# University of Durham

## EXAMINATION PAPER

May/June 2015 Examination code: PHYS3631WE01

**FOUNDATIONS OF PHYSICS 3B**

**SECTION A**. Statistical Physics
**SECTION B**. Condensed Matter Physics part 1
**SECTION C**. Condensed Matter Physics part 2

**Time allowed:** 3 hours

**Additional material provided:** None

**Materials permitted:** None

**Calculators permitted:** Yes **Models permitted:** Casio fx-83 GTPLUS or Casio fx-85 GTPLUS

**Visiting students may use dictionaries:** No

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**Instructions to candidates:**

- Answer the compulsory question that heads each of sections A, B and C. These **three** questions have a total of 15 parts and carry 50% of the total marks for the paper. Answer **one** other question from **each** section. If you attempt more than the required number of questions only those with the lowest question number compatible with the rubric will be marked: **clearly delete** those that are not to be marked. The marks shown in brackets for the main parts of each question are given as a guide to the weighting the markers expect to apply.
- **ANSWER EACH SECTION IN A SEPARATE ANSWER BOOK**
- Do **not** attach your answer booklets together with a treasury tag, unless you have used more than one booklet for a single section.

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**Information**

A list of physical constants is provided on the next page.

## Information

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| Elementary charge: | $e = 1.60 \times 10^{-19}$ C |
| Speed of light: | $c = 3.00 \times 10^{8}\,\mathrm{m\,s^{-1}}$ |
| Boltzmann constant: | $k_{\mathrm{B}} = 1.38 \times 10^{-23}\,\mathrm{J\,K^{-1}}$ |
| Electron mass: | $m_{\mathrm{e}} = 9.11 \times 10^{-31}$ kg |
| Gravitational constant: | $G = 6.67 \times 10^{-11}\,\mathrm{N\,m^{2}\,kg^{-2}}$ |
| Proton mass: | $m_{\mathrm{p}} = 1.67 \times 10^{-27}$ kg |
| Planck constant: | $h = 6.63 \times 10^{-34}$ J s |
| Permittivity of free space: | $\epsilon_0 = 8.85 \times 10^{-12}\,\mathrm{F\,m^{-1}}$ |
| Magnetic constant: | $\mu_0 = 4\pi \times 10^{-7}\,\mathrm{H\,m^{-1}}$ |
| Molar gas constant: | $R = 8.31\,\mathrm{J\,K^{-1}\,mol^{-1}}$ |
| Avogadro's constant: | $N_{\mathrm{A}} = 6.02 \times 10^{23}\,\mathrm{mol^{-1}}$ |
| Gravitational acceleration at Earth's surface: | $g = 9.81\,\mathrm{m\,s^{-2}}$ |
| Stefan-Boltzmann constant: | $\sigma = 5.67 \times 10^{-8}\,\mathrm{W\,m^{-2}\,K^{-4}}$ |
| Astronomical Unit: | AU = $1.50 \times 10^{11}$ m |
| Parsec: | pc = $3.09 \times 10^{16}$ m |
| Solar Mass: | $M_\odot = 1.99 \times 10^{30}$ kg |
| Solar Luminosity: | $L_\odot = 3.84 \times 10^{26}$ W |



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**SECTION A**. STATISTICAL PHYSICS

Answer Question 1 and **either** Question 2 **or** Question 3.

1. (a) Consider an assembly of $N$ weakly-interacting, distinguishable particles contained in a fixed volume $V$, with fixed internal energy $U$. Are the various distributions $\{n_i\}$ of the particles in single-particle states equally probable, or do they have different probabilities? State briefly what distinguishes the Boltzmann distribution from other distributions $\{n_i\}$ of the assembly of distinguishable particles. [4 marks]

   (b) In a gas of $N$ weakly-interacting, identical, Bose particles in a fixed volume $V$, with fixed total energy $U$, the $i$-th single-particle energy level has energy $\epsilon_i$ and degeneracy $g_i$. Consider a distribution $\{n_i\}$ of the $N$ bosons in single-particle energy levels, where $n_i$ bosons have energy $\epsilon_i$. Show that the number of microstates $\Omega[\{n_i\}]$ corresponding to the distribution $\{n_i\}$ is given by

   $$\Omega[\{n_i\}] = \prod_i \frac{(n_i + g_i)!}{n_i! g_i!}.$$

   What is the limit of $\Omega[\{n_i\}]$ for a dilute gas, $g_i \gg n_i$? [4 marks]

   (c) Derive the density of states in $k$-space, $g(k)\,\delta k$, for a free particle in three dimensions. [4 marks]

   (d) Derive the density of states in energy, $g(\epsilon)\,\delta\epsilon$, for a particle with energy $\epsilon = \alpha\, k^{3/2}$ in three dimensions. [4 marks]

   (e) The volume occupied by a $^3$He atom (spin 1/2) in liquid helium is $46 \times 10^{-30}$ m$^3$. Use this information to give numerical estimates for the Fermi energy and the Fermi temperature for $^3$He atoms in liquid $^3$He. [4 marks]

  

2. A system of $N$ classical weakly-interacting particles is in contact with a heat bath at temperature $T$. The energy associated with each independent degree of freedom of the particles is quadratic, e.g., the energy of the degree of freedom $x$ is $\epsilon = a\,x^2$, with $a > 0$.

   (a) Using the Boltzmann distribution, obtain the average single-particle energy for the degree of freedom $x$. Show that the internal energy $U$ of the system of $N$ particles, when there are $\eta$ such degrees of freedom is:

   $$U = \eta\,\frac{N k_{\mathrm{B}} T}{2}.$$

   This result is known as the Equipartition Theorem. [4 marks]

   [Hint: $\int_{-\infty}^{\infty} dx\, \exp(-b\,x^2) = \sqrt{\pi/b}\,,\ b > 0$. To obtain the integral $\int_{-\infty}^{\infty} dx\, x^2\, \exp(-b\,x^2)$ differentiate both sides with respect to $b$.]

   (b) Using the Equipartition Theorem, obtain the heat capacities under constant volume of:

   (i) A gas of $N$ monoatomic neon atoms at high temperatures.

   (ii) A gas of $N$ diatomic molecules of oxygen ($O_2$) at high temperatures. Are all the degrees of freedom of $O_2$ excited at all temperatures?

   [4 marks]

The vibrations of a diatomic molecule can be approximated as one dimensional harmonic oscillations, with energies $\epsilon_n^{\mathrm{vibr}} = (n+1/2)h\nu$, with $n = 0, 1, \ldots$, where $\nu$ is the frequency of the oscillation.

   (c) Derive the single-particle partition function $Z_1^{\mathrm{vibr}}$ for the vibrations of a diatomic molecule. [3 marks]

   [Hint: $1 + \omega + \omega^2 + \ldots = (1-\omega)^{-1}$, for $|\omega| < 1$. ]

   (d) Derive the vibrational energy, $U^{\mathrm{vibr}}$, and heat capacity at constant volume, $C_V^{\mathrm{vibr}}$, for a gas of $N$ molecules of $O_2$. Compare your answer with that of part (b). [4 marks]

   (e) Write the expression for the characteristic temperature for the excitation of vibrations, $T^{\mathrm{vibr}}$, in a diatomic molecule. [1 mark]

   (f) The characteristic temperature for vibrations in $O_2$ is $T^{\mathrm{vibr}} = 2200$ K. At room temperature (293 K) what is the vibrational heat capacity $C_V^{\mathrm{vibr}}$ and the percentage contribution of the vibrations to the total heat capacity of $O_2$ gas at constant volume? [4 marks]

  

3. (a) Derive the single-particle partition function, $Z_1$, for a free particle of mass $M$ in three dimensions, constrained to a box of volume $V$, in thermal equilibrium at temperature $T$. [4 marks]

[Hint: $\int_0^\infty dx\, \exp(-b\,x^2) = (1/2)\sqrt{\pi/b}\,,\ b > 0$. To obtain the integral $\int_0^\infty dx\, x^2\, \exp(-b\,x^2)$ differentiate both sides with respect to $b$.]

(b) Give a criterion for the dilute gas limit in terms of the thermal de Broglie wavelength $\lambda_\mathrm{D} = h/\sqrt{2\pi M k_\mathrm{B} T}$. [2 marks]

(c) The free energy for a gas of $N$ weakly interacting particles in a volume $V$ at temperature $T$ is given by $F = -k_\mathrm{B} T \ln Z_N$, where $Z_N$ is the $N$-particle partition function. Find the free energy of:

(i) A gas of distinguishable particles.

(ii) A gas of indistinguishable particles.

(iii) Explain why there is a difference between the answers to parts (c)(i) and (c)(ii).

[4 marks]

(d) Show that the entropy for a classical gas of monatomic distinguishable particles is:

$$S = N k_\mathrm{B} \ln V T^{3/2} + \frac{3}{2} N k_\mathrm{B} \left[ \ln \frac{2\pi M k_\mathrm{B}}{h^2} + 1 \right].$$

[4 marks]

$$\left[ \text{Hint:}\ \ S = \frac{U - F}{T}\,, \quad U = k_\mathrm{B} T^2 \frac{\partial \ln Z_N}{\partial T} \right]$$

(e) A classical gas of distinguishable monatomic particles is in thermal equilibrium at temperature $T = 300$ K in a container of volume $V$. The gas is allowed to expand adiabatically (without change in its entopy) until it occupies twice the initial volume. What is the temperature of the gas after the expansion? [4 marks]

(f) Mention two examples of cooling under constant entropy. [2 marks]

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**SECTION B**. CONDENSED MATTER PHYSICS part 1
Answer Question 4 and **either** Question 5 **or** Question 6.

4. (a) Show that the group velocity of an electron at the bottom of an energy band in the nearly-free electron model is given by

$$v_{\mathrm{group}} = \frac{\hbar k}{m^*},$$

where $\hbar k$ is the crystal momentum of the Bloch electrons and $m^*$ is the effective mass of the electron. Use this to show that a completely filled band makes no contribution to the current carried by a crystal. [4 marks]

(b) Sketch a diagram of the three lowest energy bands of a linear lattice of ions in the nearly-free electron approximation in the extended (Brillouin) zone scheme. Redraw your diagram in both the reduced and periodic zone schemes. [4 marks]

(c) If a magnetic field, $B$, is applied perpendicular to the plane of an electron orbit the diamagnetic response can be shown to be described as the change in magnetic moment,

$$\Delta \underline{m} = -\frac{(e^2 r^2 \underline{B})}{4m^*},$$

where $r$ is the radius of the electron orbit and $m^*$ is the effective mass of the electron. Explain how this change in magnetic moment leads to the Langevin result for the diamagnetic susceptibility of a solid,

$$\chi_{\mathrm{d}} = -\frac{(\mu_0 N Z e^2)}{6m^*} < r^2 >,$$

composed of $N$ atoms per unit volume each with $Z$ electrons.
[4 marks]

(d) Sketch the magnetic field dependence of the magnetisation of a paramagnet at low temperature. Indicate on your sketch the region where Curie's Law is applicable. [4 marks]

(e) Provide a brief explanation of what is meant by direct exchange and superexchange. [4 marks]

5. (a) Describe the de Haas-van Alphen effect and show how oscillations occur at equal intervals of $\frac{1}{B}$ such that

$$\Delta\left(\frac{1}{B}\right) = \frac{2\pi e}{\hbar S},$$

where $S$ is the extremal area of the Fermi surface normal to the direction of the magnetic field $B$. [6 marks]

(b) The area of an electron orbit in $k-$space in a magnetic field $B$ is given by

$$S_n = (n+\gamma)\frac{2\pi e}{\hbar}B,$$

where $S_n$ is the area of the $n$th orbit where $n$ is an integer and $\gamma$ is a phase correction (normally taken to be $\frac{1}{2}$ for free electrons). Use this equation to explain why metals display a magneto-oscillatory behaviour at low temperatures. [4 marks]

(c) Metallic gold has an electron density of $5.9 \times 10^{28}$ m$^{-3}$. Calculate the Fermi energy of this monovalent element. [4 marks]

(d) De Haas-van Alphen measurements of the Fermi surface of a single crystal of gold, at low temperatures and high magnetic fields, show its Fermi surface to be slightly distorted from a spherical shape. Experiments find the magnetic moment has a period of $2.0 \times 10^{-5}$ T$^{-1}$ over a wide range of field directions. In the [111] direction a large period of $6.0 \times 10^{-4}$ T$^{-1}$ is observed, whilst in the [110] direction another extremal orbit is observed with a period of $5.0 \times 10^{-5}$ T$^{-1}$. Calculate the extremal areas ($S$) of these orbits and explain their nature, and discuss what can be inferred about the size and shape of the resulting Fermi surface. [6 marks]

  

6. A ferromagnetic solid contains $Eu^{2+}$ ions arranged in a primitive cubic arrangement with a unit cell lattice parameter of $a = 0.70$ nm. The Curie temperature of the material is 200 K, and each europium ion has 7 electrons in its $4f$ shell. At very low temperatures close to absolute zero the magnetocrystalline anisotropy is described by the constants $K_1(0) = 5.4 \times 10^5$ J m$^{-3}$ and $K_2(0) = 5.1 \times 10^3$ J m$^{-3}$.

   (a) For a cubic crystal structure the magnetocrystalline anisotropy energy density is given by

   $$U_{\text{anis}} = K_1(\alpha_1^2\alpha_2^2 + \alpha_1^2\alpha_3^2 + \alpha_2^2\alpha_3^2) + K_2(\alpha_1^2\alpha_2^2\alpha_3^2),$$

   where $\alpha_1 = \cos\theta_1$ , $\alpha_2 = \cos\theta_2$ , $\alpha_3 = \cos\theta_3$ are the direction cosines of the magnetisation with respect to the [100], [010] and [001] directions. Use this information to demonstrate that $< 100 >$ directions in the crystal are 'easy' axes for magnetisation, whereas $< 111 >$ are 'hard' directions for magnetisation. [6 marks]

   (b) Use Hund's rules to calculate the saturation magnetisation of the ferromagnetic solid at absolute zero. [4 marks]

   [The value of the Bohr magneton is $\mu_B = 9.27 \times 10^{-24}$ J T$^{-1}$.]

   (c) The self energy density of a completely magnetised thin plate is

   $$U = \frac{1}{2}\mu_0 D M_{\text{sat}}^2.$$

   Use your value of the saturation magnetisation, $M_{\text{sat}}$, from part (b) to calculate the self energy density of a thin square plate made from the ferromagnetic solid if it is completely magnetised in the direction perpendicular to the plane of the plate. The plate has a thickness of 0.100 mm and its sides are of length 1.00 m. Under these conditions the demagnetising factor, $D$, has a value of 1.00. [2 marks]

   (d) The [100] crystallographic direction lies perpendicular to the plane of the plate. The energy per unit area of a Bloch wall can be shown to be

   $$\sigma_{\text{BW}} = \pi S\sqrt{\frac{2\text{J}K}{a}},$$

   where $K$ is the magnetocrystalline anisotropy energy, $S$ is the total spin angular momentum number and J is the exchange integral. Calculate the energy per unit area of a 180° domain wall formed in this material at absolute zero, stating any assumptions that you may make. [4 marks]

   (e) For the above plate use your value of $\sigma_{\text{BW}}$ from part (d) to estimate the number of domain walls in the ferromagnet at $T = 0$ K by dividing the self energy by the energy of a single domain wall. [4 marks]

**SECTION C**. CONDENSED MATTER PHYSICS part 2

Answer Question 7 and **either** Question 8 **or** Question 9.

7. (a) A sample of silicon is purified until it only contains donor impurities with concentration $N_{\mathrm{D}} = 1.00 \times 10^{18}$ donors $\mathrm{m}^{-3}$. Compute the temperature below which the sample ceases to show intrinsic behaviour, given that the energy band gap is $E_g = 1.10$ eV, and the conduction and valence band effective densities of states are $N_{\mathrm{C}} = 6.00 \times 10^{25}$ $\mathrm{m}^{-3}$ and $N_{\mathrm{V}} = 3.00 \times 10^{25}$ $\mathrm{m}^{-3}$. For simplicity, assume $N_{\mathrm{C}}$ and $N_{\mathrm{V}}$ are constant. [4 marks]

   (b) A p-n junction is constructed by combining a p-type and an n-type germanium semiconductor. Given that the built-in voltage is 0.30 V at 300 K, compute the corresponding built-in voltage at 325 K. The energy band gap for germanium is $E_g = 0.66$ eV. [4 marks]

   [ Hint: The following expressions for the chemical potentials of the p- and n-type materials, $\mu_p = k_{\mathrm{B}}T \ln\left[\frac{N_{\mathrm{V}}}{N_{\mathrm{A}}}\right], \mu_n = E_g - k_{\mathrm{B}}T \ln\left[\frac{N_{\mathrm{C}}}{N_{\mathrm{D}}}\right]$, may be used without derivation. Here $N_{\mathrm{C}}$ and $N_{\mathrm{V}}$ are the conduction and valence band effective densities of states, $N_{\mathrm{A}}$ is the density of the acceptor impurities in the p-type region, and $N_{\mathrm{D}}$ is the density of donor impurities in the n-type region. For simplicity, $N_{\mathrm{C}}, N_{\mathrm{V}}, N_{\mathrm{A}}$ and $N_{\mathrm{D}}$ can be assumed to be constant with temperature. ]

   (c) A superconducting material has a critical magnetic field of 0.05 T. Using this material, what is the maximum current that can be carried by a wire of diameter 1 mm? [4 marks]

   (d) Given that the penetration depth and coherence length of a given superconducting material are 100 nm and 300 nm respectively, argue whether the material is a type I or type II superconductor. [4 marks]

   (e) Sketch how the real part of the polarizability of a solid depends on frequency when the contributing polarization mechanisms are electronic, ionic, and dipolar in nature. For each contribution, label whether it is of resonance or relaxation type. [4 marks]

8. A 2-D semiconductor has energy, $E$, as a function of wavevector, $\underline{k}$, given by

$$E(\underline{k}) = Ak_x^2 + Bk_y^2 + Ck_x^2k_y^2,$$

where $A$, $B$ and $C$ are positive constants and $|k|^2 = k_x^2 + k_y^2$. Write down an expression for the components of the inverse effective mass, $(1/m^*)_{ij}$, and determine the components in the case of the above 2-D semiconductor. [6 marks]

Sketch the form of the constant energy contours of $E(\underline{k})$ in the $(k_x, k_y)$-space plane when $A = B = C$. [4 marks]

What are the directions of electron acceleration if an electric field is applied in the (1,0) and (1,1) directions? Assume that the wavevector of the electron is $\underline{k} = (0, 0)$ and that $A = B = C$. [6 marks]

Derive the conditions on $A$, $B$ and $C$ such that the material has an isotropic response. This means the direction of the acceleration is always the same as that of the force, and the magnitude of the acceleration depends only on the magnitude of the force, not its direction or the wavevector $\underline{k}$. [4 marks]

[Hint: For the material to be isotropic the inverse effective mass tensor has to be a multiple of the unity matrix, i.e. $(1/m^*)_{ij} = \lambda\delta_{ij}$, where $\lambda$ is a constant scalar.]

9. A ferroelectric material can be described by the following Landau free energy

$$G(P,T) = g_0 + \frac{1}{2}g_2P^2 + \frac{1}{4}g_4P^4 + \frac{1}{6}g_6P^6,$$

where $P$ is the polarization, $g_2 = \gamma(T - T_0)$, $T$ is the temperature of the system, and $T_0$ is the so-called Curie temperature. $\gamma$, $g_0$, $g_4\,(< 0)$ and $g_6\,(> 0)$ are constants in the model.

The critical (transition) temperature, $T_\mathrm{c}$, is defined as the temperature at which the ferroelectric state is equal in free energy to the dielectric state. In this model, show that

$$T_\mathrm{c} = T_0 + \frac{3|g_4|^2}{16\gamma g_6},$$

and that the spontaneous polarization in the ferroelectric state, $P_\mathrm{s}$, is given by

$$P_\mathrm{s}^2 = \frac{|g_4| + \sqrt{|g_4|^2 - 4g_2g_6}}{2g_6},$$

with $|g_4|$ defined as the absolute value of the $g_4$ coefficient. [8 marks]

A metastable state corresponds to a minimum free energy state which has a higher energy than the global minimum. Show that the ferroelectric state is metastable between $T_\mathrm{c} < T \leq T_1$, with $T_1 = T_0 + |g_4|^2/4\gamma g_6$. Similarly, show that the dielectric state is metastable between $T_0 \leq T < T_\mathrm{c}$. [5 marks]

At $T_\mathrm{c} = 110$ K, a ferroelectric material is measured to have a spontaneous polarization $P_\mathrm{s} = 0.1$ C/m$^2$. Given that $\gamma/g_6 = 2 \times 10^{-6}$ C$^4$/m$^8$K, compute $T_0$ and $T_1$. [4 marks]

Based on the model described above, sketch how the polarization will depend on temperature. Will the system show any hysteretic behaviour? Clearly label where $T_0$, $T_\mathrm{c}$ and $T_1$ are in the sketch. [3 marks]