Emergent States of Matter

HOMEWORK SHEET 4 and 5

HW4: Due 5pm Fri 6 April 2018.
HW5: Due 5pm Fri 13 April 2018.

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

Question 4–1.
In this question, you will derive the excitation spectrum for Bogoliubov quasi-particles, starting from an equation of motion for the condensate known as the Gross-Pitaevskii equation. You will be surprised at how easy it is from this approach, compared to the operator approach.

(a) Writing the field operator $\hat{\psi}(\mathbf{r},t) = \psi_0(\mathbf{r},t) + \tilde{\psi}(\mathbf{r},t)$, find the equation satisfied by $\tilde{\psi}$, by substituting into the Heisenberg equation of motion with the Bogoliubov Hamiltonian. Here the notation is as in the lectures: note that $\psi_0(\mathbf{r},t)$ is the wave function for a condensate in some general superposition of plane wave states.

(b) We are interested in small fluctuations about the uniform state of the condensate. Verify that the uniform state is $\psi_0 = \sqrt{n_0}\exp(-i\mu t/\hbar)$, with $\mu = U_0 n_0$, and hence derive the linearised equation of motion for $\tilde{\psi}$.

(c) Define $\delta\psi = \tilde{\psi}\exp(i\mu t/\hbar)$. Show that

$$\left(i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2\nabla^2}{2m}\right)\delta\psi - n_0 U_0\left(\delta\psi + \delta\psi^+\right) = 0,$$

where $\delta\psi^+$ is the Hermitian conjugate of $\delta\psi$.

(d) From this equation, and its Hermitian conjugate, obtain an equation for the quantity $(\delta\psi - \delta\psi^+)$ and seek a solution of the form $\exp i(\mathbf{k}\cdot\mathbf{x} - \epsilon(\mathbf{k})t/\hbar)$ to find $\epsilon(\mathbf{k})$. Explain briefly the interpretation of $\epsilon(\mathbf{k})$.

Question 4–2: Solution of a minimal model for a superconductor.

Only do parts (a) - (c) for this week's homework. In 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 μ 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: $u_k = u_{-k}$, $v_{-k} = -v_k$. 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 α_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:

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

HW 5. If you want you can start it now. DUE DATE FRI APRIL 13 5pm

(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 the 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 ξ_k in terms of $E(k)$ and the constant Δ.

(f) Now, using its definition and your result for ξ_k, show that Δ 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 ω_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 Δ 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) Define the condensation energy $E_c \equiv H(U) - H(0)$. Show that $E_c < 0$, i.e. the free electron gas has a higher energy than the state of the system which is the ground state of $H(U)$. [You should be able to calculate that $E_c = -N(0)\Delta^2/2$, assuming that $\Delta \ll \hbar\omega_D$, but you do not need to do this.]

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

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

(j) 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 $m_k \neq 0$. Then the energy of the system is the ground state energy you have already calculated + the terms (ii). Show that the energy of the system is then for the form: $H = H_{Groundstate} + \sum_k \epsilon(k) m_k$ and determine the quasi-particle excitation spectrum $\epsilon(k)$. Plot your result for $\epsilon(k)$ a function of k, indicating clearly where k_f is and μ.