})$$

The factor 2 in front is from unnormalized way of writing the spin wave function. We omit it in the final answer. The expectation value for the spin of the pair is then:

$$\mathbf{S} = \langle \hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2 \rangle = i\hbar \int \frac{d^3k}{(2\pi)^3}\ \boldsymbol{\Delta}(\mathbf{k}) \times \boldsymbol{\Delta}^*(\mathbf{k})$$

Answer of exercise 2

The mean-field BCS Hamiltonian is

$$\mathcal{H} = E_0^{mf} + \sum_{\mathbf{k}} h_{\mathbf{k}} \qquad h_{\mathbf{k}} = \xi_{\mathbf{k}}(a^\dagger_{\mathbf{k}\uparrow}a_{\mathbf{k}\uparrow} + a^\dagger_{-\mathbf{k}\downarrow}a_{-\mathbf{k}\downarrow}) - (\Delta_{\mathbf{k}} a^\dagger_{\mathbf{k}\uparrow}a^\dagger_{-\mathbf{k}\downarrow} + \Delta^*_{\mathbf{k}} a_{-\mathbf{k}\downarrow}a_{\mathbf{k}\uparrow})$$

For each pair ($\mathbf{k}\uparrow$, $-\mathbf{k}\downarrow$) consider a basis in Fock space made up of 4 states: $|\, n_{\mathbf{k}\uparrow}, n_{-\mathbf{k}\downarrow}\,\rangle = (|\,0,0\,\rangle, |\,1,0\,\rangle, |\,0,1\,\rangle, |\,1,1\,\rangle)$ that we will label (in this order) as $|\, i = 1,2,3,4\,\rangle$.

(a) We can create a table of action:

$$\begin{aligned} h_{\mathbf{k}}|\,0,0\,\rangle &= -\Delta_{\mathbf{k}}|\,1,1\,\rangle \\ h_{\mathbf{k}}|\,1,0\,\rangle &= \xi_{\mathbf{k}}|\,1,0\,\rangle \\ h_{\mathbf{k}}|\,0,1\,\rangle &= \xi_{\mathbf{k}}|\,0,1\,\rangle \\ h_{\mathbf{k}}|\,1,1\,\rangle &= 2\xi_{\mathbf{k}}|\,1,1\,\rangle - \Delta^*_{\mathbf{k}}|\,0,0\,\rangle \end{aligned}$$

that one can cast into matrix form, $h_{ij} = \langle\, i\,|h_{\mathbf{k}}|\,j\,\rangle$, and use it to find its eigenvalues and eigenvectors in this basis: $\psi_{n=1,2,3,4} = \sum_{i=1}^4 c_i|\,i\,\rangle$

$$h_{ij} = \begin{pmatrix} 0 & 0 & 0 & -\Delta^*_{\mathbf{k}} \\ 0 & \xi_{\mathbf{k}} & 0 & 0 \\ 0 & 0 & \xi_{\mathbf{k}} & 0 \\ -\Delta_{\mathbf{k}} & 0 & 0 & 2\xi_{\mathbf{k}} \end{pmatrix} \quad \Rightarrow \quad \hat{h}\psi_n = E_n\psi_n \quad \Leftrightarrow \quad \begin{pmatrix} 0 & 0 & 0 & -\Delta^*_{\mathbf{k}} \\ 0 & \xi_{\mathbf{k}} & 0 & 0 \\ 0 & 0 & \xi_{\mathbf{k}} & 0 \\ -\Delta_{\mathbf{k}} & 0 & 0 & 2\xi_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = E \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix}$$

It is easy to find the 4 eigenstates:

$$\psi_1 = \begin{pmatrix} u_{\mathbf{k}} \\ 0 \\ 0 \\ v_{\mathbf{k}} \end{pmatrix} = u_{\mathbf{k}}|\,0,0\,\rangle + v_{\mathbf{k}}|\,1,1\,\rangle \qquad E_1 = \xi_{\mathbf{k}} - \sqrt{\xi^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2}$$

$$\psi_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = |\,1,0\,\rangle \qquad E_2 = \xi_{\mathbf{k}}$$

$$\psi_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = |\,0,1\,\rangle \qquad E_3 = \xi_{\mathbf{k}}$$

$$\psi_4 = \begin{pmatrix} -v^*_{\mathbf{k}} \\ 0 \\ 0 \\ u^*_{\mathbf{k}} \end{pmatrix} = -v^*_{\mathbf{k}}|\,0,0\,\rangle + u^*_{\mathbf{k}}|\,1,1\,\rangle \qquad E_1 = \xi_{\mathbf{k}} + \sqrt{\xi^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2}$$

with

$$\boxed{u_{\mathbf{k}} = \frac{E_{\mathbf{k}} + \xi_{\mathbf{k}}}{\sqrt{(E_{\mathbf{k}} + \xi_{\mathbf{k}})^2 + |\Delta_{\mathbf{k}}|^2}} \qquad v_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{\sqrt{(E_{\mathbf{k}} + \xi_{\mathbf{k}})^2 + |\Delta_{\mathbf{k}}|^2}} \qquad |u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1 \qquad E_{\mathbf{k}} = \sqrt{\xi^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2}}$$

With these definitions all the states are properly normalized and orthogonal.

(b) We write the lowest energy state

$$|\,BCS\,\rangle = u_{\mathbf{k}}|\,0,0\,\rangle + v_{\mathbf{k}} a^\dagger_{\mathbf{k}\uparrow}a^\dagger_{-\mathbf{k}\downarrow}|\,0,0\,\rangle$$

with the same coefficients as defined above. Acting with $b_{\mathbf{k}\uparrow} = u_{\mathbf{k}}a_{\mathbf{k}\uparrow} - v_{\mathbf{k}}a^\dagger_{-\mathbf{k}\downarrow}$ on this gives (omitting obvious vanishing terms):

$$b_{\mathbf{k}\uparrow}|\,BCS\,\rangle = (u_{\mathbf{k}}a_{\mathbf{k}\uparrow} - v_{\mathbf{k}}a^\dagger_{-\mathbf{k}\downarrow})(u_{\mathbf{k}} + v_{\mathbf{k}}a^\dagger_{\mathbf{k}\uparrow}a^\dagger_{-\mathbf{k}\downarrow})|\,0,0\,\rangle = u_{\mathbf{k}}v_{\mathbf{k}}(a_{\mathbf{k}\uparrow}a^\dagger_{\mathbf{k}\uparrow}a^\dagger_{-\mathbf{k}\downarrow} - a^\dagger_{-\mathbf{k}\downarrow})|\,0,0\,\rangle$$

$$= u_{\mathbf{k}} v_{\mathbf{k}} (a^\dagger_{-\mathbf{k}\downarrow} - a^\dagger_{\mathbf{k}\uparrow} a_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow} - a^\dagger_{-\mathbf{k}\downarrow}) |\, 0, 0 \,\rangle = 0$$

where we used anticommutation relations of fermionic operators.

To construct $b_{\mathbf{k}\downarrow}$ we look at another part of BCS state:

$$|\, BCS \,\rangle = u_{-\mathbf{k}} |\, 0, 0 \,\rangle + v_{-\mathbf{k}} a^\dagger_{-\mathbf{k}\uparrow} a^\dagger_{\mathbf{k}\downarrow} |\, 0, 0 \,\rangle$$

and to make sure we have similar cancellation we need to change sign in front of the creation part since additional -1 sign appear due to $a_{\mathbf{k}\downarrow} a^\dagger_{-\mathbf{k}\uparrow} = -a^\dagger_{-\mathbf{k}\uparrow} a_{\mathbf{k}\downarrow}$:

$$b_{\mathbf{k}\downarrow} = u_{-\mathbf{k}} a_{\mathbf{k}\downarrow} + v_{-\mathbf{k}} a^\dagger_{-\mathbf{k}\uparrow} \boxed{= u_{\mathbf{k}} a_{\mathbf{k}\downarrow} + v_{\mathbf{k}} a^\dagger_{-\mathbf{k}\uparrow}}$$

and also

$$\boxed{b_{-\mathbf{k}\downarrow} = u_{\mathbf{k}} a_{-\mathbf{k}\downarrow} + v_{\mathbf{k}} a^\dagger_{\mathbf{k}\uparrow}} \qquad b_{-\mathbf{k}\downarrow} |\, BCS \,\rangle = 0$$

(c) To express other states through the $|\, BCS \,\rangle$ ground state we act with creation $b^\dagger$ operators on it:

$$\boxed{\psi_2 = b^\dagger_{\mathbf{k}\uparrow} |\, BCS \,\rangle} = (u^*_{\mathbf{k}} a^\dagger_{\mathbf{k}\uparrow} - v^*_{\mathbf{k}} a_{-\mathbf{k}\downarrow})(u_{\mathbf{k}} + v_{\mathbf{k}} a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow}) |\, 0, 0 \,\rangle = (|u_{\mathbf{k}}|^2 a^\dagger_{\mathbf{k}\uparrow} - |v_{\mathbf{k}}|^2 a_{-\mathbf{k}\downarrow} a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow}) |\, 0, 0 \,\rangle$$

$$= (|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2) a^\dagger_{\mathbf{k}\uparrow} |\, 0, 0 \,\rangle = |\, 1, 0 \,\rangle = \psi_2 \qquad \boxed{E_2 - E_1 = \xi_{\mathbf{k}} - (\xi_{\mathbf{k}} - E_{\mathbf{k}}) = E_{\mathbf{k}} = \sqrt{\xi^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2}}$$

$$\boxed{\psi_3 = b^\dagger_{-\mathbf{k}\downarrow} |\, BCS \,\rangle} = |\, 0, 1 \,\rangle \qquad \boxed{E_3 - E_1 = \xi_{\mathbf{k}} - (\xi_{\mathbf{k}} - E_{\mathbf{k}}) = E_{\mathbf{k}} = \sqrt{\xi^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2}}$$

These are single particle excitations.

$$\boxed{\psi_4 = b^\dagger_{\mathbf{k}\uparrow} b^\dagger_{-\mathbf{k}\downarrow} |\, BCS \,\rangle} = (u^*_{\mathbf{k}} a^\dagger_{\mathbf{k}\uparrow} - v^*_{\mathbf{k}} a_{-\mathbf{k}\downarrow}) a^\dagger_{-\mathbf{k}\downarrow} |\, 0, 0 \,\rangle = -v^*_{\mathbf{k}} |\, 0, 0 \,\rangle + u^*_{\mathbf{k}} |\, 1, 1 \,\rangle$$

$$\boxed{E_4 - E_1 = (\xi_{\mathbf{k}} + E_{\mathbf{k}}) - (\xi_{\mathbf{k}} - E_{\mathbf{k}}) = 2E_{\mathbf{k}} = 2\sqrt{\xi^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2}}$$

This is the excited state of the pair, two-particle excitation.