CH 107 Quiz

October 14, 2017 **Time: 2 Hours** **Full marks: 18**

Answers should be brief and to the point. <u>Answer all parts of the same question **together**</u>.
Use <u>**Pen**</u> to write your answers (<u>**including sketches**</u>). Provide arguments to earn full credit.

Question 1

(a) $\psi = \frac{sin^2 x}{x^2}$. How many nodes does ψ have, if x is in radian and $-3\pi \le x \le 3\pi$. **6 × 1.0 mark**

(b) Why is the general form of probability density $\psi^*\psi$ and not ψ^2 ?

(c) $\psi = A \sin kx + B \cos kx\,;\ -\infty \le x \le \infty$.

Does ψ satisfy all conditions of acceptability, as per Born interpretation? Explain.

(d) Show that quantum number of a particle, confined in a one dimensional infinite potential well, can only take up integer values.

(e) Why can the quantum number of the particle in part (d) not have a value of zero? Explain.

(f) A particle is in a 2-dimensional square infinite potential well. By some means, the box becomes a rectangular one. This is reflected in the increase in the number of lines in the absorption spectrum of the system. Explain.

Question 2

(a) i) How many radial and angular nodes are there in $4p_x$ orbital? **1.0 marks**

ii) Draw a schematic contour diagram for this orbital, showing all radial and angular nodes clearly. Indicate the sign on each lobe. Label the axes. **2.0 marks**

(b) Where is the probability of finding an electron in the following orbital greatest? **3.0 marks**

$$\psi = \frac{1}{162}\left(\frac{1}{\pi a_0^3}\right)^{1/2}\left(\frac{r}{a_0}\right)^2 e^{-r/3a_0}\sin^2\theta\, e^{-2i\phi}$$

~~Question 3~~

(a) Consider an atom with two electrons, 1 and 2. The operator for the square of the total spin of these two electrons is

$$\widehat{S_{total}}^2 = (\widehat{S_1} + \widehat{S_2})^2 = \widehat{S_1}^2 + \widehat{S_2}^2 + 2(\widehat{S_{1x}.S_{2x} + S_{1y}.S_{2y} + S_{1z}.S_{2z}})$$

Given: $S_x\alpha = \frac{\hbar}{2}\beta,\quad S_x\beta = \frac{\hbar}{2}\alpha,\quad S_y\alpha = \frac{i\hbar}{2}\beta,\quad S_y\beta = \frac{i\hbar}{2}\alpha,\quad S_z\alpha = \frac{\hbar}{2}\alpha,\quad S_z\beta = -\frac{\hbar}{2}\beta$

and $\widehat{S_i}^2 = S_{ix}^2 + S_{iy}^2 + S_{iz}^2$ for i = 1 and 2.

i) Write the spin wavefunction for the electronic part of the atom when both the electrons have α spin. ~~**0.5 mark**~~

ii) With appropriate proof, determine if this wavefunction is an eigenfunction of $\widehat{S_{total}}^2$ ~~**3.5 marks**~~

(b) What is the shielding constant (σ) for the electrons in helium atom? Use the expression: **2.0 marks**

$I.E. = (I.E.\ of\ H\ atom).\left(\frac{Z-\sigma}{n}\right)^2$, given I.E. of He = 2.372 × 10^6 J mol^{-1}, I.E. of H = 1.313× 10^6 J mol^{-1}

CH 107 Quiz

October 13, 2018 **Time: 1.5 hours** **Full Marks: 18**

<u>Answer all the parts of the same question</u> **<u>together</u>**. Answer should be to the point, however, arguments have to be provided for full credit. Use **<u>only Pen</u>** to write your answers (**<u>including sketches</u>**).

An equation sheet is provided along with the question paper

Question 1

(a) Consider a particle in a 1-D box of length L, in the quantum state of n = 3. What is (are) the value(s) of position for which the probability-density of finding the particle is maximum? *No explanation is required*. **1 mark**

(b) Consider a particle in a square 2-D box of length L, where the maximum value of both the quantum-numbers n_x and n_y is 3. Evaluate the transition energy (in terms of $\beta = h^2/8mL^2$) from the *lowest degenerate* (equal energy) state to the *2nd lowest degenerate* state. **2 marks**

(c) What is an orbital? **1 mark**

(d) The force acting between the electron and the proton in H-atom is given by $F = -e^2/4\pi\varepsilon_0 r^2$. Evaluate the average (expectation) value of the force (in terms of e, ε_0, a_0) when the electron is in the 1s state, for which the normalized wavefunction is given by: $\psi_{1s} = \frac{1}{\sqrt{\pi}}(1/a_o)^{3/2}\exp(-r/a_o)$. **2 marks**

Question 2

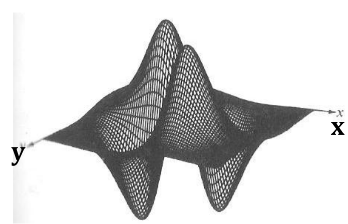
(a) Consider the following orbitals for hydrogen atom (a_0 = Bohr radius): **2 marks**

$$\psi_1 = \frac{1}{81}\left(\frac{1}{\pi a_0^3}\right)^{1/2}\left(\frac{r}{a_0}\right)^2 e^{-r/3a_0}\,\mathrm{Cos}\theta\mathrm{Sin}\,\theta e^{i\phi} \qquad \psi_2 = \frac{1}{81}\left(\frac{1}{\pi a_0^3}\right)^{1/2}\left(\frac{r}{a_0}\right)^2 e^{-r/3a_0}\,\mathrm{Cos}\theta\mathrm{Sin}\,\theta e^{-i\phi}$$

(i) Take appropriate linear combinations of these two orbitals to generate two new real orbitals.
(ii) Express any one of these real orbitals as $f(r).F(x,y,z)$, and hence identify the real orbital.

(b) Given the angular part of an orbital is $Y(\theta,\varphi) = (7/6\pi)^{1/2}cos\theta(5cos^2\theta - 3)$, what are the values of ***l*** and ***m***? **2 marks**

(c) Using the surface plot of a hydrogenic orbital depicted, sketch its contour plot in the xy plane. Draw at least 3 contour lines of different (arbitrary) values for the entire surface plot and identify the nodes. **2 marks**



Question 3

(a) ~~What is orbital approximation for a 2 electron system such as the He atom?~~ **1 ~~mark~~**

~~(b)~~ ~~Starting from the electronic Hamiltonian for the He-atom, derive the expression for the ground state electronic energy (in terms of hydrogenic energies) via neglect of the inter-electronic repulsion.~~ **~~2 marks~~**

(c) The state of the electron in a hydrogenic atom (Z = 1) is described by the normalized wavefunction below: (the subscripts denote the hydrogenic quantum numbers n, l and m in their standard format) **3 marks**

$$\Psi(r,\theta,\varphi) = -\sqrt{\frac{1}{3}}R_{4,2}(r)Y_{2,-1}(\theta,\varphi) + \sqrt{\frac{2}{9}}R_{3,2}(r)Y_{2,1}(\theta,\varphi) - \frac{2i}{3}R_{1,0}(r)Y_{0,0}(\theta,\varphi) .$$

(i) If the electronic energy of the atom in this state is measured, what are *all* the values that can be found?
(ii) Similarly, if the total orbital angular momentum is measured, what are *all* the values that can be found?
(iii) Upon a large number of measurements on identical such systems, *evaluate* the most probable value of the total orbital angular momentum in this state?