Chapter Homework

1. The energy levels of hydrogenlike atoms are given by: $E_n = -\frac{1}{2}\frac{e^2}{4\pi\varepsilon_0 a_0}\frac{Z^2}{n^2}$

   (a) Calculate the wavelength, in nm, of the n=6 to n=3 radiative transition in He^+.

   (b) Calculate the ionization energy of He^+, in eV

   Note: $\frac{e^2}{4\pi\varepsilon_0 a_0} = 2625\ kJ/mol$

2. The 1s and 2s wavefunctions of hydrogenlike atoms are:

$$\psi_{1s} = A_{1s}e^{-Zr/a_0} \qquad \psi_{2s} = A_{2s}\left(1-\frac{Zr}{2a_0}\right)e^{-Zr/2a_0}$$

   (a) Prove the ψ_{1s} and ψ_{2s} are orthogonal to each other.

   (b) Calculate the normalization constant, A_{1s}.

   (c) Calculate the most probable value of r for an electron in a 1s orbital.

   (d) Calculate $\langle r \rangle$ for an electron in a 1s orbital (Note: first normalize the radial distribution function).

   (e) Calculate the probability that the electron in a 1s orbitl is between r=0 and $r=2a_0/Z$

   (f) Calculate the probability that r is in the range: $a_0/Z \le r \le 4a_0/Z$

   (g) Calculate the average potential energy of an electron in a =1s orbital.

   (h) Show that the Radial component of ψ_{1s} is an eigenfunction of the radial Schrödinger equation (below) with $l = 0$

3. The $2p_x$ wavefunction of hydrogenlike atoms is given by:

$$\psi_{2px} = Are^{-Zr/2a_0}\sin\theta\cos\phi$$

   (a) Calculate the most probably value of r for an electron in a $2p_x$ orbital.

   (b) Calculate $\langle r^2 \rangle$ for an electron in a $2p_x$ orbital (Note: first normalize the radial distribution function).

4. One of the wavefunctions of hydrogenlike atoms is:

$$\psi = A\cdot R(r)\cdot Y_{lm}(\theta,\varphi) = Ar^2e^{-Zr/3a_0}\sin^2\theta e^{2i\varphi}$$

   (a) Show that $Y_{lm}(\theta,\phi)$ is an eigenfunction of the L^2 operator (below). What is the eigenvalue?

(b) Show that $Y_{lm}(\theta,\phi)$ is an eigenfunction of the L_z operator (below). What is the eigenvalue?

(c) Set up the product of 3 integrals in spherical polar coordinates required to calculate $\langle y^2 \rangle$. You do NOT have to perform the integrals.

5. Two of the complex hydrogen atom d (l=2) wavefunctions are:

$$\psi_{n22}(r,\theta,\varphi) = R_{n2}(r)\cdot\sin^2\theta\cdot e^{2i\varphi} \qquad \psi_{n2-2}(r,\theta,\varphi) = R_{n2}(r)\cdot\sin^2\theta\cdot e^{-2i\varphi}$$

Use the Euler Relations below to show how these can be combined to yield two real forms of the hydrogen atom d wavefunctions.

DATA

$h = 6.63\text{x}10^{-34}$ J·s
$\hbar = h/2\pi = 1.05\text{x}10^{-34}$ J·s
$c = 3.00\text{x}10^{8}$ m/s $= 3.00\text{x}10^{10}$ cm/s
$N_A = 6.02\text{x}10^{23}$ mol^{-1}
$k = 1.38\text{x}10^{-23}$ J/K
R = 8.31 J/mol-K
R = 8.31 Pa-m^3/mol-K
$m_e = 9.11\text{x}10^{-31}$ kg (electron mass)

1 J = 1 kg·m^2/s^2
1 Å = 10^{-10} m
$k\cdot N_A = R$
1 amu = $1.66\text{x}10^{-27}$ kg
1 atm. = $1.013\text{x}10^{5}$ Pa
1 eV = $1.60\text{x}10^{-19}$ J

$$\int_0^\infty x^n e^{-ax}\,dx = \frac{n!}{a^{n+1}}$$

$$\int_0^2 x^2 e^{-x}\,dx = 0.647$$

$$\int_0^4 x^2 e^{-x}\,dx = 1.524$$

$$\int_0^8 x^2 e^{-x}\,dx = 1.972$$

Radial Schrödinger Equation: $-\frac{\hbar^2}{2m}\left[\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} - \frac{l(l+1)}{r^2} + \frac{2Z}{a_0 r}R\right] = ER$

L_z Operator: $\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial\varphi}$

L^2 Operaor: $L^2 = -\hbar^2\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right\}$

Euler Relations: $e^{ix} = \cos(x) + i\sin(x)$ and $e^{-ix} = \cos(x) - i\sin(x)$