Name:

Chem 3322 practice for test #2

I want complete, detailed answers to the questions. Show all your work to get full credit.

$$\int_{-\infty}^{\infty} e^{-cx^2} = \frac{\sqrt{\pi}}{\sqrt{c}} \tag{1}$$

$$\int_{-\infty}^{\infty} x^2 e^{-cx^2} = \frac{\sqrt{\pi}}{2c^{3/2}} \tag{2}$$

$$\int r^2 e^{-c\,r}\, dr = -\frac{e^{-c\,r}(2 + 2c\,r + c^2 r^2)}{c^3} \tag{3}$$

The Schrödinger time dependent equation is, for $\psi(x,t)$

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\psi(x,t) \tag{4}$$

The Schrödinger time independent equation is, for $\psi(x)$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{5}$$

A wavefunction $\psi(x,y,z,t)$ is normalized if $\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi^* \psi dx\, dy\, dz = 1$

The particle in a one dimensional box energy levels are

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \qquad \text{n} = 1, 2, 3, ... \tag{6}$$

energy levels of the particle on a ring:

$$E_n = \frac{n^2\hbar^2}{2mR^2} \qquad \text{n} = 0, 1, 2, ... \tag{7}$$

energy levels of the harmonic oscillator: $E_n = (n + 1/2)\hbar\omega$, n = 0, 1, 2, ...

ground state wavefunction of the harmonic oscillator:

$$\psi(x) = \left(\frac{2\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2} \tag{8}$$

with

$$\alpha = \frac{m\omega}{2\hbar} \qquad \text{and} \qquad \omega = (k/m)^{1/2} \tag{9}$$

where k is the force constant and m is the mass.

Speed of light = c = 3.0×10^8 m/s

electron mass = 9.11×10^{-31} kg

Avogadro's constant = $N_A = 6.022 \times 10^{23}$ mol^{-1}

Planck constants: h = 6.6262×10^{-34} Js and $\hbar = 1.05459 \times 10^{-34}$ Js

Boltzmann's constant k_B=1.38066×10^{-23}J K^{-1}

$\pi = 3.14159$

mass conversion from amu to kg: 1.66×10^{-27} kg/amu

Relationship between the wavelength of a photon and its energy

$$\lambda = \frac{hc}{E} \tag{10}$$

Volume of a sphere is $4\pi r^3/3$ and the surface area is $4\pi r^2$

Problem 1

Recall that the operator corresponding to the x-component of momentum is

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x} \tag{11}$$

Also recall that the classical formula for kinetic energy is $mv^2/2 = p^2/2m$.

a) Consider the wavefunctions $\psi_n(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right)$ which are the solutions to the time-independent Schroedinger equation for the 1-dimensional particle in a box. Are these wavefunctions $\psi_n(x)$ eigenfunctions of the momentum operator? If so, give the eigenvalue(s).

b) Are these wavefunctions $\psi_n(x)$ eigenfunctions of the kinetic energy operator? If so, give the eigenvalue(s).

c) Explain your answer to (b) on physical grounds.

Problem 2

a) State the textbook's version of the correspondence principle to relate the behavior of quantum and classical mechanics (hint: something about large quantum numbers).

b) Illustrate and explain your answer to (a) using either the harmonic oscillator or the particle in a box model.

c) State the version of the correspondence principle we used in class to relate the behavior of quantum and classical mechanics in order to derive the form of the momentum operator.

d) Illustrate and explain your answer to (c) using either the harmonic oscillator or the particle in a box model.

FIG. 1: A representation of the 1s, 2s, and 3s orbitals.

Problem 3

Shown in Fig. 1 is a representation of the three-dimensional 1s, 2s, and 3s orbitals.

a) Sketch the (one-dimensional) radial wavefunction for each of these three orbitals.

b) The probability of finding the electron very close to the nucleus is (almost) zero. How can this fact be explained, since Fig. 1 and part (a) would seem to suggest otherwise? Your answer may include a sketch if appropriate.

c) Calculate the probability that a hydrogen 1s electron is within a distance $a_0 = 5.2918 \times 10^{-11}$ m from the nucleus. Recall that the Jacobian for spherical polar coordinates is $r^2 \sin\theta$. Also, Eq (3) is helpful. The 1s wavefunction is

$$\psi(r, \theta, \phi) = \pi^{-1/2} a_0^{-3/2} e^{-r/a_0} \tag{12}$$