Trent: PHYS 2620H – Atomic, Molecular and Nuclear Physics: 2011-2012

Midterm: Friday Mar 2, 2012

Allowed: Formula sheet (given), calculator, 1 hour 50 minutes
Answer all of question one (worth 40% of the marks), and two out of the remaining three questions

Advice: Don't cram your answers into too small a space – explain your working

Do all of this first question:

1. a) Determine the energy separation (in eV) between the two lowest energy levels of:
   i) an electron confined to a 1-dimensional infinite well of length 1 nm.
   ii) a helium atom (mass number 4) confined to the same infinite well as in (i)

b) From your formula sheet find the radial probability density, $P(r)$, for a hydrogen atom in the $n = 3, \ell = 2, m_\ell = 0$ state (a $3d_{z^2}$ orbital). Make a rough sketch of this function, find the position of its maximum.

c) The hydrogen atom's energy eigenfunctions are written down on your formula sheet in a way such that the radial and the angular functions are each separately normalized. Check that the normalization constant for the angular function corresponding to $\ell = 2, m_\ell = +1$ is indeed correct.

d) Carefully, but using only a few sentences with a diagram or two, describe the principle behind the Stern-Gerlach experiment. Suppose it were experimentally feasible to send a beam of hydrogen atoms in the 3d state into such an experiment. If the electron (and proton) had no spin, how many peaks of atom intensity are expected to be observed, and why?

e) Given an electron with principal quantum number $n = 3$, find and list using the $\{n, \ell, m_\ell, m_s\}$ notation all 18 possible states, and group them according to whether they are in the 3s, 3p, or 3d orbitals. For each of these orbitals what are the possible values of *j*, the total angular momentum quantum number, and of m_j, the magnetic total angular momentum quantum number?

Do two out of these three remaining questions:

2. To a good approximation the hydrogen chloride molecule (HCl) behaves vibrationally as a quantum harmonic oscillator of spring constant 480 N/m and with a mass given by that of the hydrogen atom. Assume that it is in its ground vibrational state:
a) Find the classical turning points for this oscillator.
b) Sketch on the same plot the potential energy function, and the ground state wavefunction of this system. Denote the approximate location of the classical turning points in the ground state.
c) What wavelength of light would be just right to excite this molecule to its next-highest vibrational energy state?

3. a) Consider an infinite-well potential of length L containing five identical non-interacting particles. What is the minimum possible total energy of this system in each case if the particles have spin angular momentum quantum number: i) $s = 1/2$, ii) $s = 1$ and iii) $s = 3/2$?

b) Consider two different, perfectly acceptable, wavefunctions for two electrons in an atom, ψ_a and ψ_b:

$$\psi_a(1,2) = \phi(\vec{r}_1, \vec{r}_2) \uparrow_1 \uparrow_2$$
$$\psi_b(1,2) = \chi(\vec{r}_1, \vec{r}_2) \frac{1}{\sqrt{2}} (\uparrow_1 \downarrow_2 - \downarrow_1 \uparrow_2)$$

i) In each case is the <u>spin</u> part of the wavefunction symmetric, antisymmetric or asymmetric (no symmetry), with respect to exchange of the two electrons' labels?
ii) In each case, is the <u>spatial</u> part of the wavefunction symmetric, antisymmetric or asymmetric under particle exchange? Explain why.
iii) For which of the two wavefunctions ψ_a and ψ_b do the electrons have a very low likelihood of both being in a region of space such that they are very close to each other?

4. Spin-orbit coupling in atoms can be represented by a term in the Hamiltonian operator of the form:

$$\hat{H}_{SO} = \frac{\mu_0 e^2}{4\pi m^2 r^3} \hat{\boldsymbol{S}} \cdot \hat{\boldsymbol{L}},$$

where r is the radial coordinate of the electron under consideration, m the electron mass, $\hat{\boldsymbol{S}}$ the electron spin angular momentum operator , and $\hat{\boldsymbol{L}}$ the electron orbital angular momentum operator.
a) What is the result of operating on a $2p$ state with the $\hat{\boldsymbol{L}}^2$ operator? What about the $\hat{\boldsymbol{S}}^2$ operator?
b) Demonstrate that the $\hat{H}_{SO}$ operator has dimensions of energy [note that $\mu_0 \varepsilon_0 \equiv 1/c^2$].
c) Provide in two or three sentences the simple physical arguments that justify the form of this expression for $\hat{H}_{SO}$.
d) For the $2p$ states of hydrogen, what two possible values of total electronic angular momentum quantum number, j, are allowed?