Final Exam

April 29th, 2006

Allowed: Time – three hours 2 sides of 8½×11" paper containing equations only (no text) Formula sheet (given) Calculator

Each question carries equal marks. Answer three out of the four questions.

For each problem <u>briefly explain</u> the equations you choose to use – simply writing down a set of equations from your formula sheet will not earn any marks.

Don't cram your answers into too small a space – try to spread out your answers.

1. A particle of mass *m* has a potential energy given by $V(x) = \frac{1}{2}kx^2$. It is in the first excited energy state:

$$(x) = A x \exp\left(-\left(\frac{mk}{h^2}\right)^{\frac{1}{2}} \frac{x^2}{2}\right)$$

where A is a normalization constant.

a) Calculate in terms of *A* the expectation values of *x*, *p* and p^2 in this state. (Hint: Use symmetry where possible and explain why).

b) Write down a formula representing the vibrational energies of a HF molecule in terms of an effective spring constant, k, and the masses $m_{\rm H}$, $m_{\rm F}$ of the constituent atoms.

c) Given that the wavelength of the light emitted by HF in a transition from $v = 1 \rightarrow v = 0$ state is 2.4 µm, find the value of *k* that characterizes the H..F bond. (The atomic mass of F is 19 amu).

2.a) A beam of silver atoms (107 amu, electronic level ${}^{2}S_{1/2}$) with velocity 5×10^{2} m/s along the *y*-axis passes through a region of length 0.2 m in which the magnetic field has the following properties:

$$B_y = 0$$
 $B_z \approx 1T$ $\frac{\partial B_z}{\partial z} = 200 \text{ T/m}$ $B_x(x, z) = -B_x(-x, z)$ $B_z(x, z) = B_z(-x, z)$

i) Sketch the form of the **B**-field in the *xz* plane.

ii) Find the force acting on an atom in this region.

iii) Calculate the distance from the y-axis that an atom will emerge from the magnetic field.

b) i) Define what is meant by the terms *fermion*, *boson*, *antisymmetric total wavefunction* and *symmetric total wavefunction*. Give concrete examples for each of these terms.

ii) Write down (with a brief explanation) the time-independent Schrodinger equation for the helium atom, neglecting any effects due to electron spin.

iii) Now neglect the term representing interaction between the two electrons. Write down the total (space **and** spin) two-electron wavefunction of the ground state for this system in terms of the explicit coordinates of the two electrons, labelled 1 and 2. What energy (in eV) would this state have?

3. The following table shows the wavelengths of the visible emission lines in the Balmer series of atomic hydrogen and the Pickering series of singly-ionized helium. For each species the transitions are given a label starting at *a*.

H / nm	$^{4}\text{He}^{+}/\text{nm}$
a 656.28	a 656.01
<i>b</i> 486.13	<i>b</i> 541.16
c 434.05	<i>c</i> 485.93
d 410.17	d 456.16
	e 433.87
	f 419.99
	g 410.00

a) Write down the equation in terms of fundamental constants for the energy eigenstates of i) the hydrogen atom and ii) the He^+ ion (neglect the effects of electron spin).

b) By comparing these formulae with the data in the table, explain all transitions shown using an energy level diagram for each species.

c) Why do four pairs of lines (e.g. b for H and c for He⁺) have closely similar wavelengths?

d) From the four pairs of transitions with similar wavelength, deduce a value for the ratio of the masses of the proton and the electron.

4. Atomic spin-orbit coupling can be represented by a term

$$\hat{H}_{so} = \frac{1}{2m^2c^2} \frac{1}{r} \frac{\partial V(r)}{\partial r} \hat{\mathbf{l}} \cdot \hat{\mathbf{s}}$$

in the single electron Hamiltonian, where *r* is the radial coordinate of the electron, *m* the electron mass, $\hat{\mathbf{l}}$ the orbital angular momentum operator and $\hat{\mathbf{s}}$ the electron spin angular momentum operator. *V*(*r*) is the electrostatic potential energy.

a) What is the result of operating on a 2*p* state by the $\hat{\mathbf{l}}^2$ operator? What about the $\hat{\mathbf{s}}^2$ operator?

b) Demonstrate that the \hat{H}_{so} operator has dimensions of energy.

c) Give simple physical arguments that justify the form of this expression for \hat{H}_{so} .

d) For the 2*p* electronic states of hydrogen, what two possible values of *j* are allowed?

V(r) is the Coulomb interaction with the nucleus of atomic number Z. Then for a 2p electron

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{24} \left(\frac{Z}{a_0} \right)^3$$

e) Using these expressions, calculate (**both** in symbols **and** numerically in eV) the energy splitting between the two possible i levels for a 2p electron in hydrogen due to the spin-orbit interaction.

f) How many m_j states are shifted up, and how many are shifted down? Show that the centre of gravity of the states (i.e. the average energy) is unchanged due to the spin-orbit interaction.