CH107: Physical Chemistry Quiz 19th October, 2013 1.5 hours

Answer each question in a separate page. Calculators may be used. Use PEN to write all answers, including sketches. Read questions carefully and keep answers to-the-point. Provide arguments to earn full credit.

Answer all questions. Total 24 Marks – Will be graded on best 20 marks answered

h=6.626x10^{-34}Js; c=3x10^{8} ms^{-1};m_e=9.1x10^{-31}kg;m_p=1.672x10^{-27} kg; e=6x10^{-19}C; 1eV=1.6x10^{-19} J;k_B=1.308 x 10^{-23} JK^{-1}

1A. Assume the function Bx(a-x) is a solution for a particle in 1-D well potential of length a (limit 0-a); B = const.

(i) Does this function satisfy all the necessary conditions to be a well-behaved wavefunction? [1]
(ii) Obtain the energy expression for the particle (of mass m) and compare it with the one obtained using trigonometric functions. [2]
(iii) Evaluate the normalization constant for the wavefunction, if it can be normalized at all. [1]

1B. Draw contours of equal probability for (1,2) and (2,2) states of a particle in a 2D square-well potential. [2]

2A. What is the expression for energy of an un-normalized wavefunction? [1]

2B. Does the following wavefunction represent a stationary or a non-stationary state? Explain!

$$\Psi(x,t) = \varphi_1(x)\exp\left(-iE_1t/\hbar\right) + \varphi_2(x)\exp\left(-iE_2t/\hbar\right)$$

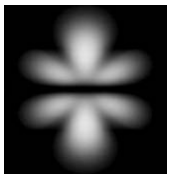
; Note: E_1, E_2 are constants [2]

2C. Consider a single electron moving in a circular orbit of radius r around a nucleus. What percentage error is introduced in the value of energy of (a) m = 0 and (b) m = 1 states, if the mass of the electron, m_e is used in the energy expression instead of the reduced mass μ. Note: m is the relevant quantum number. [2]

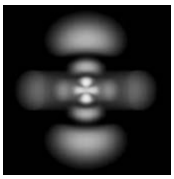
3A. The force acting between the electron and the proton in H-atom is given by $F = -e^2/4\pi\varepsilon_0 r^2$ **Calculate the expectation value (in terms of** e, ε_0, a_0**) of the force when an electron is in 1s state.** $\psi_{1s} = \frac{1}{\sqrt{\pi}}(1/a_o)^{3/2}\exp(-r/a_o)$ **[2]**

3B. Identify the radial and angular nodes in the following projections of electron density, and hence identify the orbitals.

(i)



(ii)



Note: The vertical direction is the z-axis. [2]

3C. The d orbitals have a nomenclature $d_{z^2}, d_{xy}, d_{yz}, d_{xz}, d_{x^2-y^2}$**. Show how the following orbital** $\psi_{3d} = \left(\sqrt{2}/81\sqrt{2\pi}\right)(1/a_o)^{3/2}(r/a_o)^2\exp(-r/3a_o).\sin^2\theta\sin 2\phi$ **can be expressed in the form f(r).F(x,y). From the derived expression, identify the nodal line(s)/plane(s)/surface(s) for this 3d orbital. [3]**

4A. What is a spin orbital? [1]

4B. Express the electronic Hamiltonian of Li atom in terms of 1-e Hydrogenic Hamiltonians and other terms. Under what conditions of the Hamiltonian can the corresponding Schrodinger Equation be solved? [3]

4C. What are the possible (acceptable) spin-functions for a 3 electron system? Hint. Use symmetry arguments to nullify spin-functions which distinguish between electrons. [2]

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