UNIVERSITY OF LONDON
MSci EXAMINATION May 2007
for Internal Students of Imperial College of Science, Technology and Medicine
This paper is also taken for the relevant Examination for the Associateship

QUANTUM THEORY OF MATTER

For Fourth-Year Physics Students
Thursday 24th May 2007: 14.00 to 16.00

Answer THREE questions.
Choose at least ONE question from EACH section.
All questions carry equal marks.

Marks shown on this paper are indicative of those the Examiners anticipate assigning.

General Instructions

Write your CANDIDATE NUMBER clearly on each of the THREE answer books provided.

If an electronic calculator is used, write its serial number in the box at the top right hand corner of the front cover of each answer book.

USE ONE ANSWER BOOK FOR EACH QUESTION.

Enter the number of each question attempted in the horizontal box on the front cover of its corresponding answer book.

Hand in THREE answer books even if they have not all been used.

You are reminded that the Examiners attach great importance to legibility, accuracy and clarity of expression.
SECTION A

1. A homogeneous quantum fluid of $N$ interacting bosonic atoms can be modelled by the Hamiltonian ($u > 0$):

$$\hat{H} = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 + u \sum_{i<j} \delta(r_i - r_j).$$

(i) Explain briefly why this delta-function interaction is a reasonable model for inter-atomic interactions, e.g. in liquid helium. [2 marks]

(ii) The dynamics of this system can be described by the Gross-Pitaevskii (GP) equation for the condensate wavefunction $\psi(r, t)$:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + u(|\psi|^2 - \bar{n})\psi,$$

where $\bar{n}$ is the mean number density of bosons in the system.

(a) Explain the physical origin of the three terms on the right-hand side of the GP equation. [3 marks]

(b) Consider small fluctuations around the ground state and write the wavefunction as $\psi = \sqrt{\bar{n}} + \delta \psi(r, t)$ with $|\delta \psi| \ll \sqrt{\bar{n}}$. Show that $\delta \psi$ approximately obeys the equation:

$$i\hbar \frac{\partial}{\partial t} \delta \psi = \left[ -\frac{\hbar^2}{2m} \nabla^2 + u\bar{n} \right] \delta \psi + u\bar{n} \delta \psi^*,$$

where $\delta \psi^*$ denotes the complex conjugate of $\delta \psi$. [4 marks]

(c) Consider the trial solution $\delta \psi = a_k \exp[i(k \cdot r - \omega_k t)] + b_k \exp[-i(k \cdot r - \omega_k t)]$ where $a_k$ and $b_k$ are independent of space and time. Using this trial solution, show that the natural frequency $\omega_k$ for a travelling wave with wavevector $k$ in this system is given by:

$$\omega_k = k \left[ \frac{u\bar{n}}{m} \left( 1 + \frac{k^2 \xi^2}{4} \right) \right]^{1/2},$$

where $\xi = \hbar/(mu\bar{n})^{1/2}$. [4 marks]

(d) This homogenous quantum fluid has excited states that have definite momentum and energy. How is the frequency $\omega_k$ at a given $k$ related to the energy $E(P)$ of an excited state with momentum $P$? [1 mark]

(e) State the Landau criterion for superfluidity in terms of the excitations of a quantum liquid, i.e. in terms of the energies $E$ and momenta $P$ of these excitations. Discuss whether this Bose system should be a superfluid. [3 marks]
In fact, the many-body Hamiltonian $\hat{H}$ can be solved in one dimension without any approximations, providing exact solutions for the excited states. The momenta $p$ and energies $E$ where there are excited states are shown as the shaded area in Fig.1. This means that, at any given momentum $p$, there is a continuous range of possible excitations. This is in sharp contrast to the results of the approximate Gross-Pitaevskii treatment which indicates that there is only one excitation with a definite energy $E = E(p)$ at a given momentum $p$.

![Figure 1](image)

Figure 1: Each point in the shaded region of the $p$-$E$ plane represents a possible excited state with momentum $p$ and energy $E$. ($p_0 = 2\pi \hbar \bar{n}$.)

(a) Is this one-dimensional system a superfluid? Explain your reasoning in terms of the Landau criterion. [1 mark]

(b) The exact results indicate that the Gross-Pitaevskii theory completely fails to describe this one-dimensional system. Discuss why. [2 marks]

[TOTAL 20 marks]
2. (i) In the presence of a magnetic field $B$, the mechanical momentum of a particle with charge $q$ is given by $-i\hbar\nabla - qA$ where $A$ is the vector potential corresponding to the magnetic field: $B = \nabla \times A$. Explain how the phase $\theta(r)$ of the condensate wavefunction for the superconductor varies under the gauge transformation

$$A \rightarrow A + \nabla \chi$$

for some time-independent scalar function $\chi(r)$. [3 marks]

(ii) A ring of an $s$-wave superconductor contains a superconductor-insulator-superconductor (SIS) junction. The insulator is thin enough that Cooper pairs can tunnel between the two superconductors. Suppose the superconductor has phases $\theta_L$ and $\theta_R$ on two sides (L and R) of the insulating layer. The Josephson pair tunnelling current $I_p$ across the junction from L to R is given by

$$I_p = I_c \sin \Theta_{LR},$$

where $\Theta_{LR}$ is the gauge-invariant phase difference between the two sides of the junction. The dimensions of the ring are larger than the penetration depth of the superconductor.

(a) In the absence of any magnetic flux, the phase difference $\Theta_{LR}$ is given by $\theta_R - \theta_L$. Write down this gauge-invariant phase difference $\Theta$ when there is a non-zero vector potential $A(r)$. Show that your expression is invariant under a gauge transformation. [2 marks]

(b) Show that the gauge-invariant phase difference across the junction is given by:

$$\Theta_{LR} = \frac{2e}{\hbar} \oint A \cdot d\mathbf{r},$$

where the line integral is taken around a closed loop around the ring which traverses the junction from R to L. (Ignore any flux that penetrates the junction itself.) [5 marks]

(c) Is the enclosed flux quantised in units of $\Phi_0 = \hbar/2e$? Explain. [2 marks]
(iii) For a ring containing several junctions, it can be shown that the sum of all the
gauge-invariant phase differences across the junctions around the ring is given by
\((2e/h) \oint A \cdot dr\) (see Fig.2).

For instance, for three junctions as depicted in Fig.2, [DO NOT PROVE]
\[ \Theta_{12} + \Theta_{34} + \Theta_{56} = \frac{2e}{\hbar} \oint A \cdot dr, \]
where the line integral is a closed loop around the ring in the \textit{anticlockwise} direction.

(a) A two-junction SQUID is made by attaching superconducting leads to a ring
with two identical SIS junctions with critical current \(I_c\) (see Fig.3). Using the
above result for multiple junctions, show that the current through this SQUID
cannot exceed:
\[ I_{\text{max}} = 2I_c \cos \left( \frac{\pi \Phi}{\Phi_0} \right) \]
where \(\Phi\) is the magnetic flux enclosed by the ring.
[Note: \(\sin a + \sin b = 2\sin \left( \frac{a+b}{2} \right) \cos \left( \frac{a-b}{2} \right) \).]

(b) A theory suggests that a superconductor-ferromagnet-superconductor (SFS)
junction introduces a phase shift of \(\pi\) for Cooper pair tunnelling so that the tunnelling
current across such a junction becomes \(I_p = I_c \sin(\Theta + \pi) = -I_c \sin \Theta\).
Suppose that we can fabricate a two-junction SQUID where one of the two
junctions is an SFS junction and the other is a SIS junction. Assuming that the
two junctions have a similar \(I_c\), describe how the theoretical \(\pi\)-shift hypothesis
can be tested by measuring the current through this device.

[5 marks]

[3 marks]

[TOTAL 20 marks]
3. A neutral superfluid of $N$ bosonic atoms of mass $m$ is confined between two concentric cylindrical walls of similar radii. The inner wall has radius $R$ and the outer wall has radius $R + d$ with $d \ll R$. They have length $l$. Assume that this superfluid is well approximated as a totally condensed Bose condensate.

(i) Write down the superfluid velocity $v$ in terms of the phase $\theta(r)$ of the condensate wavefunction $\psi_c(r) = \sqrt{n}e^{i\theta}$. [2 marks]

(ii) Show that circulation $K \equiv \oint v \cdot dr$ around a closed loop in the superfluid is quantised in units of $\hbar/m$. [3 marks]

(iii) What is the local superfluid velocity $v(r)$ in this fluid when there is a circulation of $K = nK\hbar/m$? You should give the direction and magnitude of the superflow in cylindrical polar coordinates $(r, \phi, z)$. [3 marks]

(iv) Hence write down the condensate wavefunction $\psi_c(r, \phi, z)$ of the condensate in cylindrical polar coordinates. You may assume that the density $n(r)$ is constant. (You may need to use the cylindrical polar form for the gradient operator: $\nabla = \hat{r}\partial/\partial r + \hat{\phi}r^{-1}\partial/\partial \phi + \hat{z}\partial/\partial z$.) [2 marks]

(v) The angular momentum operator for a single particle is $-i\hbar\partial/\partial \phi$ in cylindrical polars. What is the total angular momentum $L_z$ of the system with a circulation of $K = nK\hbar/m$? [1 mark]

(vi) Show that the kinetic energy of the superfluid with circulation $K = nK\hbar/m$ in this container is given by:

$$E_K = n_K^2 \frac{\hbar^2 \pi l \bar{n}}{m} \ln \left( 1 + \frac{d}{R} \right),$$

where $\bar{n}$ is the average number density of the atoms. [4 marks]

(vii) The container is rotated around its axis of symmetry at an angular frequency $\omega$. Show that, for $d \ll R$, the superfluid does not rotate at all if the container is rotating at a frequency $\omega \ll \omega_c \approx \hbar/2mR^2$.

You can assume that the energy $E'$ of the superfluid in the rotating frame where the walls are at rest is related to the energy $E$ in the lab frame by $E' = E - \omega L_z$. You should nevertheless explain why we need to work in the rotating frame. [3 marks]

(viii) What is the relative velocity between the fluid and inner container wall as a function of the rotation frequency $\omega$ when $\omega > \omega_c$. You may give your answer using a sketch of the relative velocity against the rotation frequency. [2 marks]

[TOTAL 20 marks]
SECTION B

4. (i) Consider the creation and annihilation operators, \( \hat{c}_{k\sigma}^\dagger \) and \( \hat{c}_{k\sigma} \), for a fermion with momentum \( \hbar k \) and spin \( \sigma \) (=↑ or ↓).

(a) Write down anticommutation relations for these operators:
\[ \{ \hat{c}_{k\sigma}, \hat{c}_{q\sigma'}^\dagger \}, \{ \hat{c}_{k\sigma}^\dagger, \hat{c}_{q\sigma'} \} \text{ and } \{ \hat{c}_{k\sigma}, \hat{c}_{q\sigma'} \}. \]

(b) Show that these fermions obey the Pauli exclusion principle.

(ii) The BCS wavefunction is of the form
\[ |\text{BCS} \rangle = \prod_k (u_k + v_k \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\downarrow}^\dagger) |\text{vac} \rangle \]
where \( |\text{vac} \rangle \) is the vacuum state with no electrons. The coherence factors \( u_k \) and \( v_k \) are real and are given by:
\[ v_k^2 = 1 - u_k^2 = \frac{1}{2} \left[ 1 - \frac{\epsilon_k}{(\epsilon_k^2 + \Delta^2)^{1/2}} \right] \]
where \( \Delta \) is the BCS energy gap and \( \epsilon_k = \hbar^2 k^2 / 2m - E_F \) gives the energies of non-interacting electrons as measured from the Fermi level \( E_F \).

(a) What are \( u_k \) and \( v_k \) for a non-interacting Fermi gas?

(b) Sketch, as a function of \( k = |k| \), the probability of finding a Cooper pair with a spin-up electron at momentum \( \hbar k \) and a spin-down electron at momentum \( -\hbar k \) in the BCS ground state. Indicate any relevant wavevector scales in your diagram.

(c) Hence or otherwise, write down the average number of electrons in the BCS ground state in terms of the coherence factors.

(iii) An excited state (with momentum \( \hbar q \) and spin ↑) of the BCS superconductor is \( |q \uparrow \rangle \equiv \gamma_{q\uparrow}^\dagger |\text{BCS} \rangle \) where the creation operator \( \gamma_{q\uparrow}^\dagger \) is:
\[ \gamma_{q\uparrow}^\dagger = A_{q\uparrow} \hat{c}_{q\uparrow}^\dagger - B_{q\downarrow} \hat{c}_{-q\downarrow} \]
with real \( A_q \) and \( B_q \).

(a) The excited state has spin \( S = 1/2 \) and so should be a fermionic excitation. Show that this condition means that we must have \( A_q^2 + B_q^2 = 1 \).

(b) It can be shown that \( A_q = u_q \) and \( B_q = v_q \). In terms of the coherence factors, what is the charge of the excited state \( |q \uparrow \rangle \) compared to the charge of the ground state?

(c) By considering the action of \( \gamma_{q\uparrow}^\dagger \) on \( (u_q + v_q \hat{c}_{q\uparrow}^\dagger \hat{c}_{-q\downarrow}^\dagger) |\text{vac} \rangle \), find the probability of finding a spin-up electron with momentum \( \hbar q \) in the excited state \( |q \uparrow \rangle \).

Write down also the probability of finding a Cooper pair with a spin-up electron at momentum \( \hbar q \) and a spin-down electron at momentum \( -\hbar q \) in this state.

[TOTAL 20 marks]
5. Bosonic atoms can be trapped optically in an ‘optical lattice’ which is a periodic potential $V(\mathbf{r})$ generated by standing waves of a set of laser beams. The single-particle levels in this potential have orthonormal wavefunctions $\phi_\alpha(\mathbf{r})$ with energies $\epsilon_\alpha (\alpha = 1, 2, 3, \ldots)$. In other words, they are eigenfunctions of the single-particle Hamiltonian:

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r})\right] \phi_\alpha(\mathbf{r}) = \epsilon_\alpha \phi_\alpha(\mathbf{r}).$$

The optical lattice is designed so that the two single-particle levels with lowest energy ($\alpha = 1, 2$) are degenerate. Let us set this energy to be zero, i.e. $0 = \epsilon_1 = \epsilon_2 < \epsilon_3 < \ldots$

(i) (a) Consider the operators $\hat{c}_\alpha^\dagger$ and $\hat{c}_\alpha$ which create and annihilate respectively a boson in level $\alpha$. Write down the commutation relations for $\hat{c}_\alpha$ and $\hat{c}_\alpha^\dagger$. In other words, what are $[\hat{c}_\alpha, \hat{c}_\beta^\dagger]$, $[\hat{c}_\alpha, \hat{c}_\beta]$ and $[\hat{c}_\alpha^\dagger, \hat{c}_\beta]^\dagger$? [3 marks]

(b) Many bosons are trapped in the optical lattice. Write down the Hamiltonian $\hat{H}_0$ for the system in second-quantised form (i.e. using $\hat{c}_\alpha$ and $\hat{c}_\alpha^\dagger$) if the bosons do not interact with each other. [2 marks]

(ii) The bosons have a pairwise interaction $U(\mathbf{r} - \mathbf{r}') = u \delta(\mathbf{r} - \mathbf{r}')$. This contributes a term $\hat{H}_{\text{int}}$ to the Hamiltonian:

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}},$$

$$\hat{H}_{\text{int}} = \frac{1}{2} \int d^3\mathbf{r} \int d^3\mathbf{r}' \hat{\psi}^\dagger (\mathbf{r}) \hat{\psi}^\dagger (\mathbf{r}') U(\mathbf{r} - \mathbf{r}') \hat{\psi} (\mathbf{r}') \hat{\psi} (\mathbf{r}),$$

where $\hat{\psi}$ and $\hat{\psi}^\dagger$ are the boson field operators. These field operators can be rewritten using the set of orthonormal wavefunctions $\phi_\alpha$ as the basis:

$$\hat{\psi}(\mathbf{r}) = \sum_\alpha \phi_\alpha(\mathbf{r}) \hat{c}_\alpha \quad \text{and} \quad \hat{\psi}^\dagger(\mathbf{r}) = \sum_\alpha \phi_\alpha^*(\mathbf{r}) \hat{c}_\alpha^\dagger.$$

Consider the subset of many-boson states where the bosons are condensed in the two degenerate levels of lowest energy ($\alpha = 1, 2$). Let $|N_1, N_2\rangle$ denote the many-boson state with $N_1$ bosons condensed in level 1 and $N_2$ bosons in level 2.

(a) Use the state $|N, 0\rangle$ (with $N$ bosons condensed into $\alpha = 1$) as a variational wavefunction. Show that the variational energy $\langle \hat{H} \rangle$ of this trial state is

$$E(N, 0) = \frac{U_{11}}{2} N (N - 1).$$

where $U_{\alpha\beta} = u \int |\phi_\alpha(\mathbf{r})|^2 |\phi_\beta(\mathbf{r})|^2 d^3r$.

[You may find the formulae at the end of this question useful.] [4 marks]
(b) In the Hartree approximation, a particle $i$ in level $\alpha$ sees the density profile of another particle $j$ in state $\beta$ as presenting a potential energy of $u_{\alpha\beta}(r) = u|\phi_\beta(r)|^2$. By considering the probability density of finding the particle $i$ at position $r$, show that the average interaction energy between particles $i$ and $j$ is $U_{\alpha\beta}$. Hence, show that $E(N, 0)$ is simply the Hartree interaction energy for all particles condensed into level 1. [3 marks]

(c) Show that the variational energy for the state $|N_1, N_2\rangle$ is

$$E(N_1, N_2) = \frac{U_{11}}{2}N_1(N_1 - 1) + \frac{U_{22}}{2}N_2(N_2 - 1) + 2U_{12}N_1N_2.$$  

[3 marks]

(d) The design of the optical lattice means that $U_{11} = U_{22}$ for symmetry reasons. $U_{12}$ is also very similar to $U_{11}$ and $U_{22}$. By comparing the variational energies for $|N, 0\rangle$ and $|N/2, N/2\rangle$, show that, in the case of attractive interactions, a system of $N$ bosons would prefer to condense into the two degenerate levels in equal numbers instead of condensing into just one of the levels. [2 marks]

(e) Show that the Hartree interaction energy for the state $|N_1, N_2\rangle$ is $E(N_1, 0) + E(0, N_2) + U_{12}N_1N_2$ and so does not account for all the interaction energy of the system. [2 marks]

(f) What would be our conclusion for the condensation of attractive bosons if we only considered the Hartree contribution to the energy? [1 mark]

[TOTAL 20 marks]

[You may use the fact that, for boson creation and annihilation operators, $\hat{a}^\dagger$ and $\hat{a}$:

$$\hat{a}^\dagger|n\rangle = \sqrt{n + 1}|n\rangle \quad \text{and} \quad \hat{a}|n\rangle = \sqrt{n}|n - 1\rangle,$$

where $|n\rangle$ denotes the state with $n$ bosons.]
6. A homogeneous system of bosons of mass $m$ interacting via a Coulombic repulsion can be described by the Hamiltonian:

$$\hat{H} \simeq \int \frac{\hbar^2}{2m} |\nabla \hat{\psi}|^2 d^3r + \frac{u}{2} \int \int \frac{(\hat{n}(\mathbf{r}) - \bar{n})(\hat{n}(\mathbf{r}') - \bar{n})}{|\mathbf{r} - \mathbf{r}'|} d^3r \, d^3r'$$

where $\bar{n}$ is the density of a uniform background of opposite charge which attracts the bosons. This can be expressed in terms of the density $\hat{n}$ and the phase $\hat{\theta}$ of the Bose field $\hat{\psi} = \exp(i\hat{\theta})\sqrt{\bar{n}}$. For small density and phase fluctuations, the kinetic term in this Hamiltonian can be approximated by:

$$\hat{H}_0 = \bar{n} \sum_{k \neq 0} \epsilon_k \left( \hat{\theta}_k \hat{\theta}_{-k} + \frac{1}{4} \hat{v}_k \hat{v}_{-k} \right)$$

where $\bar{n}$ is the average boson density, $\epsilon_k = \frac{\hbar^2 k^2}{2m}$ and the Fourier transforms of the density and phase fluctuations are defined by:

$$\hat{\theta}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{k \neq 0} e^{i\mathbf{k} \cdot \mathbf{r}} \hat{\theta}_k \quad \text{and} \quad \hat{n}(\mathbf{r}) = \bar{n} \left( 1 + \frac{1}{\sqrt{V}} \sum_{k \neq 0} e^{i\mathbf{k} \cdot \mathbf{r}} \hat{\nu}_k \right)$$

for a system of volume $V$.

(i) What is the average density of the bosons in the ground state? [1 mark]

(ii) Show that the interaction part of the Hamiltonian can be written as

$$\hat{H}_1 = \bar{n}^2 \sum_{k \neq 0} \frac{2\pi u}{k^2} \hat{v}_k \hat{v}_{-k}.$$  

You may use the formula: $\int \frac{e^{i\mathbf{q} \cdot \mathbf{R}}}{R} d^3\mathbf{R} = \frac{4\pi}{q^2}$. [4 marks]

(iii) Hence, show that the total Hamiltonian can be written in the form:

$$\hat{H} = \hat{H}_0 + \hat{H}_1 = \frac{1}{2} \sum_{k \neq 0} E_k \left[ 2\bar{n} l_k^2 \hat{\theta}_k \hat{\theta}_{-k} + \bar{n} \frac{l_k^2}{2} \hat{v}_k \hat{v}_{-k} \right].$$

You should identify $E_k$ and $l_k^2$ in terms of $k$, $\epsilon_k$, $u$ and $\bar{n}$. [5 marks]

(iv) We can define $\sqrt{\bar{n}} \hat{\theta}_k = (\hat{a}_k + \hat{a}_k^\dagger)/2l_k$ and $\sqrt{\bar{n}} \hat{v}_k = il_k (\hat{a}_k - \hat{a}_k^\dagger)$. It can be shown that $[\hat{a}_k \hat{a}_q^\dagger] = \delta_{k,q}$. [DO NOT PROVE.]

What is the physical significance of this commutation relation for $\hat{a}_k$ and $\hat{a}_q^\dagger$? [2 marks]
(v) Show that the Hamiltonian can be written as:

\[ \hat{H} = \sum_{k \neq 0} \left[ \epsilon_k \left( \epsilon_k + \frac{8\pi u \bar{n}}{k^2} \right) \right]^{1/2} \left( \hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} \right). \]

You should explain the physical significance of this final expression for the Hamiltonian. [4 marks]

(vi) Show that the excitations in this Coulombic system have an energy gap of \( E_g = (4\pi \hbar^2 u \bar{n}/m)^{1/2} \). [1 mark]

(vii) A neutral superfluid with short-range interactions (e.g. of the form \( u\delta(r - r') \)) has gapless excitations. In other words, the energy of an excitation with momentum \( \bar{\hbar}k \) vanishes in the limit of \( k \to 0 \). What is the physical reason behind this? Why is this reasoning not applicable to this Coulombic superfluid? [3 marks]

[ TOTAL 20 marks ]

End