Imperial College London
BSc/MSci EXAMINATION May 2012

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

SOLID STATE AND ATOMIC PHYSICS

For 3rd-Year Physics Students

Friday, 25th May 2012: 10:00 to 12:00

Answer ALL parts of Section A, ONE question from Section B and ONE question from Section C.
Marks shown on this paper are indicative of those the Examiners anticipate assigning.

General Instructions

Complete the front cover of each of the 4 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 4 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 (Compulsory)

1. (i) The element boron has atomic number $Z = 5$. With explanations, give its ground state configuration, specifying the n and l quantum numbers for each electron. For this ground configuration write down any allowed term, and the possible J quantum numbers. [4 marks]

(ii) Using a one-electron model of a neutral atom, the energy level structure of one-electron atoms can be calculated using quantum defect theory, where an energy level E_{nl} is given by:

$$E_{nl} = -\frac{R_\infty}{n^{*2}} \, ,$$

where n^* is the effective principal quantum number and $R_\infty = 109\,737.315\ \mathrm{cm}^{-1}$.

For sodium, the wavelength of the $4p\,{}^2P$ - $3s\,{}^2S$ transition is 330.4 nm.

Given the quantum defect $\delta_s = 1.373$ for the $3s\,{}^2S$ term, calculate the quantum defect for the $4p\,{}^2P$ term.

Explain in detail why the quantum defects of the $4p\ {}^2P$ and $3s\,{}^2S$ terms differ.

[4 marks]

(iii) Explain the physical origin of the Stark effect. [2 marks]

[Total 10 marks]

2. The energies of an electron moving in a periodic potential form continuous bands separated by gaps of forbidden values of the energy. Use this fact to discuss the following:

(i) The physical origin of the band gaps. [3 marks]

(ii) The differences between metals and insulators. What is the main distinguishing feature between insulators and semiconductors? [2 marks]

(iii) The reason why most elemental crystalline solids are metals. [2 marks]

(iv) The difference between donors and acceptors in semiconductors, including the position of the donor and acceptor levels. [3 marks]

[Total 10 marks]

SECTION B

3. (i) For an atom in a magnetic field the Hamiltonian may be written:

$$\hat{H}_{mag} = \zeta_{LS}\,\hat{\mathbf{L}} \cdot \hat{\mathbf{S}} + \frac{\mu_B}{\hbar}(\hat{\mathbf{L}} \cdot \hat{\mathbf{B}} + 2\hat{\mathbf{S}} \cdot \hat{\mathbf{B}})$$

(a) Explain what the terms in this Hamiltonian represent. In this context, what is meant by the strong field limit ? [3 marks]

(b) Show that, in a strong magnetic field, with only $B_z \neq 0$, the energy shift is given by: $\Delta E_{mag} = \mu_B B_z (M_L + 2M_S)$. [2 marks]

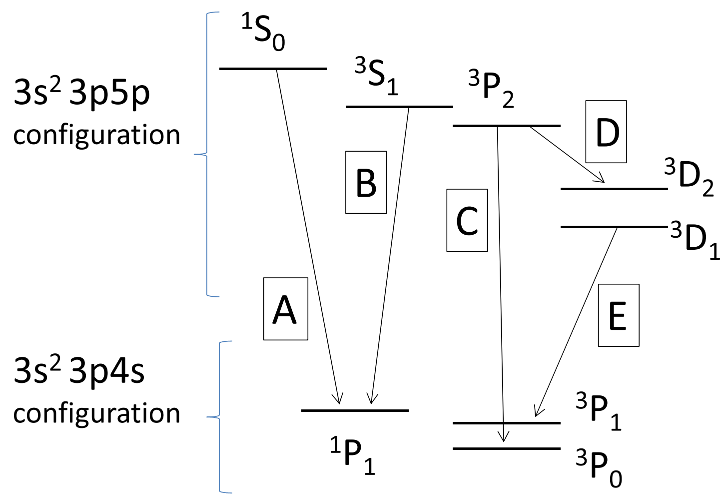
(c) For the element lithium, consider the splitting of two terms, upper term $1s^2 2p\,^2P$ and lower term $1s^2 2s\,^2S$, in the presence of a strong magnetic field. Draw an energy level diagram showing these terms, and the states arising from level splitting in the magnetic field. In your diagram label the states with quantum numbers. Use units of $\mu_B B_z$ to indicate the energy shift of each state from the field free term energies. [4 marks]

(d) The lithium 670.8 nm line, transition $1s^2 2p\,^2P$ - $1s^2 2s\,^2S$, is seen to be composed of components (transitions between states) in a magnetic field. Calculate the separation (in cm^{-1}) between the extreme components of this transition when it is observed in the spectrum of the cool magnetic star HD154708. This star has a mean magnetic field strength 2.45 T, which is a high magnetic field strength in the case of lithium.

[Bohr magneton μ_B = 0.4669 cm^{-1} T^{-1}, and relevant selection rules are $\Delta M_s = 0$, $\Delta M_l = 0, \pm 1$] [4 marks]

(ii) (a) What is an *allowed transition*? List the selection rules for allowed transitions. [3 marks]

(b) Comment on each of the transitions shown in the partial energy level diagram for the silicon atom below: are they allowed? and if not, why not? [4 marks]



[Total 20 marks]

4. (i) Considering multi-electron atoms, explain what is meant by:

(a) *the residual electrostatic interaction*

(b) *the LS coupling approximation*

(c) *the spin-orbit interaction* [5 marks]

(ii) (a) In the context of diatomic molecules, explain, with a sketch, what the following are: an *electronic spectrum*, a *pure rotation spectrum* and also a *vibration-rotation spectrum*.
Comment also on which spectral regions these three types of spectra may lie in. [4 marks]

(b) The vibrational energy levels of a molecule, ϵ_v, can be calculated using:

$$\epsilon_v = \bar{\omega}_e \, (v \; + \; 1/2) - \; x_e \, \bar{\omega}_e \, (v + 1/2)^2$$

What is the significance of x_e?
Write down expressions, in terms of the constants $\bar{\omega}_e$ and x_e, for the energies of the lowest three vibrational levels in a diatomic molecule.
[3 marks]

(c) Calculate the central wavenumbers for the fundamental and first overtone transitions of HCl given $\bar{\omega}_e$ = 2990.6 cm^{-1} and x_e = 0.0174.
Explain why and in what way the observed vibrational spectrum would differ if the temperature of the molecules was raised very significantly from low to high temperature. [3 marks]

(d) The force constant is defined as $k_f = 4\pi^2\bar{\omega}_e^2 c^2\mu$, where c is the speed of light, and μ is the reduced mass. The mass number of Cl is 35. Calculate the force constant for HCl. [2 marks]

(e) The transitions calculated in (c) are not observed with N_2 or O_2, why ?
Comment also on why nitrogen and oxygen (the largest components of our atmosphere) are not *"greenhouse gases"*. [3 marks]

[Total 20 marks]

SECTION C

5. Consider an intrinsic two-dimensional semiconductor in which the valence and conduction bands are described by the free-electron dispersion relation corresponding to a region of area $L \times L$. The density of states is independent of energy,

$$D(E)\,dE = A\,dE\,,$$

where $A = m^* L^2/\hbar^2\pi$ is a constant and m^* is the effective mass of the electron.

(i) The numbers of electrons N in the conduction band and holes P in the valence band are given by

$$N = A_c \int_{E_c}^{\infty} \frac{dE}{e^{(E-\mu)/k_B T} + 1}\,, \qquad P = A_v \int_{0}^{E_v} \frac{dE}{e^{(\mu-E)/k_B T} + 1}\,,$$

in which $A_v = m_v^* L^2/\hbar^2\pi$, $A_c = m_c^* L^2/\hbar^2\pi$, where m_v^* and m_c^* are the effective masses in the valence and conductions bands, respectively, E_v and E_c are their band edges, and the bottom of the valence band is the zero of energy. Change the integration variable in these expressions to $x = (E - \mu)/k_B T$ and evaluate the resulting integrals. [6 marks]

(ii) Use the relation $N = P$ and the Boltzmann-type approximation, where $\ln(1+x) \approx x$ for small x, to obtain

$$m_c^* e^{-\beta(E_c-\mu)} = m_v^*\Big[e^{\beta(E_v-\mu)} - e^{-\beta\mu}\Big]\,.$$

[5 marks]

(iii) Solve this expression for μ and show that the dominant terms yield

$$\mu = \tfrac{1}{2} k_B T \ln\!\left(\frac{m_v^*}{m_c^*}\right) + \tfrac{1}{2}(E_v + E_c)\,.$$

[4 marks]

(iv) Using appropriate diagrams, explain the qualitative dependence of the chemical potential on temperature if (i) $m_v^* = m_c^*$, (ii) $m_v^* > m_c^*$, and (iii) $m_v^* < m_c^*$.
[5 marks]

[Total 20 marks]

6. The Drude theory of electrical conduction regards the electrons in a metal as free between instantaneous collisions separated by an average collision time τ.

(i) The equation for the velocity v of an electron of mass m and charge e moving in a time-dependent electric field $E(t) = E_0 e^{-i\omega t}$ is, in the Drude theory,

$$m\frac{dv}{dt} + \frac{mv}{\tau} = eE(t)\,.$$

Determine the solution $v(t)$. [4 marks]

(ii) The electrical current j in a metal with a density n of electrons is $j = nev$. Use your result in (i) to show that Drude's theory produces Ohm's law, $j = \sigma E$, with

$$\sigma = \frac{ne^2\tau}{m(1 - i\omega\tau)}\,.$$

[2 marks]

(iii) For a field $\mathbf{E} = \mathbf{i}\,E_0 e^{i(kx-\omega t)}$, show that the dispersion relation within a linear conducting medium with permittivity ϵ and permeability μ and which satisfies Ohm's law is obtained from the Maxwell equations

$$\nabla \times \mathbf{E} + \mu\frac{\partial \mathbf{H}}{\partial t} = 0\,, \qquad \nabla \times \mathbf{H} = \mathbf{J} + \epsilon\frac{\partial \mathbf{E}}{\partial t}\,,$$

with $\nabla \cdot \mathbf{E} = 0$, as

$$k^2 = \mu\epsilon\omega^2\left(1 + \frac{i\sigma}{\epsilon\omega}\right) \equiv \mu\epsilon\omega^2\varepsilon(\omega)\,.$$

This defines the complex dielectric function $\varepsilon(\omega)$.

The following identity might be useful: $\nabla\times(\nabla\times\mathbf{V}) = \nabla(\nabla\cdot\mathbf{V}) - \nabla^2\mathbf{V}$. [6 marks]

(iv) Consider the limit $\omega\tau \gg 1$. Referring to the equation of motion in (i), describe in words the motion of the electron in this limit. Show that $\varepsilon(\omega)$ reduces to

$$\varepsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2}\,,$$

where the plasma frequency $\omega_p^2 = ne^2/\epsilon m$. [3 marks]

(v) Explain the difference between the situations where $\omega < \omega_p$ and $\omega > \omega_p$. For many metals, ω_p lies in the ultraviolet range of frequencies. What does this tell you about the appearance of metals in visible light? [5 marks]

[Total 20 marks]