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KEELE UNIVERSITY

EXAMINATIONS, 2009/10

Level III

Friday 30th April 2010, 09.30 – 11.30

PHYSICS/ASTROPHYSICS

PHY-30009

QUANTUM PHYSICS OF ATOMS AND MOLECULES

Candidates should attempt to answer THREE questions.

NOT TO BE REMOVED FROM THE EXAMINATION HALL

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1. Consider a particle of mass m in the potential

$$V_1(x) = \begin{cases} \infty & x < 0 \\ V_0 x & x \geq 0 \end{cases}$$

for which the eigenstate of the ground state is approximated by the normalized trial function

$$\psi(x) = \begin{cases} 0 & x < 0 \\ \frac{1}{\sqrt{2}}\lambda^{3/2} x e^{-\lambda x/2} & x \geq 0 \end{cases}$$

(a) Explain *briefly* how the variational principle can be used to determine an optimal value for the parameter λ and why this value of λ will give an upper limit to the energy of the ground state. [15]

(b) Use $\psi(x)$ to estimate the expectation value for the potential energy of the particle, $\langle V \rangle$, in terms of λ and V_0. [20]

(c) The expectation value for the kinetic energy of the particle calculated using $\psi(x)$ is

$$\langle T \rangle = \frac{1}{4}\left(\frac{\hbar^2}{2m}\right)\lambda^2.$$

i. Use the variational principle to calculate the optimal value of λ. [25]

ii. Hence, show that the energy of the ground state of the potential $V_1(x)$ is approximately $2.476 V_0^{\frac{2}{3}} \left(\frac{\hbar^2}{2m}\right)^{\frac{1}{3}}$. [10]

(d) Consider an electron in the potential $V_1(x)$ with $V_0 = 6.2\,\mathrm{eV\,nm^{-1}}$.

i. Calculate an upper limit to the ground state energy of the electron in this case. [20]

ii. The numerically determined value for the energy of the ground state is 2.615 eV. What can you conclude about the trial function ψ? [10]

[You may find the following integral to be useful

$$\int_0^\infty x^n e^{-\alpha x}\, dx = \frac{n!}{\alpha^{n+1}}$$]

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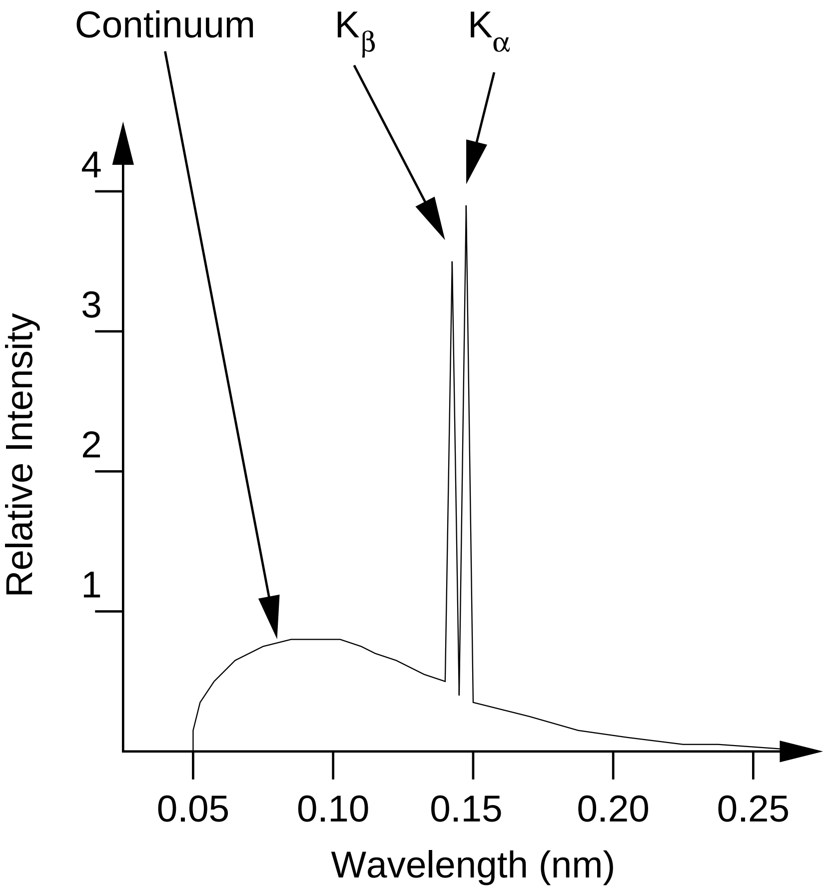
2. (a) The figure below shows the spectrum of X-rays emitted from a sample of zinc when bombarded by high energy electrons.



i. Describe the physical origin of the features labelled "Continuum", "K_α" and "K_β" in this spectrum. [20]

ii. Show that the K_α line appears at the wavelength expected for your interpretation of its origin given in part i. [20]

iii. Estimate the energy of the incident electrons. Explain your method clearly. [15]

(b) Describe briefly the physical origin of the K-edge and L-edge features in the X-ray absorption spectrum of metals. [15]

(c) Estimate the photon energy at the K-edge for zinc. [10]

(d) Explain briefly why the L-edge shows "fine-structure" in the form of three closely spaced edges. [20]

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3. Magnesium atoms have two optically active electrons. In the ground state the electrons have the configuration $3s^2$ and occupy an energy level with the spectroscopic notation $^1S_0$. In one possible excited state these electrons have the configuration $3s^1\,3p^1$.

(a) Sketch the energy levels for the electrons in the excited state using spectroscopic notation to label each state. Your sketch should indicate the correct ordering of the energy levels according to Hund's rules and the relative spacing of different levels. You do not need to provide an energy scale for your sketch. [20]

(b) The ^3P multiplet of the $3s^1\,3p^1$ state has experimentally determined energies (relative to the ground-state) of 2709.443 meV, 2711.930 meV and 2716.979 meV. Show that the splitting of these energy levels is consistent with the LS-coupling scheme. [25]

(c) State the selection rules that govern allowed transitions from the $3s^1\,3p^1$ state. Hence, list the only transition from the excited state to the $^1S_0$ energy level of the ground state that is not forbidden. [25]

(d) The Landé g-factor for an energy level is given by

$$g = 1 + \frac{j'(j'+1) + s'(s'+1) - \ell'(\ell'+1)}{2j'(j'+1)}.$$

In the absence of any external fields, the transition in part (c) produces a single spectral line at 285.2127 nm. Calculate the wavelengths of the spectral lines produced by the same transition in the presence of an external magnetic field of 0.2 T. [30]

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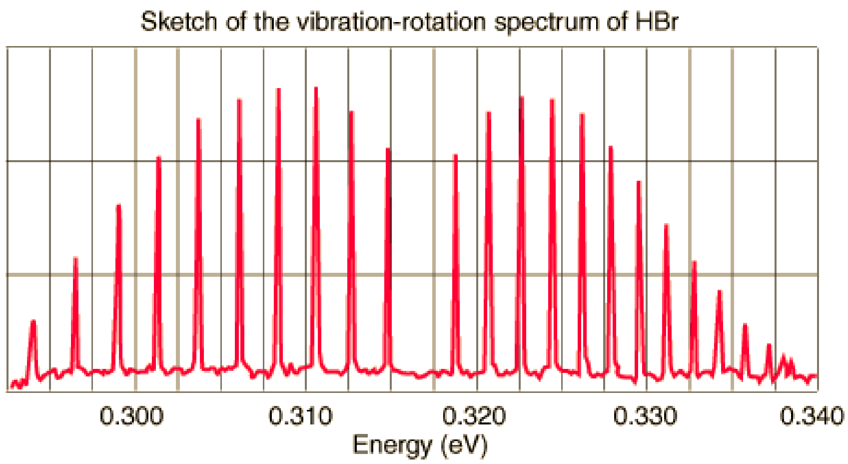
4. The figure below shows the absorption as a function of wavelength for the HBr at 300K.



(a) Describe the main features of this spectrum and describe their physical origin. State the relevant quantum numbers for the initial and final state where possible. [30]

(b) Use the spectrum above to show that the length of the bond in the HBr molecule is approximately 0.15 nm. Explain your method clearly. [25]

(c) Show that the peak intensity in this absorption spectrum occurs at the expected location for a gas at T=300K. Explain your method clearly. [45]

You may use the following results without proof in your answers.

- Energy of a rigid rotator: $E_R = \frac{\hbar^2}{2\mathcal{I}}J(J+1)$, $J = 0, 1, \ldots$, where $\mathcal{I}$ is the moment of inertia.
- Moment of inertia for two masses with separation a: $I = \mu a^2$ where μ is the reduced mass.
- Energy of a simple harmonic oscillator: $E_\nu = (\nu + \frac{1}{2})\hbar\sqrt{k/\mu}$, $\nu = 0, 1, 2, \ldots$, where k is the spring constant and μ is the reduced mass.

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5. (a) Why is the bond length in the H_2 molecule shorter than the bond length in the H_2^+ molecule? [15]

(b) Why are the spins of the electrons in the H_2 molecule anti-parallel? [25]

(c) Why is the H_3^+ molecule highly unstable? [20]

(d) Describe the appearance and physical origin of the Raman spectrum that is observed when laser light is scattered from rotational energy levels in molecular hydrogen. [40]

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