Condensed Matter Physics (FKA091)

Problem Set 4

Deadline: 15-12-2016

To be handed in to:

Oleksandr Balabanov

Soliden building 3008

oleksandr.balabanov@physics.gu.se

Problem 1 (7 pt): As I discussed in class, a number-conserving theory for a conventional superconductor can be obtained by making coherent superpositions of BCS ground states of definite phase,

$$|\psi(N)\rangle = \int_0^{2\pi} d\phi \, e^{i\phi N/2} |\psi(\phi)\rangle.$$

a) Show by an explicit calculation that $|\psi(N)\rangle$ contains N electrons.

b) In class I claimed that the distribution of terms with different particle numbers in the BCS ground state peaks sharply about the average number $\langle N\rangle$ when $\langle N\rangle$ is macroscopic. In other words, the distribution of a_N in

$$|\psi\rangle = \sum_N a_N \, |\psi(N)\rangle$$

is sharply peaked about its mean value $\langle N\rangle$ for large $\langle N\rangle$. Can you calculate a_N?

c) The fact that a definite (indefinite) phase of the superconducting ground state implies an indefinite (definite) particle number (and vice versa) reflects the fact that phase and particle number are canonically conjugate variables and are subject to a Heisenberg uncertainty relation. Show this explicitly!

Problem 2 (8 pt): In class we discussed how to diagonalize the BCS Hamiltonian using a Bogoliubov transformation. In this problem you are asked to reconsider the problem, in a slightly different guise, but again working with a Bogoliubov transformation.

Consider a superconductor described by the following mean-field BCS Hamiltonian (written in second quantization)

$$\hat{H} = \int d^3\boldsymbol{r} \sum_{\sigma} \left[\hat{\Psi}^\dagger(\boldsymbol{r},\sigma) H_e \hat{\Psi}(\boldsymbol{r},\sigma) + U(\boldsymbol{r}) \hat{\Psi}^\dagger(\boldsymbol{r},\sigma) \hat{\Psi}(\boldsymbol{r},\sigma) \right] \tag{1}$$

$$+ \int d^3\boldsymbol{r} \left[\Delta(\boldsymbol{r}) \hat{\Psi}^\dagger(\boldsymbol{r},\uparrow) \hat{\Psi}^\dagger(\boldsymbol{r},\downarrow) + \Delta^*(\boldsymbol{r}) \hat{\Psi}(\boldsymbol{r},\downarrow) \hat{\Psi}(\boldsymbol{r},\uparrow) \right] \tag{2}$$

where $\hat{\Psi}^\dagger(\boldsymbol{r},\sigma)$ creates an electron of spin σ at position $\boldsymbol{r}$, $H_e = -\frac{\hbar^2}{2m}\nabla^2$ is a kinetic term, $U(\boldsymbol{r})$ is an external potential that we assume to be spin-independent for simplicity (this is not true in general, for example magnetic field breaks this form), $\Delta(\boldsymbol{r})$ is BCS order parameter.

Let's diagonalize the BCS Hamiltonian. This means that we aim to find fermionic operators $\hat{\gamma}_{n,\sigma}$ such that

$$\hat{H} = E + \sum_{n,\sigma} \epsilon_n \hat{\gamma}^\dagger_{n,\sigma} \hat{\gamma}_{n,\sigma} \tag{3}$$

where E is some constant and ϵ_n is a quasi-particle energy corresponding to $\hat{\gamma}_{n,\sigma}$. The energies ϵ_n and operators $\hat{\gamma}_{n,\sigma}$ can be found by solving the so-called Bogoliubov-de Gennes equations, derived using a Bogoliubov transformation.

a) (Bogoliubov transformation) We notice that $\hat{H}$ contains only quadratic terms in $\hat{\Psi}$ and $\hat{\gamma}$ and therefore they have to depend linearly on each other. After taking care of some issues with spin-dependence we introduce the following proportionality relations

$$\hat{\Psi}(\boldsymbol{r},\uparrow) = \sum_n \left[\hat{\gamma}_{n,\uparrow} u_n(\boldsymbol{r}) - \hat{\gamma}^\dagger_{n,\downarrow} v_n^*(\boldsymbol{r}) \right]$$

$$\hat{\Psi}(\boldsymbol{r},\downarrow) = \sum_n \left[\hat{\gamma}_{n,\downarrow} u_n(\boldsymbol{r}) + \hat{\gamma}^\dagger_{n,\uparrow} v_n^*(\boldsymbol{r}) \right]$$

Both operators $\hat{\Psi}$ and γ have to obey fermionic anti-commutation relations and this places some restrictions on the functions $u_n(\boldsymbol{r})$ and $v_n(\boldsymbol{r})$. Derive these restrictions.

b) (Bogoliubov-de Gennes equations)

1. Calculate the commutators $[\hat{H}, \gamma_{n,\downarrow}]$ and $[\hat{H}, \gamma_{n,\uparrow}]$ using $\hat{H}$ from equation (3).

2. Calculate the commutators $[\hat{H}, \hat{\Psi}(\boldsymbol{r}, \downarrow)]$ and $[\hat{H}, \hat{\Psi}(\boldsymbol{r}, \uparrow)]$ using $\hat{H}$ from equations (1) and (2).

3. Now, transform $\hat{\Psi}(\boldsymbol{r})$ in **2**. using the Bogoliubov transformation and simplify the equation using **1**. Separate the terms corresponding to different operators. If you have done everything correctly, you should get two equations looking very similar to a Schrödinger equation. These equations are called Bogoliubov-de Gennes (BdG) equations and they are very useful because one may use them to solve non-homogeneous problems in superconductivity (like effects of boundaries, impurities, etc.)

c) (Particle-hole symmetry) Let a pair of functions $\{u(\boldsymbol{r}), v(\boldsymbol{r})\}$ be a solution to BdG equations with energy ϵ. Show that $\{v^*(\boldsymbol{r}), -u^*(\boldsymbol{r})\}$ is also a solution but with energy $-\epsilon$.

This is a so-called particle-hole symmetry (PHS). It is an intrinsic property of BCS theory and it comes from the fact that $\hat{\gamma}_n$ and E are not uniquely defined through relation (3). Show explicitly that they are not uniquely defined. *Hint: use fermionic anti-commutation relations for some $\hat{\gamma}$ and then use a new set of operators $\hat{\gamma}' = \hat{\gamma}^\dagger$ to obtain an equation in the form* (3) *but with new operators and constant E'.*

How do you think PHS can be broken in BCS theory?