Imperial College London

BSc/MSci EXAMINATION May 2012

This paper is also taken for the relevant Examination for the Associateship

QUANTUM THEORY OF MATTER

For 4th-Year Physics Students

Tuesday, 29th May 2012: 14:00 to 16:00

Answer THREE questions.
There are two sections. 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

Complete the front cover of each of the THREE answer books provided.

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

USE ONE ANSWER BOOK FOR EACH QUESTION.

Enter the number of each question attempted in the 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 Examiners attach great importance to legibility, accuracy and clarity of expression.

SECTION A

1. (i) The Bose-Einstein distribution for a state of energy ϵ may be written as

$$f(\epsilon) = \frac{1}{\exp\{\beta(\epsilon - \mu)\} - 1}.$$

What does $f(\epsilon)$ describe?

What are β and μ and how are they determined?

What type of particles obey this expression?

Give an example of a particle for which $\mu = 0$ always but otherwise is described by the Bose-Einstein distribution.

Give an example of a particle for which μ can take different values and whose distribution is described by the Bose-Einstein distribution. [5 marks]

(ii) Suppose that the density of states in a material is of the form

$$g(\epsilon) = \frac{(\epsilon - \epsilon_0)^\alpha}{E^{1+\alpha}} \;\text{ if }\; \epsilon \geq \epsilon_0\,, \qquad \text{and} \qquad g(\epsilon) = 0 \;\text{ if }\; \epsilon < \epsilon_0$$

where E is a constant with units of energy, α is a fixed parameter and ϵ_0 is the ground state. Show that the number of particles in the system, N, is given by

$$N = (\beta E)^{-1-\alpha} J(z, \alpha) \qquad \text{where} \qquad J(z, \alpha) = \int_0^\infty dx\, \frac{x^\alpha}{e^x z^{-1} - 1}\,,$$

and $z = \exp\{\beta(\mu - \epsilon_0)\}$.

Rearrange this equation to find the function $T_0(N)$ where

$$1 = \left(\frac{T}{T_0(N)}\right)^{1+\alpha} J(z, \alpha)\,.$$

[5 marks]

(iii) Show that for fixed N, $\alpha > -1$, and high temperatures $T \gg T_0(N)$ that $\mu \approx -(1 + \alpha) k_B T \ln(T/T_0(N))$ justifying any expansions and approximations used. [5 marks]

(iv) Show that for given N that a condensate will form at a temperature

$$T_c = T_0(N)[J(1, \alpha)]^{-1/(1+\alpha)}$$

By considering the behaviour of the integrand of $J(1, \alpha)$ near $x = 0$ and for large x, explain why we find a non-zero critical temperature, $0 < T_c < \infty$, for for $\alpha > 0$.

For black body radiation, the density of states has $\alpha = 2$. Explain why no condensate is observed for black body radiation. [5 marks]

[Total 20 marks]

2. A Gross-Pitaevskii equation for the dynamics of the condensate wavefunction ψ_c of a Bose-Einstein condensate (BEC) is

$$i\hbar\frac{\partial\psi_c}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi_c + u|\psi_c|^2\psi_c - \mu\psi_c \tag{1}$$

where $m > 0$, $\mu < 0$ and $u > 0$.

(i) Explain why this Gross-Pitaevskii equation cannot be a quantum mechanical Schrödinger equation and thus why ψ_c can not be a quantum mechanical wave-function.

What is ψ_c in terms of the phase transition between the normal phase and that with a Bose-Einstein condensate?

How is ψ_c related to the density of bosons in the condensate n?

How are μ and u related to the physical properties of the bosons? [6 marks]

(ii) Find the ground state solution for ψ_c when there is a Bose-Einstein condensate and justify your derivation.

Hence show that $\mu = u\bar{n}$ where $\bar{n}$ is the average density of bosons. [4 marks]

(iii) What are the dimensions of ψ_c?

Show that the Gross-Pitaevskii equation of Eqn. 1 may be written in a dimensionless form where

$$i\frac{\partial f}{\partial\tau} = -\frac{1}{2}\tilde{\nabla}^2 f + (|f|^2 - 1)f \tag{2}$$

where $\tilde{\nabla} = \xi\nabla$ and $\tau = t/t_0$. You must give an explicit expressions for the healing length ξ and time scale t_0 in terms of the parameters of the Gross-Pitaevskii equation (1). [5 marks]

(iv) What physically is conserved by the dynamics of the Gross-Pitaevskii equation? Demonstrate this by showing that the continuity equation $\dot{\rho} + \nabla.\boldsymbol{j} = 0$ holds for appropriate definitions of ρ and $\boldsymbol{j}$ in terms of ψ_c which you must give. You may use dimensionless quantities or not, as you prefer. [5 marks]

[Total 20 marks]

3. The Ginzburg-Landau Free energy describes time-independent configurations in a superconductor and is

$$F = \int d^3\boldsymbol{r} \left(\frac{\hbar^2}{2m^*}|\boldsymbol{D}\psi|^2 + a(T)|\psi|^2 + b(T)|\psi|^4 + \frac{1}{2\mu_0}B^2 \right) . \qquad (1)$$

where the magnetic field is the curl of the vector potential $\boldsymbol{A}$, i.e. $\boldsymbol{B} = \nabla \times \boldsymbol{A}$. Here $\boldsymbol{D}$ is the covariant derivative where $\boldsymbol{D} = \nabla - (iq/\hbar)\boldsymbol{A}$ and q is the electric charge of the Cooper pair.

The gauge transformation for the fields in the Ginzburg-Landau Free energy (1) are

$$\psi \to \psi' = e^{iq\theta}\psi \,, \qquad \boldsymbol{A} \to \boldsymbol{A}' = \boldsymbol{A} + \hbar\nabla\theta \,, \qquad (2)$$

where $\theta(\boldsymbol{r})$ is an arbitrary function of spatial coordinate $\boldsymbol{r}$.

(i) Show that $\boldsymbol{D}\psi \to \boldsymbol{D}'\psi' = (\nabla - i(q/\hbar)\boldsymbol{A}')\psi' = e^{iq\theta}\boldsymbol{D}\psi$ under (2).
Hence show that the Ginzburg-Landau Free energy (1) is invariant under gauge transformations (2).
Also show that the physical current $\boldsymbol{J}$ is gauge invariant where

$$\boldsymbol{J} = -\frac{i\hbar q}{m^*}\left(\psi^*(\boldsymbol{D}\psi) - (\boldsymbol{D}\psi)^*\psi\right) . \qquad (3)$$

[5 marks]

(ii) For a type I superconductor in its superconducting phase the magnetic field is excluded from the bulk of the superconductor. Use this to derive the ground state solution deep inside such a superconductor.
What are appropriate forms for the functions $a(T)$ and $b(T)$ for temperatures T near the critical temperature T_c?
By comparing the $|\boldsymbol{D}\psi|^2$ and $a(T)|\psi|^2$ terms, or otherwise, find an expression for the coherence length ξ up to numerical factors. [5 marks]

(iii) In a type I superconductor the magnetic field varies on length scales λ_L, the London penetration depth, which is much shorter than the coherence length. Find an expression for λ_L in terms of the parameters of equation (1) (up to numerical constants). *Hints* use dimensional analysis or use the ansatz that at the edge of an infinite slab of superconductor occupying $z \geq 0$ the magnetic field falls off as $\exp\{-z/\lambda_L\}$.
Hence show that there is a constraint on the parameters of the Ginzburg-Landau Free energy describing a type I superconductor that (up to numerical constants)

$$\kappa = \lambda_L/\xi \propto \sqrt{\frac{(m^*)^2 b}{\hbar^2\mu_0 q^2}} \qquad (4)$$

Comment on the temperature dependence of this ratio in Ginzburg-Landau theory.
Sketch how the magnetic field and the condensate field vary in two physical situations:

[*This question continues on the next page . . .*]

(a) at the boundary of a large slab of type I superconductor in an external magnetic field,

(b) around a flux line in a type II superconductor.

In each case you should indicate how this relates to λ_L, ξ and κ.

[10 marks]

[Total 20 marks]

SECTION B

4. N identical particles of mass M are confined to lie in a ring. Their positions r_i and momenta p_i ($i = 1, \ldots, N$) are real and are components of N-dimensional vectors $\boldsymbol{r}$ and $\boldsymbol{p}$. The classical behaviour is defined by the Hamiltonian

$$H = \left[\sum_{i=1}^{N} \frac{p_i^2}{2M} + \frac{M\omega^2}{2} \sum_{i,j=1}^{N} r_i A_{ij} r_j \right] = \left[\frac{\boldsymbol{p}.\boldsymbol{p}}{2M} + \frac{M\omega^2}{2} \boldsymbol{r}^{\mathsf{T}}.\mathsf{A}.\boldsymbol{r} \right] . \qquad (1)$$

The matrix A is dimensionless, real and symmetric, but there may be significant interactions between any pair of particles, so $A_{ij} = A_{ji}$ are real numbers and generally $O(1)$. We can always decompose the matrix A as $\mathsf{A} = \mathsf{U}^{\mathsf{T}}\Lambda\mathsf{U}$ where Λ is a diagonal matrix with the real eigenvalues of A, λ_i, lying along the diagonal, and U may always be chosen to be a real orthogonal matrix so that $\mathsf{U}^* = \mathsf{U}$, $\mathsf{U}^{-1} = \mathsf{U}^{\mathsf{T}}$, and $\mathsf{U}^{\mathsf{T}}\mathsf{U} = \mathsf{U}\mathsf{U}^{\mathsf{T}} = \mathbb{1}$ where $\mathbb{1}$ is the unit matrix.

(i) Define new position coordinates $R_i = \sum_j U_{ij} r_j$ (i.e. $\boldsymbol{R} = \mathsf{U}\boldsymbol{r}$). The appropriate conjugate momentum to the i-th position is $\Pi_i = \sum_j U_{ij} p_j$ (i.e. $\Pi = \mathsf{U}\boldsymbol{p}$). The R_i and Π_i are real and you may assume this without proof.
Show that the classical Hamiltonian (1) may be written in terms $\omega_i^2 = \omega^2 \lambda_i$ as (only one of these two forms is required)

$$H = \sum_{i=1}^{N} \left[\frac{1}{2M} \Pi_i \Pi_i + \frac{M\omega_i^2}{2} R_i R_i \right] = \left[\frac{1}{2M} \Pi^{\mathsf{T}}.\Pi + \frac{M\omega^2}{2} \boldsymbol{R}^{\mathsf{T}}.\Lambda.\boldsymbol{R} \right] .$$

[5 marks]

(ii) In quantum mechanics the variables r_i and p_i are replaced by the operators $\hat{r}_i$ and $\hat{p}_i$ where $\hat{r}_i$ and $\hat{p}_i$ are all Hermitian operators and $[\hat{r}_j, \hat{p}_i] = i\hbar\delta_{i,j}$, and $[\hat{r}_j, \hat{r}_i] = [\hat{p}_j, \hat{p}_i] = 0$. Define $\hat{R}_i = \sum_j U_{ij} \hat{r}_i$ and $\hat{\Pi}_i = \sum_j U_{ij} \hat{p}_j$. The $\hat{R}_i$ and $\hat{\Pi}_i$ are then hermitian operators and you may assume this without proof.
Show that $\hat{R}_i$ and $\hat{\Pi}_i$ satisfy the same commutation relations as $\hat{r}_i$ and $\hat{p}_i$, that is $[\hat{R}_i, \hat{\Pi}_j] = i\hbar\delta_{i,j}$ and $[\hat{R}_i, \hat{R}_j] = [\hat{\Pi}_i, \hat{\Pi}_j] = 0$. [5 marks]

(iii) We define the annihilation operators $\hat{a}_i = (\hat{R}_i/L_i + i\hat{\Pi}_i L_i/\hbar)/\sqrt{2}$ with length scales $L_i = (\hbar/M\omega_i)^{1/2}$. What is the creation operator $\hat{a}_i^\dagger$?
Compute the commutators $[\hat{a}_i, \hat{a}_j^\dagger]$ and $[\hat{a}_i, \hat{a}_j]$ and $[\hat{a}_i^\dagger, \hat{a}_j^\dagger]$. [4 marks]

(iv) The quantum Hamiltonian $\hat{H}$ is the classical Hamiltonian (1) with the variables r_i and p_i replaced by the operators $\hat{r}_i$ and $\hat{p}_i$. Show that $\hat{H}$ may be rewritten as

$$\hat{H} = \sum_{i=1}^{N} \hbar\omega_i \left(\hat{a}_i^\dagger \hat{a}_i + \frac{1}{2} \right) .$$

Hence, without further detailed calculation, deduce the energy eigenstates of this system. You may quote standard results for a single quantum harmonic oscillator. [6 marks]

[Total 20 marks]

5. A Fock space for bosons may be defined in terms of the normalised basis states $|n\rangle$ built from the creation operator $\hat{a}^\dagger$ acting on the vacuum state $|0\rangle$ as follows

$$[\hat{a}, \hat{a}^\dagger] = 1 \, , \, \hat{a}|0\rangle = 0 \, , \, \hat{a}|n\rangle = \sqrt{n}|n-1\rangle \, , \, \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \, . \tag{1}$$

(i) Show that

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle \, .$$

We define a *coherent state* $|\lambda\rangle_{\text{coh}}$ to be an eigenstate of the annihilation operator $\hat{a}$ so that

$$\hat{a}|\lambda\rangle_{\text{coh}} = \lambda|\lambda\rangle_{\text{coh}} \, . \tag{2}$$

Why are the eigenvalues λ not necessarily real?

Show that the normalised coherent state is (up to an arbitrary phase)

$$|\lambda\rangle_{\text{coh}} = \exp\{-|\lambda|^2/2\} \exp\{\lambda\hat{a}^\dagger\}|0\rangle \tag{3}$$

Hint:- Express $|\lambda\rangle_{\text{coh}}$ as a superposition of basis states $|n\rangle$, $|\lambda\rangle_{\text{coh}} = \sum_n c_n|n\rangle$, and find a recursion relation for the coefficients c_m in this expansion by considering $\langle m|\hat{a}|\lambda\rangle_{\text{coh}}$. [8 marks]

(ii) In quantum field theory, the coherent states for a bosonic field ψ, $|\psi\rangle$, may be defined as the eigenstates for the field operator $\hat{\psi}$ where

$$\hat{\psi}(\boldsymbol{r}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}.\boldsymbol{r}} \hat{a}_{\boldsymbol{k}} \, ,$$

i.e. $\hat{\psi}(\boldsymbol{r})|\psi\rangle = \psi(\boldsymbol{r})|\psi\rangle$. Find the explicit form for the coherent states $|\psi\rangle$ of field ψ in terms of the Fourier transform $\psi(k)$ of $\psi(\boldsymbol{r})$.

[4 marks]

(iii) The Hamiltonian for a Bose gas may be approximated as

$$\hat{H} = \int d^3\boldsymbol{r} \left[-\frac{\hbar^2}{2m}\hat{\psi}^\dagger(\boldsymbol{r})\nabla^2\hat{\psi}(\boldsymbol{r}) - \mu\hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r}) + \frac{u}{2}\hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})\hat{\psi}(\boldsymbol{r}) \right] \, .$$

Describe the physics behind each of the three terms.

Find the coherent state $|\psi_0(\boldsymbol{r})\rangle$ for which the energy expectation value $E = \langle\psi_0|\hat{H}|\psi_0\rangle$ is minimised assuming a large volume (i.e. ignore any boundary effects).

What is the relationship between the minimum energy coherent state $|\psi_0\rangle$ and the original vacuum $|0\rangle$ in the infinite volume limit. Comment briefly on what this tell us about the physics described by these two different vacuum states?

[8 marks]

[Total 20 marks]

6. The BCS wavefunction is

$$|\mathrm{BCS}\rangle = \prod_{\mathrm{k}} (u_{\mathrm{k}} + v_{\mathrm{k}} \hat{c}^{\dagger}_{\mathrm{k}\uparrow} \hat{c}^{\dagger}_{-\mathrm{k}\downarrow}) |0_c\rangle\,, \tag{1}$$

$$\text{with} \qquad \{\, \hat{c}_{\mathrm{k}\sigma}, \hat{c}^{\dagger}_{\mathrm{q}\eta} \,\} = \delta_{\mathrm{kq}} \delta_{\sigma\eta}\,, \qquad \{\, \hat{c}_{\mathrm{k}\sigma}, \hat{c}_{\mathrm{q}\eta} \,\} = \{\, \hat{c}^{\dagger}_{\mathrm{k}\sigma}, \hat{c}^{\dagger}_{\mathrm{q}\eta} \,\} = 0\,. \tag{2}$$

Here $\hat{c}_{\mathrm{k}\sigma}$ and $\hat{c}^{\dagger}_{\mathrm{k}\sigma}$ are the annihilation and creation operators for electrons of momentum $\mathbf{k}, \mathbf{q}$ and spin $\sigma, \eta = \uparrow, \downarrow$. These obey the usual fermionic canonical anti-commutation relations The vacuum state $|0_c\rangle$ satisfies $\hat{c}_{\mathrm{k}\sigma}|0_c\rangle = 0$ and $\langle 0_c | 0_c \rangle = 1$.

(i) Show that $\hat{c}^{\dagger}_{\mathrm{k}\sigma} \hat{c}^{\dagger}_{\mathrm{k}\sigma} = 0$ for each $\mathbf{k}$ and σ value (no sum over $\mathbf{k}$ or σ). Relate this to the Pauli exclusion principle.
Show that $\hat{c}^{\dagger}_{\mathrm{k}\sigma} \hat{c}_{\mathrm{k}\sigma}$ is the number operator for the state labelled $(\mathbf{k}, \sigma)$.
Note there is no sum over $\mathbf{k}$ or σ in either case. [4 marks]

(ii) Let 1 and 2 label two distinct states so that $\hat{c}_1$ and $\hat{c}_2$ are annihilation operators for these two different states. If we define a two-dimensional vector $\widehat{\boldsymbol{C}}$ as

$$\widehat{\boldsymbol{C}} = \begin{pmatrix} \hat{c}_1 \\ \hat{c}^{\dagger}_2 \end{pmatrix}$$

then the anticommutation relations (2) are $\{\widehat{C}_i, \widehat{C}_j\} = \{\widehat{C}^{\dagger}_i, \widehat{C}^{\dagger}_j\} = 0$ and $\{\widehat{C}_i, \widehat{C}^{\dagger}_j\} = \delta_{ij}$ with $i, j = 1, 2$ (no need to prove this).
By using a two-dimensional vector notation

$$\widehat{\boldsymbol{B}} = \begin{pmatrix} \hat{b}_1 \\ \hat{b}^{\dagger}_2 \end{pmatrix}$$

or otherwise, show that for *complex* parameters u and v the transformation

$$\hat{b}_1 = u\hat{c}_1 - v\hat{c}^{\dagger}_2\,, \qquad \hat{b}_2 = v\hat{c}^{\dagger}_1 + u\hat{c}_2 \tag{3}$$

is canonical if $|u|^2 + |v|^2 = 1$. That is show that the b annihilation and creation operators obey the same anticommutation relations (2). [6 marks]

(iii) Show that the BCS state $|\mathrm{BCS}\rangle$ is annihilated by the operators

$$\hat{\gamma}_{\mathrm{k}\uparrow} = u_{\mathrm{k}} \hat{c}_{\mathrm{k}\uparrow} - v_{\mathrm{k}} \hat{c}^{\dagger}_{-\mathrm{k}\downarrow}\,. \tag{4}$$

Having proved equation (4) you may then assume that $\hat{\gamma}_{\mathrm{k}\downarrow} = u_{\mathrm{k}} \hat{c}_{\mathrm{k}\downarrow} + v_{\mathrm{k}} \hat{c}^{\dagger}_{-\mathrm{k}\uparrow}$ in the rest of this question. [7 marks]

(iv) What operators describe the quasiparticle excitations in a BCS superconductor and what quantum numbers can you associate with these operators?
In a BCS superconductor with BCS gap Δ, the coherence factors u_{k} and v_{k} are given by:

$$|v_{\mathrm{k}}|^2 = 1 - |u_{\mathrm{k}}|^2 = \frac{1}{2}\left[1 - \frac{\epsilon_{\mathrm{k}}}{(\epsilon_{\mathrm{k}}^2 + \Delta^2)^{1/2}}\right] \tag{5}$$

where $\epsilon_{\mathrm{k}} = \hbar^2 k^2/2m - E_{\mathrm{F}}$ is the free-electron energy relative to the Fermi level.
In what regime are the quasiparticles neither electron-like nor hole-like?
[3 marks]

[Total 20 marks]