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Exercise sheet online at http://www.thp.uni-koeln.de/∼jinhong/qft2

Quantum Field Theory II
Problem Set 9

Please hand in your solution of the exercise marked with (*), for which we offer correction, in the mail box until Monday 12am.

1. Mean-field free energy of the ferromagnet

The goal of this exercise to demonstrate a "Mexican Hat" potential in the ferromagnet calculating the mean-field free energy. In the previous problem set, we derive the effective action for the ferromagnet solution of the Hubbard model. In the momentum and frequency space, the effective action is written as

$$S_{\rm MF}(\phi_0) = -\sum_{\boldsymbol{k},\omega_n} \operatorname{Tr}\ln\left(\epsilon_{\boldsymbol{k}} - \mu - i\omega_n - \frac{\phi_0}{2}\sigma_z\right) + \frac{\phi_0^2}{2J}N\beta. \tag{1}$$

Here N is the total number of sites in the Hubbard model. Note that the mean-field solution ϕ_0 acts like an effective magnetic field in z direction that leads to a splitting of the Fermi surface into 2 components. The mean-field free energy per site is defined as $F_{\rm MF} \equiv S_{\rm MF}/(\beta N)$ and after the Matsubara summation and the analytic continuation, it is given by

$$F_{\rm MF} = -\frac{1}{\beta}\int d\epsilon \nu(\epsilon) \sum_{\sigma=\pm} \ln\left(1 + e^{-\beta(\epsilon-\mu-\sigma\phi_0/2)}\right) + \frac{\phi_0^2}{2J}, \tag{2}$$

where $\nu(\epsilon) \equiv \sum_{\boldsymbol{k}} \delta(\epsilon - \epsilon_{\boldsymbol{k}})$ is the density of states per spin and site. From now, let us focus on zero temperature case.

a) Check that when $\phi_0 = 0$, the free energy is just expressed as the integral over the energy of all occupied states.

b) Expanding the free energy to the fourth order in small ϕ_0, show that the free energy is written as

$$F_{\rm MF} = F_0 + \frac{\phi_0^2}{2}\left(\frac{1}{J} - \frac{\nu(\mu)}{2}\right) + 2\frac{1}{4!}\left(\frac{\phi_0}{2}\right)^4\left(-\frac{\partial^2\nu(\epsilon)}{\partial\epsilon^2}\Big|_{\epsilon=\mu}\right). \tag{3}$$

c) Show that when $J\nu(\mu) > 2$ and $\partial^2\nu(\epsilon)/\partial\epsilon^2|_{\epsilon=\mu} < 0$, the free energy forms a "Mexican Hat" potential. The former condition $J\nu(\mu) > 2$ is called Stoner criterion. Show that the second condition can be achieved in three dimensions.

2. Variational BCS wave function (*)

In this exercise, we determine the ground state wave function of a superconductor using a variational calculation. We consider a more simplified version of the pairing Hamiltonian

$$\hat{K} = \hat{H} - \mu\hat{N} = \sum_{\boldsymbol{k}\sigma} \xi_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \frac{1}{\mathcal{V}} \sum_{\boldsymbol{k}} \sum_{\boldsymbol{l}\neq\boldsymbol{k}} V_{\boldsymbol{kl}} c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow} c_{-\boldsymbol{l}\downarrow} c_{\boldsymbol{l}\uparrow} \tag{4}$$

than that considered in the lecture. Here the attractive potential $V_{\boldsymbol{kl}}$ is active only in the vicinity of the Fermi surface

$$V_{\boldsymbol{kl}} = \begin{Bmatrix} -V & |\xi_{\boldsymbol{k}}|, |\xi_{\boldsymbol{l}}| < \omega_D \\ 0 & \text{otherwise} \end{Bmatrix}, \tag{5}$$

and ω_D is the natural ultraviolet cutoff given by the Debye frequency. The celebrated BCS wave function, written in terms of some unknown coefficients $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$, is given by

$$|\Psi\rangle = \prod_{\boldsymbol{k}} \left(u_{\boldsymbol{k}} + v_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow} \right) |0\rangle. \tag{6}$$

Here $|0\rangle$ is the vacuum, and $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$ satisfy the normalization condition

$$|u_{\boldsymbol{k}}|^2 + |v_{\boldsymbol{k}}|^2 = 1. \tag{7}$$

a) Show that the ground state expectation value of $\hat{K}$ as a function of $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$ is given by

$$\langle\Psi|\hat{K}|\Psi\rangle = 2\sum_{\boldsymbol{k}} \xi_{\boldsymbol{k}} |v_k|^2 + \frac{1}{\mathcal{V}} \sum_{\boldsymbol{k}} \sum_{\boldsymbol{l}\neq\boldsymbol{k}} V_{\boldsymbol{kl}} v^*_{\boldsymbol{k}} u_{\boldsymbol{k}} v_{\boldsymbol{l}} u^*_{\boldsymbol{l}}. \tag{8}$$

Minimize Eq. (8) with the constraint Eq. (7). Choosing the suitable real parameterization

$$u_{\boldsymbol{k}} = \sin\theta_{\boldsymbol{k}} \qquad v_{\boldsymbol{k}} = \cos\theta_{\boldsymbol{k}}, \tag{9}$$

and taking the derivative of the expectation value in $\theta_{\boldsymbol{k}}$, derive the gap equation

$$\tan 2\theta_k = \frac{1}{\mathcal{V}} \sum_{\boldsymbol{l}} V_{\boldsymbol{kl}} \frac{\sin 2\theta_{\boldsymbol{l}}}{2\xi_{\boldsymbol{k}}} \equiv -\frac{\Delta_{\boldsymbol{k}}}{\xi_{\boldsymbol{k}}}. \tag{10}$$

b) Introducing $E_{\boldsymbol{k}} = (\xi_k^2 + \Delta_{\boldsymbol{k}}^2)^{1/2}$, we see that Eq. (10) leads to $\cos(2\theta_{\boldsymbol{k}}) = -\xi_{\boldsymbol{k}}/E_{\boldsymbol{k}}$ and $\sin(2\theta_{\boldsymbol{k}}) = \Delta_{\boldsymbol{k}}/E_{\boldsymbol{k}}$. Rewrite $u^2_{\boldsymbol{k}}$ and $v^2_{\boldsymbol{k}}$ in terms of $\xi_{\boldsymbol{k}}$, $\Delta_{\boldsymbol{k}}$, and $E_{\boldsymbol{k}}$ and also the gap equation as

$$\Delta_{\boldsymbol{k}} = -\frac{1}{2\mathcal{V}} \sum_{\boldsymbol{l}\neq\boldsymbol{k}} \frac{V_{\boldsymbol{kl}}}{E_{\boldsymbol{l}}} \Delta_{\boldsymbol{l}}. \tag{11}$$

Using the expression for $V_{\boldsymbol{kl}}$, find a non-trivial solution ($\Delta_{\boldsymbol{k}} = \Delta \neq 0$) of Eq. (11). To which physical state corresponds the $\Delta = 0$ solution? Find the expression of $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$ for Δ.

c) Having $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$, you can now calculate the ground state energy. Calculate the condensation energy defined as

$$\delta E_{\text{cond}} \equiv \langle\Psi|\hat{K}|\Psi\rangle - \langle F|\hat{K}|F\rangle. \tag{12}$$

Here the Fermi sea $|F\rangle = \prod_{\xi_k<0} c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{\boldsymbol{k}\downarrow}$. Prove that the BCS wave function is more stable than the Fermi sea showing that the condensation energy is negative.

d) Use the ground state wave function to calculate the fluctuations δN of the particle number that

$$\delta N = \sqrt{\langle N^2 \rangle - \bar{N}^2}, \tag{13}$$

where $\bar{N}$ is the average number of particle. Are those fluctuations large compared to the average?

3. Tunneling density of states of a superconductor

The goal of the exercise is to obtain the tunneling density of states which probes the spectrum to add or remove an electron from a superconductor. Let us consider the mean-field Hamiltonian of

$$\hat{H} - \mu \hat{N} = \sum_{\boldsymbol{k}} \Psi_{\boldsymbol{k}}^{\dagger} (\xi_{\boldsymbol{k}} \tau_3 + \Delta \tau_1) \Psi_{\boldsymbol{k}}, \tag{14}$$

where the $\Psi_{\boldsymbol{k}} = (c_{\boldsymbol{k}\uparrow}, c_{-\boldsymbol{k}\downarrow}^{\dagger})^T$ are the so-called Nambu spinors and $\xi_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}} - \mu$. Calculate the density of states of the Nambu spinors using the formula of the density of states

$$\nu(\epsilon) = -\frac{1}{\pi} \sum_{\boldsymbol{k}} \mathrm{Im} \left[(G_{\boldsymbol{k}}(\epsilon + i\eta))_{11} \right]. \tag{15}$$

The Green's function $G_{\boldsymbol{k}}$ for $\Psi_{\boldsymbol{k}}$ is the 2×2 matrix in the Nambu spinor basis. Assume the density of states for non-interacting particles is energy-independant. Why there is no density of states at the Fermi energy? Why there is a divergence close to $\epsilon = \pm\Delta$? What is the limit of your result for $\Delta \to 0$?