Emergent States of Matter

HOMEWORK SHEET 5

Due 5pm Fri 2 Nov 2012.

Please attempt these questions without looking at textbooks, if you can. You will learn more by thinking about these problems yourself.

Question 5-1: Solution of a minimal model for a superconductor.

You did parts (a) - (c) for last week’s week’s homework. In this HW 5, you will complete the calculation.

Consider the Hamiltonian due to Bardeen, Cooper and Schrieffer (BCS)

$$H(U) = \sum_k E(k)(c_k^+ c_k + c_{-k}^+ c_{-k}) - U \sum_{kk'} c_{k'}^+ c_{k'} c_{-k'} c_{-k}$$

where $U > 0$, and the $c_k$ are fermionic annihilation operators. In the first term, $k$ includes the spin degree of freedom, and a sum over $k$ also indicates a sum over the spin. The kinetic energy term is measured with respect to the Fermi energy $\mu$ and is given by $E(k) = \hbar^2 k^2 / 2m - \mu$. Notice that when $U = 0$, this Hamiltonian describes a free Fermi gas. In the second term, there is no sum over spin: that is, $k$ and spin are locked together by the formation of the Cooper pair, which has been put in “by hand” in the BCS Hamiltonian: $k = k \uparrow$ etc.

We will later apply some constraints on the sum in the potential energy term. This Hamiltonian is a minimal model of a superconductor. In this problem, you will use the Bogoliubov theory, following the steps we did in class to solve this Hamiltonian at zero temperature. This question, unlike most others in the class, will involve you doing some careful algebra. Don’t begin your attempt to do this question the night before the due date!

(a) Introduce quasi-particle operators by the transformation

$$\alpha_k = u_k c_k - v_k c_{-k}^+$$

where the $u_k$ and $v_k$ are positive real functions to be determined. In this problem, because we are using Fermionic operators, not Bosonic operators, there are minus signs that appear in the definition of the quasi-particles and in the behaviour of the $u_k$ and $v_k$ functions. We will impose the conditions:

$$u_k = u_{-k}, \quad v_k = v_{-k}.$$  

Show that the transformation is canonical in the sense discussed in lectures as long as $u_k^2 + v_k^2 = 1$ and verify that the quasi-particle operators satisfy the canonical Fermion anti-commutation relations.

(b) Hence express the original electron operators in terms of the quasi-particle operators.

(c) Substitute your expression for the $c_k$ in terms of the $\alpha_k$ into the kinetic energy part of the Hamiltonian. Define the quasi-particle number operator $m_k \equiv \alpha_k^+ \alpha_k$. Show that the kinetic energy is:

$$H_{kinetic} = \sum_k E(k) \left\{ 2v_k^2 + (u_k^2 - v_k^2)(m_k + m_{-k}) + 2u_k v_k (\alpha_k^+ \alpha_{-k} + \alpha_{-k} \alpha_k) \right\}$$

The sections below will be part of HW 5. If you want you can start them now.

(d) Calculate the exact expression for the potential energy in terms of the quasi-particle operators. I won’t even attempt to Tex it!

(e) Notice that the full Hamiltonian can be written as the sum of terms that are (i) constants, (ii) proportional to the number operator, (iii) Quadratic off-diagonal terms i.e. with $\alpha_k^+ \alpha_{-k}^+$, (iv) Quartic off-diagonal terms. We will make (iii) vanish by appropriate choice of the $u_k$ and $v_k$. (iv) will be ignored as being small compared to the terms remaining (they describe quasi-particle interactions which are
beyond the scope of this course). Let’s now implement this program. We will start by looking at the ground state of the system. In contrast to the weakly-interacting Bose gas, we will have to derive the existence of the condensate. We start by assuming that there are no quasi-particles so that \( m_k = 0 \). Write down the expression for the energy of the system, which will be made up of terms (i) and (iii). Set the coefficient of (iii) to zero and define the number \( \Delta \equiv U \sum_k u_k v_k \). Parameterise \( u_k^2 \equiv (1 + \xi_k)/2 \) and \( v_k^2 \equiv (1 - \xi_k)/2 \). Hence determine \( \xi_k \) in terms of \( E(k) \) and the constant \( \Delta \).

\[(f) \text{ Now, using its definition and your result for } \xi_k, \text{ show that } \Delta \text{ is given by the solution of the equation:} \]

\[
1 = \frac{U}{2} \int \frac{N(E)}{(E^2 + \Delta^2)^{1/2}} dE
\]

where \( N(E) \) is the density of states in energy. In a classic superconductor, i.e. one in which the origin of the attractive interaction \( U \) is the electron-phonon interaction, the interaction is only effective within an energy interval of width \( \hbar \omega_D \) around the Fermi surface, where \( \omega_D \) is the phonon Debye frequency. So in the integral you derived, \( N(E) \) can be approximated by its value at \( E = 0 \) (remember we are measuring all energies with respect to the chemical potential), and the limits of the integral are \( \pm \hbar \omega_D \).

Hence determine \( \Delta \) in terms of \( \hbar \omega_D, U, \) and \( N(0) \), for small \( U \), i.e. \( UN(0) \ll 1 \). Notice that your result is non-analytic in \( U \).

\[(g) \text{ Define the condensation energy } E_c \equiv H(U) - H(0). \text{ Show that } E_c < 0, \text{ i.e. the free electron gas has a higher energy than the state of the system which is the ground state of } H(U). \text{ [You should be able to calculate that } E_c = -N(0)\Delta^2/2, \text{ assuming that } \Delta \ll \hbar \omega_D, \text{ but you do not need to do this.]} \]

\[(h) \text{ To determine the wavefunction in this state, notice that the ground state } |\psi\rangle \text{ has } m_k = 0 \text{ and thus } \alpha_k |\psi\rangle = 0 \text{ for all } k. \text{ Show that the unnormalised state } \prod_k \alpha_k \alpha_{-k} |0\rangle \text{ has this property (}|0\rangle \text{ is the vacuum), where the } k \text{ vectors are “positive” in the sense of being restricted to have } k_z > 0. \text{ Determine the normalisation and hence show that } |\psi\rangle = \prod_k (u_k + v_k c_k^+ c_{-k}^+) |0\rangle \]

\[(i) \text{ Calculate } u_k \text{ and } v_k \text{ when } U = 0 \text{ taking care to distinguish between } k < k_f \text{ and } k > k_f \text{ where } k_f \text{ is the Fermi wavevector. Show that the wavefunction found in (h) just reduces to the regular free Fermion wavefunction.} \]

\[(j) \text{ Now let’s allow quasi-particles. Up to now, you just calculated the ground state energy and wavefunction of the system. We will now allow } m_k \neq 0. \text{ Then the energy of the system is the ground state energy you have already calculated } + \text{ the terms (ii). Show that the energy of the system is then for the form: } H = H_{\text{Groundstate}} + \sum_k \epsilon(k) m_k \text{ and determine the quasi-particle excitation spectrum } \epsilon(k). \text{ Plot your result for } \epsilon(k) \text{ a function of } k, \text{ indicating clearly where } k_f \text{ is and } \mu. \]