### University of Durham

### **EXAMINATION PAPER**

Year:

May/June	2018	PHYS3631-WE01
Title:		
Foundations of Physics	3B	

Examination code:

Time allowed:	3 ho	urs		
Additional material provided:	None			
Materials permitted:	None			
Calculators permitted:	Yes	Мс	odels permitted:	Casio fx-83 GTPLUS or Casio fx-85 GTPLUS
Visiting students may use dictionaries: No				

#### Instructions to candidates:

Examination session:

- 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 the answers 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.
- Slip your booklets for Sections B and C, in order, inside your booklet for Section A, before they are collected by the invigilator.

#### Information

Section A: Statistical Physics

Section B: Condensed Matter Physics part 1 Section C: Condensed Matter Physics part 2

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

Revision:	
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### Information

 $e = 1.60 \times 10^{-19} \text{ C}$ Elementary charge:  $c = 3.00 \times 10^8 \, \mathrm{m \, s^{-1}}$ Speed of light:  $k_{\rm B} = 1.38 \times 10^{-23} \; {\rm J \, K^{-1}}$ Boltzmann constant:  $\mu_{\rm B} = 9.27 \times 10^{-24} \; {\rm J} \, {\rm T}^{-1}$ Bohr magneton:  $m_{\rm e} = 9.11 \times 10^{-31} \text{ kg}$ Electron mass:  $G = 6.67 \times 10^{-11} \text{ N m}^2 \text{ kg}^{-2}$ Gravitational constant:  $m_{\rm p} = 1.67 \times 10^{-27} \text{ kg}$ Proton mass:  $h = 6.63 \times 10^{-34} \text{ J s}$ Planck constant:  $\epsilon_0 = 8.85 \times 10^{-12} \; \mathrm{F \, m}^{-1}$ Permittivity of free space:  $\mu_0 = 4\pi \times 10^{-7} \; \mathrm{H} \, \mathrm{m}^{-1}$ Magnetic constant:  $R = 8.31 \text{ J K}^{-1} \text{ mol}^{-1}$ Molar gas constant:  $N_{\rm A} = 6.02 \times 10^{23} \ {\rm mol^{-1}}$ Avogadro's constant:  $q = 9.81 \text{ m s}^{-2}$ Gravitational acceleration at Earth's surface:  $\sigma = 5.67 \times 10^{-8} \ \mathrm{W \ m^{-2} \ K^{-4}}$ Stefan-Boltzmann constant:  $AU = 1.50 \times 10^{11} \text{ m}$ 

 $pc = 3.09 \times 10^{16} \text{ m}$ 

 $M_{\odot} = 1.99 \times 10^{30} \text{ kg}$ 

 $L_{\odot} = 3.84 \times 10^{26} \text{ W}$ 

Astronomical Unit: Parsec: Solar Mass: Solar Luminosity:

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### SECTION A: STATISTICAL PHYSICS

Answer Question 1 and either Question 2 or Question 3.

- 1. (a) Explain the concepts of thermodynamic macrostate, microstate and distribution,  $(n_1, n_2, ...)$ , of particles in single-particle states. [4 marks]
  - (b) Consider the microcanonical, or (N, U, V) macrostate describing a system with fixed number of particles N, internal energy U, and volume V. Explain if there is a distribution in single particle states,  $(n_1, n_2, \ldots)$ , whose microstates have the same temperature. [4 marks]
  - (c) Give the statistical definition for the entropy of an isolated system. Show that the total entropy of a composite system made up of two independent subsystems is equal to the sum of the entropies of the subsystems. [4 marks]
  - (d) State, without derivation, the expressions for the Fermi-Dirac (FD) and Bose-Einstein (BE) distributions. Define any symbols that appear in the expressions. Explain the dilute gas limit of these distributions. [4 marks]
  - (e) Show that the density of states in k-space for a free particle in a box of volume V in three dimensions is given by

$$g(k)\delta k = \frac{V}{2\pi^2} k^2 \, \delta k,$$

and then derive the density of states in energy. [4 marks]

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2. The energy of a diatomic molecule of mass M is the sum of the translational, rotational and vibrational energies,  $\epsilon^{\rm mol} = \epsilon^{\rm tran} + \epsilon^{\rm rot} + \epsilon^{\rm vib}$  (ignoring the electronic motion). The rotational energies,  $\epsilon^{\rm rot}_l = \hbar^2 l(l+1)/(2I)$ ,  $l=0,1,\ldots$ , have degeneracy 2l+1, where I is the moment of inertia. The vibrational energies,  $\epsilon^{\rm vib}_n = (n+1/2)h\nu$ ,  $n=0,1,\ldots$ , are not degenerate and  $\nu$  is the frequency of oscillation.

Consider a gas of N diatomic molecules, in a volume V, at temperature T that is much larger than the temperature necessary to rotationally excite the molecules. The molecules in the gas can be treated as distinguishable.

(a) Show that the partition function for a molecule is the product of the partition functions for the translational, rotational and vibrational motions

$$Z^{\text{mol}} = Z^{\text{tran}} \times Z^{\text{rot}} \times Z^{\text{vib}}$$

[2 marks]

- (b) The partition function for the translational motion is  $Z^{\text{tran}} = AV/\beta^{3/2}$ , where A does not depend on V, T, and  $\beta = +1/(k_{\text{B}}T)$ . Without a derivation, give the dimensions of A and state on what quantities it must depend. [2 marks]
- (c) Estimate the characteristic temperature,  $T_{\rm rot}$ , to thermally excite the first rotational excited state in terms of  $\hbar$ , I. Show that for  $T \gg T_{\rm rot}$

$$Z^{\rm rot} = \frac{2Ik_{\rm B}T}{\hbar^2}.$$

[Hint: For  $T\gg T_{\rm rot}$  the sum  $\sum_{l=0}^{\infty}$  can be replaced by  $\int_0^{\infty}dl.$ ] [4 marks]

- (d) (i) Estimate the characteristic temperature,  $T_{\rm vib}$ , to excite the first vibrational excited state.
  - (ii) Show that for  $T \ll T_{\rm vib}$ ,  $Z^{\rm vib} = \exp(-\beta \, h \, \nu/2)$
  - (iii) Show that for  $T \gg T_{\rm vib}$ ,  $Z^{\rm vib} = 1/(\beta \, h \, \nu)$ . (See hint above.) [4 marks]
- (e) Obtain the energy, U, and the heat capacity under constant volume,  $C_{\rm V}$ , of the diatomic gas (i) at a temperature  $T_{\rm rot} \ll T \ll T_{\rm vib}$  and (ii) at a temperature  $T \gg T_{\rm vib}$ . Discuss your results in relation to the equipartition theorem. [6 marks]
- (f) Show the ideal gas law,  $PV = Nk_{\rm B}T$ , for the diatomic gas. [2 marks]

$$\left[\begin{array}{l} \text{Hint: You may use without proof} \\ U = -N \, \frac{\partial \ln Z^{\text{mol}}}{\partial \beta}, \ F = -N k_{\text{B}} T \ln Z^{\text{mol}}, \ P = -\left. \frac{\partial F}{\partial V} \right|_{T} \end{array}\right]$$

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3. (a) Ignoring the spin of particles, the density of states in k-space is given by

$$g(k)\delta k = \frac{V}{2\pi^2} k^2 \, \delta k.$$

How does the density of states in k-space change for a gas of free atoms with spin 3/2 in a box of volume V? [3 marks]

Consider now a gas of N free electrons of mass m and magnetic moment  $\mu_{\rm B}$  in a box of volume V, at zero temperature.

(b) Obtain the Fermi wavevector  $k_{\rm F}$  of the electrons in terms of the electron density N/V, when there is no external magnetic field. You may use the above expression for the density of states in k-space. [3 marks]

After applying a magnetic field B, the single-particle energies for the spin-up and spin-down electrons are  $\epsilon_k^{\uparrow} = \hbar^2 k^2/(2m) - \mu_{\rm B} B$  and  $\epsilon_k^{\downarrow} = \hbar^2 k^2/(2m) + \mu_{\rm B} B$ .

- (c) Explain why the Fermi level or chemical potential (i.e. the energy of the highest occupied single-particle state) is the same for the spin-up and spin-down electrons  $\epsilon_F^{\uparrow} = \epsilon_F^{\downarrow} = \epsilon_F$ . [3 marks]
- (d) When B is weak, only few spin-down electrons can flip spin and align with B. Explain qualitatively why it is not possible for all spin-down electrons to align with the magnetic field. [3 marks]
- (e) Obtain the density of states in energy,  $g^{\sigma}(\epsilon)\delta\epsilon$ ,  $\sigma=\uparrow,\downarrow$ , for the spin-up and spin-down electrons separately, in the presence of the magnetic field B. The density of states in k-space, given in (a) is the same for spin-up and spin-down electrons. [4 marks]
- (f) Write an equation that determines the Fermi level  $\epsilon_{\rm F}$  for the electron gas in the presence of B. You are not required to solve this equation for  $\epsilon_{\rm F}$ . [4 marks]

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

4. (a) Consider a one-dimensional chain of atoms of lattice constant a. Starting from the energy-wavevector E(k) relationship for free electrons explain why the introduction of a periodic potential causes band gaps to open up at the wavevectors  $k = \pm \pi/a$ . [4 marks]

- (b) In the presence of an applied magnetic field  $\underline{B}$  the periodicity  $\Delta\left(\frac{1}{\underline{B}}\right) = 2\pi e/(\hbar S)$  of the de Haas-van Alphen oscillations measures the extremal cross-sectional area S in k-space of the Fermi surface normal to  $\underline{B}$ . Calculate the period expected for rubidium within the free electron model given that the Fermi wavevector is  $0.70 \times 10^{10} \text{ m}^{-1}$ . [4 marks]
- (c) Use Hund's rules to find the values of the total spin, S, the total orbital angular momentum, L, and the total angular momentum, J, of an isolated erbium ion,  $Er^{3+}$ , which has 11 electrons in the 4f shell. [4 marks]
- (d) Describe the origin of ferromagnetic spin waves and ferromagnetic magnons. [4 marks]
- (e) Sketch the typical hysteresis curves of both a magnetically soft material and one that is magnetically hard. Give one example of a technological application of each material. [4 marks]

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5. (a) All materials show some degree of diamagnetism, a small temperature-independent negative magnetic susceptibility. Explain using electromagnetic theory the origin of diamagnetism. [4 marks]

(b) Using either Langévin's classical approach, or a quantum mechanical derivation, show that the diamagnetic susceptibility,  $\chi_d$ , of a solid composed of N atoms per unit volume (each with Z electrons of mass  $m_e$ ) is given by

$$\chi_d = -\frac{\mu_0 N Z e^2}{6m_e} \langle r^2 \rangle,$$

where  $\langle r^2 \rangle$  is the mean square distance of the electrons from the nucleus. [6 marks]

- (c) Bismuth (Z=83, relative atomic mass = 209.0) is a diamagnetic material with a density of  $9.747 \times 10^3$  kg m<sup>-3</sup>. Calculate the magnetic susceptibility of bismuth given that the root mean square atomic radius is 0.155 nm. [6 marks]
- (d) A magnetic field strength of 3000 A m<sup>-1</sup> is applied to a sample of bismuth of mass 10 g. Calculate the magnetic moment induced in the sample by this applied field. [4 marks]

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6. (a) Antiferromagnetism is a property displayed by a class of materials that have a net magnetisation of zero. Explain how these materials are related to ferromagnetic materials and how they can be considered as magnetic even though their net magnetisation is strictly zero. Give an example of an antiferromagnetic material. [4 marks]

(b) The classical Weiss mean field theory of ferromagnetism interprets the magnetisation, M, of a ferromagnetic solid as being composed of both the applied magnetic field  $B_0$  and an 'internal' magnetic field, or exchange field,  $B_{\rm E}$ , arising from the interacting magnetic moments in the solid such that,

$$B_{\rm E} = \lambda M$$

where  $\lambda$  is a constant. Show how this concept can be transferred to antiferromagnets leading to the magnetisation being given by

$$M = M_S B_J \left( \frac{g_J \mu_B J |\lambda| M}{k_B T} \right),$$

where  $B_J$  is the Brillouin function,  $g_J$  is the Landé g-value and J is the total angular momentum quantum number. [4 marks]

(c) The internal magnetic field will disappear for temperatures above the Néel temperature  $T_{\rm N}$  defined by

$$T_{\rm N} = \frac{g_J \mu_{\rm B} (J+1)|\lambda| M_S}{3k_{\rm B}} = \frac{n|\lambda| \mu_{eff}^2}{3k_{\rm B}}.$$

Sketch the form of the temperature dependence of the magnetic susceptibility,  $\chi$ , of an antiferromagnetic single crystal assuming that  $\chi$  is measured in a small magnetic field. Identify on your sketch the Néel temperature,  $T_{\rm N}$ , and briefly explain the behaviour of the features of  $\chi$  below  $T_{\rm N}$ . [6 marks]

(d) An organic solid containing isolated unpaired electrons (free radicals) has a paramagnetic component of the magnetic susceptibility at 1 K of  $7.8 \times 10^{-5}$ . The susceptibility reduces with increasing temperature, eventually becoming negative at high temperatures. The susceptibility vanishes at 980 K and its value at 1 K is 75% of the calculated paramagnetic value. Give a detailed explanation of the likely origins of these features and obtain a form for the actual temperature dependence of the susceptibility. [6 marks]

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# **SECTION C:** CONDENSED MATTER PHYSICS part 2 Answer Question 7 and **either** Question 8 **or** Question 9.

7. (a) The band gap  $(E_q)$  in eV of a  $CdS_xTe_{1-x}$  alloy varies as,

$$E_g = 1.54 - 0.9x + 1.84x^2.$$

The alloy is being evaluated as a potential semiconductor material for a light emitting diode. Determine the wavelength range of light that can be extracted from such a device. [4 marks]

- (b) At room temperature, a semiconductor with a  $2\times10^{13}$  cm<sup>-3</sup> intrinsic carrier concentration contains donor impurities at a concentration of  $3\times10^{15}$  cm<sup>-3</sup>. Calculate the electron and hole concentrations at room temperature. State any assumptions you make. [4 marks]
- (c) Sketch the variation of magnetic field with temperature for Type I and Type II superconductors, clearly identifying the phase fields in each diagram.

If the critical magnetic field of a Type I superconductor is 0.05T, calculate the maximum current than can be carried in a 1.00 mm diameter wire in the superconducting state. [4 marks]

(d) Starting from the London equation

$$\underline{\nabla} \times \underline{j} = -\frac{nq^2}{m}\underline{B},$$

derive the London penetration depth

$$\lambda_L = \left(\frac{m}{\mu_0 n q^2}\right)^{1/2}$$

for a plane boundary (x = 0) separating a superconducting material (x > 0) from the vacuum (x < 0). The magnetic field  $\underline{B}$  is along the z-direction.  $\underline{j}$  is the current density, while n is the density of electrons, each with charge q and mass m. [4 marks]

(e) At a given temperature  $BaTiO_3$  has a polarisation of 0.15  $Cm^{-2}$  and relative permittivity of 1200. Calculate the local electric field at each dipole. [4 marks]

[Hint: proceed via the Clausius-Mossotti relation]

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8. In a pn junction a p-doped region of the semiconductor (acceptor concentration  $N_a$ ) is coupled to a n-doped region (donor concentration  $N_d$ ). The relative permittivity of the semiconductor is  $\epsilon_r$ . The junction is at x=0 and the depletion layer edges are at  $x=-w_p$  and  $x=w_n$  for the p- and n-doped regions respectively.

- (a) Calculate the electric field distribution in the device, and sketch a graph of electric field as a function of position. [4 marks]
- (b) Derive an expression for the built-in voltage  $(\phi_{bi})$  by calculating the change in electric potential within the device. [4 marks]
- (c) Show that if  $N_a \gg N_d$  the depletion layer is largely confined to the *n*-doped region. [2 marks]
- (d) Calculate the electric field distribution in a device where  $N_a$  is constant, but the donor concentration varies linearly from zero at the junction position to  $N_d$  at  $x = w_n$ . Show that charge neutrality is preserved for this device. [7 marks]
- (e) The current for a pn junction under a 0.20 V reverse bias at room temperature is 10  $\mu$ A. Calculate the 0.20 V forward bias current at room temperature. [3 marks]

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9. The Landau free energy of a ferroelectric material has the form

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

where P is the polarisation and T the temperature.  $g_2 = \gamma (T - T_o)$ , where  $T_o$  is the Curie temperature and the constants  $\gamma, g_4$  are both positive. The free energy of the paraelectric phase has arbitrarily been assigned a zero value.

- (a) Determine the spontaneous polarisation of the material for  $T > T_o$  and  $T < T_o$ . [4 marks]
- (b) Sketch on a single diagram the shape of the free energy vs. polarisation curve at  $T = T_o$  and  $T < T_o$ . Identify the energy barrier separating the ferroelectric and paraelectric phases. [4 marks]
- (c) An applied electric field E will add an extra term -EP to the free energy. Using a free energy vs. polarisation curve for  $T < T_o$ , determine whether the spontaneous polarisation increases or decreases under an applied electric field. [2 marks]

In a different ferroelectric material the free energy has the form

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

where  $g_2$  is the same as above,  $g_4$  is now *negative* and  $g_6$  positive. Assume no applied electric fields.

(d) Show that the spontaneous polarisation  $P_s$  for the ferroelectric material is given by

$$(P_s)^2 = \frac{-g_4 + \sqrt{g_4^2 - 4g_2g_6}}{2g_6}.$$

[6 marks]

(e) Using the above result show that the ferroelectric to paraelectric transition temperature  $T_c$  is greater than  $T_o$ . [4 marks]