## Formulas and constants:

 $hc = 12,400 \ eVA$ ;  $k_B = 1/11,600 \ eV/K$ ;  $ke^2 = 14.4 \ eVA$ ;  $m_ec^2 = 0.511 \times 10^6 \ eV$ ;  $m_p/m_e = 1836$ Relativistic energy - momentum relation  $E = \sqrt{m^2 c^4 + p^2 c^2}$  $c = 3 \times 10^8 m/s$ Lorentz force:  $\vec{F} = q\vec{E} + q\vec{v} \times \vec{B}$ Photons: E = hf; p = E/c;  $f = c/\lambda$ Planck's law :  $u(\lambda) = n(\lambda)\bar{E}(\lambda)$  ;  $n(\lambda) = \frac{8\pi}{\lambda^4}$  ;  $\bar{E}(\lambda) = \frac{hc}{\lambda}\frac{1}{e^{hc/\lambda k_B T} - 1}$ Energy in a mode/oscillator:  $E_f = nhf$ ; probability  $P(E) \propto e^{-E/k_f}$ Stefan's law :  $R = \sigma T^4$ ;  $\sigma = 5.67 \times 10^{-8} W / m^2 K^4$ ; R = cU/4,  $U = \int u(\lambda) d\lambda$ Planck:  $u(\lambda) = n(\lambda)\bar{E}(\lambda)$ ;  $n(\lambda) = \frac{8\pi}{\lambda^4}$ ;  $\bar{E}(\lambda) = \frac{hc}{\lambda} \frac{1}{e^{hc/\lambda k_B T} - 1}$ ; Wien:  $\lambda_m T = hc/4.96k_B$ Photoelectric effect:  $eV_0 = (\frac{1}{2}mv^2)_{\text{max}} = hf - \phi$ ,  $\phi = \text{work function}$ Compton:  $\lambda_2 - \lambda_1 = \frac{h}{m_s c} (1 - \cos\theta)$ ;  $\lambda_c = \frac{h}{m_s c} = 0.0243A$ ; Rutherford:  $b = \frac{kq_a Q}{m_s v^2} \cot(\theta/2)$ ;  $\Delta N \propto \frac{1}{\sin^4(\theta/2)}$ Electrostatics:  $F = \frac{kq_1q_2}{r^2}$  (force) ;  $V = \frac{kq}{r}$  (potential) ;  $U = q_0V$  (potential energy) Hydrogen spectrum:  $\frac{1}{\lambda} = R(\frac{1}{m^2} - \frac{1}{n^2})$ ;  $R = 1.097 \times 10^7 \ m^{-1} = \frac{1}{911.34}$ Bohr atom:  $r_n = r_0 n^2$ ;  $r_0 = \frac{a_0}{Z}$ ;  $E_n = -E_0 \frac{Z^2}{n^2}$ ;  $a_0 = \frac{\hbar^2}{mke^2} = 0.529A$ ;  $E_0 = \frac{ke^2}{2a} = 13.6eV$ ;  $L = mvr = n\hbar$  $E_{k} = \frac{1}{2}mv^{2}$ ;  $E_{p} = -\frac{ke^{2}Z}{r}$ ;  $E = E_{k} + E_{p}$ ;  $F = \frac{ke^{2}Z}{r^{2}} = m\frac{v^{2}}{r}$ ;  $hf = hc/\lambda = E_{n} - E_{m}$ Reduced mass:  $\mu = \frac{mM}{m+M}$ ; X-ray spectra:  $f^{1/2} = A_n(Z-b)$ ; K: b = 1, L: b = 7.4de Broglie :  $\lambda = \frac{h}{n}$ ;  $f = \frac{E}{h}$ ;  $\omega = 2\pi f$ ;  $k = \frac{2\pi}{\lambda}$ ;  $E = \hbar\omega$ ;  $p = \hbar k$ ;  $E = \frac{p^2}{2m}$ ;  $\hbar c = 1973 \ eVA$ Wave packets:  $y(x,t) = \sum a_j \cos(k_j x - \omega_j t)$ , or  $y(x,t) = \int dk a(k) e^{i(kx - \omega(k)t)}$ ;  $\Delta k \Delta x \sim 1$ ;  $\Delta \omega \Delta t \sim 1$ group and phase velocity :  $v_g = \frac{d\omega}{dk}$  ;  $v_p = \frac{\omega}{k}$  ; Heisenberg :  $\Delta x \Delta p \sim \hbar$  ;  $\Delta t \Delta E \sim \hbar$  $\Psi(x,t) = |\Psi(x,t)| e^{i\theta(x,t)}$ ;  $P(x,t) dx = |\Psi(x,t)|^2 dx$  = probability Wave function Schrödinger equation:  $-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial r^2} + V(x)\Psi(x,t) = i\hbar \frac{\partial\Psi}{\partial t}$ ;  $\Psi(x,t) = \psi(x)e^{-i\frac{\omega}{\hbar}t}$ Time – independent Schrödinger equation:  $-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi(x) = E\psi(x); \quad \int_{\infty}^{\infty} dx \ \psi^*\psi = 1$  $\infty$  square well:  $\psi_n(x) = \sqrt{\frac{2}{I}} \sin(\frac{n\pi x}{I})$ ;  $E_n = \frac{\pi^2 \hbar^2 n^2}{2mI^2}$ ;  $x_{op} = x$ ,  $p_{op} = \frac{\hbar}{i} \frac{\partial}{\partial x}$ ;  $\langle A \rangle = \int_{-\infty}^{\infty} dx \psi^* A_{op} \psi$ Eigenvalues and eigenfunctions:  $A_{op} \Psi = a \Psi (a \text{ is a constant})$ ; uncertainty:  $\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$ Harmonic oscillator:  $\Psi_n(x) = C_n H_n(x) e^{-\frac{m\omega}{2\hbar}x^2}$ ;  $E_n = (n + \frac{1}{2})\hbar\omega$ ;  $E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 = \frac{1}{2}m\omega^2 A^2$ ;  $\Delta n = \pm 1$ Step potential:  $R = \frac{(k_1 - k_2)^2}{(k_1 + k_1)^2}$ , T = 1 - R;  $k = \sqrt{\frac{2m}{\hbar^2}(E - V)}$ 

 $\psi(x) \sim e^{-\alpha x}$ ;  $T \sim e^{-2\alpha \Delta x}$ ;  $T \sim e^{-2\int_{a}^{b} \alpha(x)dx}$ ;  $\alpha(x) = \sqrt{\frac{2m[V(x) - E]}{\pi^2}}$ Tunneling : 3D square well:  $\Psi(x,y,z) = \Psi_1(x)\Psi_2(y)\Psi_3(z)$ ;  $E = \frac{\pi^2\hbar^2}{2m}(\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_2^2})$ Spherically symmetric potential:  $\Psi_{n,\ell,m}(r,\theta,\phi) = R_{n\ell}(r)Y_{\ell m}(\theta,\phi)$ ;  $Y_{\ell m}(\theta,\phi) = f_{lm}(\theta)e^{im\phi}$ Angular momentum:  $\vec{L} = \vec{r} \times \vec{p}$ ;  $L_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}$ ;  $L^2 Y_{\ell m} = \ell(\ell+1)\hbar^2 Y_{\ell m}$ ;  $L_z = m\hbar$ Radial probability density:  $P(r) = r^2 |R_{n,\ell}(r)|^2$ ; Energy:  $E_n = -13.6eV \frac{Z^2}{r^2}$ Ground state of hydrogen and hydrogen - like ions:  $\Psi_{1,0,0} = \frac{1}{\pi^{1/2}} (\frac{Z}{a_1})^{3/2} e^{-Zr/a_0}$ Orbital magnetic moment :  $\vec{\mu} = \frac{-e}{2m}\vec{L}$  ;  $\mu_z = -\mu_B m_l$  ;  $\mu_B = \frac{e\hbar}{2m_a} = 5.79 \times 10^{-5} eV/T$ Spin 1/2:  $s = \frac{1}{2}$ ,  $|S| = \sqrt{s(s+1)}\hbar$ ;  $S_z = m_s\hbar$ ;  $m_s = \pm 1/2$ ;  $\vec{\mu}_s = \frac{-e}{2m}g\vec{S}$ Total angular momentum:  $\vec{J} = \vec{L} + \vec{S}$ ;  $|J| = \sqrt{j(j+1)}\hbar$ ;  $|l-s| \le j \le l+s$ ;  $-j \le m_j \le j$  $\vec{\mu} = \frac{-e}{2m}(\vec{L} + g\vec{S})$ ; Energy in mag. field:  $U = -\vec{\mu} \cdot \vec{B}$ Orbital + spin mag moment : Two particles :  $\Psi(x_1, x_2) = +/-\Psi(x_2, x_1)$ ; symmetric/antisymmetric Screening in multielectron atoms :  $Z \rightarrow Z_{eff}$  ,  $1 < Z_{eff} < Z$ Orbital ordering: 1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 4f < 5d < 6p < 7s < 6d ~ 5f

## Justify all your answers to all (3) problems

## Problem 1 (10 pts)

For an electron in an infinite three-dimensional square well of dimensions  $L_1$ ,  $L_2$ ,  $L_3$  with  $L_1=L_2=L$ ,  $L_3>L$ :

(a) Find the five lowest energy levels if  $L_3 = \sqrt{2}L$ . Draw an energy level diagram giving the quantum numbers, the energies and the degeneracy of each level. Give the energies in

terms of  $E_0 = \frac{\hbar^2 \pi^2}{2m_e L^2}$ , and the degeneracy in brackets (e.g. (1), (2), (3)). Degeneracy is

the number of states with the same energy.

(b) Find a value of  $L_3 > L$  (not  $L_3 = L$ ) for which one of the four lowest energy levels is three-fold degenerate. For this case, draw an energy level diagram as in part (a) that shows the four lowest energy levels, their energies and degeneracies.

## Problem 2 (10 pts)

The ground state wave function for an electron in hydrogen is given by

$$\psi(r,\vartheta,\phi) = \frac{1}{(\pi a_0^3)^{1/2}} e^{-r/a}$$

(a) Give the radial wavefunction for this state, R(r). It is defined by

$$\psi(r,\vartheta,\phi) = R(r)Y(\vartheta,\phi)$$
, with  $\int d\Omega |Y|^2 = \int_0^{2\pi} d\phi \int_0^{\pi} d\vartheta \sin\vartheta |Y|^2 = 1$ 

(b) Find the ratio of the probability that the electron will be found at radius r=0.9a<sub>0</sub> to the probability that it will be found at r=a<sub>0</sub>. Find also the ratio of the probability that the electron will be found at radius r=1.1a<sub>0</sub> to the probability that it will be found at r=a<sub>0</sub>. (c) Find the uncertainty in the radial position of this electron,  $\Delta r = \sqrt{\langle r^2 \rangle - \langle r \rangle^2}$  in terms of a<sub>0</sub>. Radial averages are defined as  $\langle f(r) \rangle = \int_{0}^{\infty} dr f(r) P(r)$  with P(r) given in the

formula sheet. Use that  $\int_{0}^{\infty} dr r^{s} e^{-\lambda r} = \frac{s!}{\lambda^{s+1}}$ 

Problem 3 (10 pts)



An electron orbiting around a nucleus of charge Ze "sees" an effective magnetic field B=2.5T due to the relative motion of the electron and the nucleus. Assume its magnetic quantum number is  $m_{\ell} = -3$ .

(a) Find the magnitude of the energy shift of this electron (in eV) due to the interaction of the electron intrinsic (spin) magnetic moment with this effective magnetic field, relative to the case where this interaction is ignored.

(b) Give the sign of this shift (plus or -) when the spin quantum number  $m_s$  has the values +1/2 and -1/2. Which has higher energy, +1/2 or -1/2? Justify your answer.

(c) Suppose the value of the charge of the nucleus changes from Ze to 2Ze., and assume the state of the electron is characterized by the same quantum numbers as in (a). Will the magnitude of the energy shift found in (a) increase or decrease? By what factor? Justify your answer carefully, no credit for guesses.

<u>Hints:</u> you may use aguments based on the Bohr model. Take into account that both the radius of the orbit and the velocity of the electron will change, as well as the charge of the nucleus. Remember that the magnetic field at a distance R of a wire carrying current I is given by  $B = \mu_0 I / (2\pi R)$ . Assume the nucleus moving relative to the electron carries current I=charge/time. What is "charge" and "time" in that formula? Use the fact that the angular momentum of the electron didn't change since the quantum numbers didn't.