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*Superconductivity, superfluidity and magnetism*
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# TD8: Anderson's pseudo-spin model and BCS variational wavefunction

In this TD we will explore a very insightful approach to the BCS Hamiltonian provided by P. W. Anderson (1958). Recasting the BCS Hamiltonian in terms of pseudo-spin variables, we will be able to write down the ground state of BCS theory in a very transparent and suggestive way.
NOTE: the angle $\vartheta_{\boldsymbol{k}}$ that appears in the following is not the same as the angle $\theta_{\boldsymbol{k}}$ discussed in the lectures on BCS theory. We shall establish the relationship between the two later.

## 1 Pair operators and spin operators

Consider the pair operators

$$\hat{b}_{\boldsymbol{k}} = \hat{c}_{-\boldsymbol{k}\downarrow}\hat{c}_{\boldsymbol{k}\uparrow} \qquad \hat{b}^\dagger_{\boldsymbol{k}} = \hat{c}^\dagger_{\boldsymbol{k}\uparrow}\hat{c}^\dagger_{-\boldsymbol{k}\downarrow} \tag{1}$$

### 1.1

Show that

$$\left[\hat{b}_{\boldsymbol{k}}, \hat{b}_{\boldsymbol{q}}\right] = \left[\hat{b}^\dagger_{\boldsymbol{k}}, \hat{b}^\dagger_{\boldsymbol{q}}\right] = 0 \tag{2}$$

$$\left[\hat{b}_{\boldsymbol{k}}, \hat{b}^\dagger_{\boldsymbol{q}}\right] = (1 - n_{\boldsymbol{k},\uparrow} - n_{-\boldsymbol{k},\downarrow})\,\delta_{\boldsymbol{q},\boldsymbol{k}} \tag{3}$$

Moreover, justify that $(b^\dagger_{\boldsymbol{k}})^2 = (b_{\boldsymbol{k}})^2 = 0$.

### 1.2

Introducing the operators (Anderson's pseudospins)

$$\begin{aligned} \hat{S}^z_{\boldsymbol{k}} &= \frac{1}{2}\left(\hat{n}_{\boldsymbol{k},\uparrow} + \hat{n}_{-\boldsymbol{k},\downarrow} - 1\right) \\ \hat{S}^+_{\boldsymbol{k}} &= \hat{b}^\dagger_{\boldsymbol{k}} \\ \hat{S}^-_{\boldsymbol{k}} &= \hat{b}_{\boldsymbol{k}} \end{aligned} \tag{4}$$

show that they satisfy the commutation relations of angular momentum

$$\left[\hat{S}^+_{\boldsymbol{k}}, \hat{S}^-_{\boldsymbol{k}}\right] = 2\hat{S}^z_{\boldsymbol{k}} \qquad \left[\hat{S}^+_{\boldsymbol{k}}, \hat{S}^z_{\boldsymbol{k}}\right] = -\hat{S}^+_{\boldsymbol{k}} \tag{5}$$

Given that $(\hat{S}^+_{\boldsymbol{k}})^2 = (\hat{S}^-_{\boldsymbol{k}})^2 = 0$, what is the spin length $S$?

## 2 BCS Hamiltonian as a spin Hamiltonian

The BCS Hamiltonian for (quasi-)electrons interacting via an effective phonon-mediated interaction reads

$$\hat{\mathcal{H}} - \mu\hat{N} = \sum_{\boldsymbol{k}} (\epsilon_{\boldsymbol{k}} - \mu)\,(\hat{n}_{\boldsymbol{k},\uparrow} + \hat{n}_{\boldsymbol{k},\downarrow}) - \frac{V_0}{\mathcal{V}} \sum_{\boldsymbol{k},\boldsymbol{q}}{}' \,\hat{b}^\dagger_{\boldsymbol{k}}\hat{b}_{\boldsymbol{q}} \quad . \tag{6}$$

Here $\mathcal{V}$ is the volume, $V_0$ is the strength of the interaction, and the sum $\sum_{\boldsymbol{k},\boldsymbol{q}}{}'$ runs over momenta $\boldsymbol{k}$ and $\boldsymbol{q}$ such that $|\epsilon_{\boldsymbol{k}(\boldsymbol{q})} - \mu| \leq \epsilon_c$, where $\epsilon_c \approx \hbar\omega_D$ is the characteristic energy cutoff of the interaction.

### 2.1

Rewrite the above Hamiltonian in terms of the pseudo-spin operators. You should find

$$\hat{\mathcal{H}} - \mu\hat{N} = \sum_{\boldsymbol{k}} \left[2\,(\epsilon_{\boldsymbol{k}} - \mu) - \frac{V_0}{\mathcal{V}}\,\vartheta\,(\epsilon_c - |\epsilon_{\boldsymbol{k}} - \mu|)\right]\hat{S}^z_{\boldsymbol{k}} - \frac{V_0}{\mathcal{V}}\sum_{\boldsymbol{k}\neq\boldsymbol{q}}{}' \left(\hat{S}^x_{\boldsymbol{k}}\hat{S}^x_{\boldsymbol{q}} + \hat{S}^y_{\boldsymbol{k}}\hat{S}^y_{\boldsymbol{q}}\right) + \text{const.} \tag{7}$$

It might be useful to remember the following relationships

$$\hat{S}^+_{\boldsymbol{k}}\hat{S}^-_{\boldsymbol{k}} = \frac{1}{2} + \hat{S}^z_{\boldsymbol{k}} \qquad \frac{1}{2}\left(\hat{S}^+_{\boldsymbol{k}}\hat{S}^-_{\boldsymbol{q}} + \hat{S}^+_{\boldsymbol{q}}\hat{S}^-_{\boldsymbol{k}}\right) = \hat{S}^x_{\boldsymbol{k}}\hat{S}^x_{\boldsymbol{q}} + \hat{S}^y_{\boldsymbol{k}}\hat{S}^y_{\boldsymbol{q}} \quad . \tag{8}$$

Now, think of $\boldsymbol{k}$-space as a lattice (it is discretized after all, due to the boundary conditions), and put a $S = 1/2$ (pseudo-)spin on each lattice site. The above Hamiltonian effectively describes a system of interacting spins on a lattice. Taking the spin at lattice site $\boldsymbol{k}$, which are the sites that this spin is interacting with? And what is the value of the local magnetic field?

### 2.2

We take for the moment $V_0 = 0$. Write down the ground state for each pseudo-spin $\hat{S}_{\boldsymbol{k}}$. If you report the $\boldsymbol{k}$ points on the energy axis $\epsilon_{\boldsymbol{k}}$ (a simply sketch is sufficient) together with the associated pseudo-spin, can you find a "domain wall" at a given energy in the spin configuration? And can you anticipate qualitatively what happens when the interaction is turned on?

## 3 BCS variational wavefunction

We now look for the ground state of the interacting system ($V_0 \neq 0$) in a *factorized* form, namely in the form

$$|\Psi_0\rangle = \prod_{\boldsymbol{k}} |\vartheta_{\boldsymbol{k}}, \phi_{\boldsymbol{k}}\rangle \tag{9}$$

where

$$|\vartheta, \phi\rangle = \cos(\vartheta/2)\,|\uparrow\rangle + \sin(\vartheta/2)\,e^{i\phi}\,|\downarrow\rangle \tag{10}$$

### 3.1

Show that the above wavefunction is equivalent to the so-called BCS wavefunction

$$|\Psi_0\rangle = \prod_{\boldsymbol{k}} \left( u_{\boldsymbol{k}} + v_{\boldsymbol{k}}\ \hat{b}^\dagger_{\boldsymbol{k}} \right) |0\rangle \tag{11}$$

where the coefficients $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$ are to be identified. (Suggestion: write the vacuum $|0\rangle$ in terms of the pseudo-spin states).

### 3.2

Show that the expectation value of the spin operator $\hat{\boldsymbol{S}}$ on the $|\vartheta, \phi\rangle$ state behaves like a classical spin of length $S = 1/2$:

$$\langle \vartheta, \phi | \hat{\boldsymbol{S}} | \vartheta, \phi \rangle = \frac{1}{2} \left( \cos\phi \sin\vartheta, \sin\phi \sin\vartheta, \cos\vartheta \right) \tag{12}$$

and, moreover

$$\langle \vartheta_{\boldsymbol{k}}, \phi_{\boldsymbol{k}} | \langle \vartheta_{\boldsymbol{q}}, \phi_{\boldsymbol{q}} | \left( \hat{S}^x_{\boldsymbol{k}} \hat{S}^x_{\boldsymbol{q}} + \hat{S}^y_{\boldsymbol{k}} \hat{S}^y_{\boldsymbol{q}} \right) | \vartheta_{\boldsymbol{k}}, \phi_{\boldsymbol{k}} \rangle | \vartheta_{\boldsymbol{q}}, \phi_{\boldsymbol{q}} \rangle = \frac{1}{4} \cos\left( \phi_{\boldsymbol{k}} - \phi_{\boldsymbol{q}} \right) \sin\vartheta_{\boldsymbol{k}} \sin\vartheta_{\boldsymbol{q}} \tag{13}$$

Show that the variational energy takes the form

$$\langle \Psi_0 | \hat{\mathcal{H}} - \mu \hat{N} | \Psi_0 \rangle = \sum_{\boldsymbol{k}} \left[ \epsilon_{\boldsymbol{k}} - \mu - \frac{V_0}{2\mathcal{V}}\ \vartheta\left( \epsilon_c - |\epsilon_{\boldsymbol{k}} - \mu| \right) \right] \cos\vartheta_{\boldsymbol{k}} - \frac{V_0}{4\mathcal{V}} \sum_{\boldsymbol{k} \neq \boldsymbol{q}}{}' \cos\left( \phi_{\boldsymbol{k}} - \phi_{\boldsymbol{q}} \right) \sin\vartheta_{\boldsymbol{k}} \sin\vartheta_{\boldsymbol{q}} \tag{14}$$

Given that $V_0 > 0$ and $\vartheta_{\boldsymbol{k}} \in [0, \pi]$, what value of the $\phi_{\boldsymbol{k}}$ angles minimizes the energy?

### 3.3

Minimize the variational energy with respect to $\vartheta_{\boldsymbol{k}}$ for $|\epsilon_{\boldsymbol{k}} - \mu| < \epsilon_c$, to find the condition

$$\left( \epsilon_{\boldsymbol{k}} - \mu - \frac{V_0}{2\mathcal{V}} \right) \sin\vartheta_{\boldsymbol{k}} = -\frac{V_0}{2\mathcal{V}} \sum_{\boldsymbol{q} \neq \boldsymbol{k}}{}' \sin\vartheta_{\boldsymbol{q}} \cos\vartheta_{\boldsymbol{k}} \tag{15}$$

This condition defines a set of coupled equations.
Making an error of order $\mathcal{O}(1/\mathcal{V})$, we can neglect the term $V_0/(2\mathcal{V})$ on the left-hand side and the add the term with $\boldsymbol{q} = \boldsymbol{k}$ in the sum on the right-hand side.
Introducing then the symbol

$$\Delta = \frac{V_0}{2\mathcal{V}} \sum_{\boldsymbol{q}}{}' \sin\vartheta_{\boldsymbol{q}} \tag{16}$$

rewrite Eq. (15) in terms of $\Delta$, $\epsilon_{\boldsymbol{k}}$, $\mu$ and $\vartheta_{\boldsymbol{k}}$.

### 3.4

Solve for $\vartheta_{\boldsymbol{k}}$, to find

$$\sin\vartheta_{\boldsymbol{k}} = \frac{\Delta}{E_{\boldsymbol{k}}} \qquad \cos\vartheta_{\boldsymbol{k}} = \frac{\mu - \epsilon_{\boldsymbol{k}}}{E_{\boldsymbol{k}}} \qquad E_{\boldsymbol{k}} = \sqrt{\Delta^2 + (\epsilon_{\boldsymbol{k}} - \mu)^2} \tag{17}$$

What is the pseudo-spin orientation at the Fermi energy $\epsilon_F = \mu$? Draw schematically how the pseudo-spin orientation evolve when the energy goes from $\mu - \epsilon_c$ to $\mu + \epsilon_c$.

### 3.5

From Eq. (16) recover the (implicit) gap equation for $|\Delta|$ as seen in the lecture.

## 4 Average particle number

The BCS wavefunction, Eq. (11), does not contain a well defined particle number. In particular, $|\Psi_0\rangle$ contains all possible *even* particle numbers from 0 to $\infty$. But let us have a look at how well defined the *average* particle number is

### 4.1

Express the average particle number

$$\langle \hat{N} \rangle = \sum_{\boldsymbol{k}} \langle \hat{n}_{\boldsymbol{k},\uparrow} + \hat{n}_{\boldsymbol{k},\downarrow} \rangle \tag{18}$$

and the average square number

$$\langle \hat{N}^2 \rangle = \sum_{\boldsymbol{k},\boldsymbol{q}} \langle (\hat{n}_{\boldsymbol{k},\uparrow} + \hat{n}_{\boldsymbol{k},\downarrow}) \left( \hat{n}_{\boldsymbol{q},\uparrow} + \hat{n}_{\boldsymbol{q},\downarrow} \right) \rangle \tag{19}$$

in terms of the $\vartheta_{\boldsymbol{k}}$ angles.

### 4.2

Show that

$$\langle \delta^2 \hat{N} \rangle = \sum_{\boldsymbol{k}} \left( 1 - \langle \cos \vartheta_{\boldsymbol{k}} \rangle^2 \right) \sim \mathcal{O}(N) \tag{20}$$

How can one conclude that the sum is $\mathcal{O}(N)$? Which $\boldsymbol{k}$ states are contributing to it?

### 4.3

Conclude on the importance of the relative particle-number fluctuations.

## 5 Angle $\vartheta_{\boldsymbol{k}}$ vs. angle $\theta_{\boldsymbol{k}}$

Consider the angle $\theta_{\boldsymbol{k}}$ given in the lectures on BCS theory (such that $u_{\boldsymbol{k}} = \cos(\theta_{\boldsymbol{k}}/2)$, $v_{\boldsymbol{k}} = \sin(\theta_{\boldsymbol{k}}/2)$): what is the relationship with the angle $\vartheta_{\boldsymbol{k}}$ introduced in this exercise?