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Introduction to quantum liquids
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TD6: 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.

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)

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

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

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

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

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

where

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

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 $|\theta, \phi\rangle$ state behaves like a classical spin of length $S = 1/2$:

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

and, moreover

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

Show that the variational energy takes the form

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

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

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

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

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

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

rewrite Eq. (15) in terms of Δ, $\epsilon_{\boldsymbol{k}}$, μ and $\theta_{\boldsymbol{k}}$.

3.4) Solve for $\theta_{\boldsymbol{k}}$, to find

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

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 ∞. 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

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

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

4.2) Show that

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

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.