## Formulas and constants:

 $hc = 12,400 \ eVA$ ;  $k_B = 1/11,600 \ eV/K$ ;  $ke^2 = 14.4 \ eVA$ ;  $m_e c^2 = 0.511 \times 10^6 \ eV$ ;  $m_p / m_e = 1836$ 

Relativistic energy - momentum relation  $E = \sqrt{m^2c^4 + p^2c^2}$ ;  $c = 3 \times 10^8 m/s$ 

Photons: E = hf; p = E/c;  $f = c/\lambda$  Lorentz force:  $\vec{F} = q\vec{E} + q\vec{v} \times \vec{B}$ 

Photoelectric effect:  $eV_0 = (\frac{1}{2}mv^2)_{\text{max}} = hf - \phi$ ,  $\phi = \text{work function}$ 

Integrals:  $I_n = \int_0^\infty x^n e^{-\lambda x^2} dx$ ;  $\frac{dI_n}{d\lambda} = -I_{n+2}$ ;  $I_0 = \frac{1}{2} \sqrt{\frac{\pi}{\lambda}}$ ;  $I_1 = \frac{1}{2\lambda}$ ;  $\int_0^\infty \frac{x^3}{e^x - 1} dx = \frac{\pi^4}{15}$ 

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  $P(E) \propto e^{-E/k_BT}$ 

Stefan's law :  $R = \sigma T^4$  ;  $\sigma = 5.67 \times 10^{-8} W / m^2 K^4$  ; R = cU/4 ,  $U = \int_{0}^{\infty} u(\lambda) d\lambda$ 

Wien's displacement law :  $\lambda_m T = hc/4.96k_B$ 

Compton scattering:  $\lambda' - \lambda = \frac{h}{m_e c} (1 - \cos \theta)$ ;  $\lambda_c = \frac{h}{m_e c} = 0.0243A$ 

Rutherford scattering:  $b = \frac{kq_{\alpha}Q}{m_{\alpha}v^2}\cot(\theta/2)$  ;  $\Delta N \propto \frac{1}{\sin^4(\theta/2)}$ 

Electrostatics:  $F = \frac{kq_1q_2}{r^2}$  (force);  $U = q_0V$  (potential energy);  $V = \frac{kq}{r}$  (potential)

Hydrogen spectrum:  $\frac{1}{\lambda} = R(\frac{1}{m^2} - \frac{1}{n^2})$ ;  $R = 1.097 \times 10^7 \ m^{-1} = \frac{1}{911.3A}$ 

Bohr atom:  $r_n = r_0 n^2$ ;  $r_0 = \frac{a_0}{Z}$ ;  $E_n = -E_0 \frac{Z^2}{n^2}$ ;  $a_0 = \frac{\hbar^2}{mke^2} = 0.529A$ ;  $E_0 = \frac{ke^2}{2a_0} = 13.6eV$ ;  $L = mvr = n\hbar$ 

 $E_k = \frac{1}{2}mv^2$ ;  $E_p = -\frac{ke^2Z}{r}$ ;  $E = E_k + E_p$ ;  $F = \frac{ke^2Z}{r^2} = m\frac{v^2}{r}$ ;  $hf = hc/\lambda = E_n - E_m$ 

Reduced mass:  $\mu = \frac{mM}{m+M}$ ; X-ray spectra:  $f^{1/2} = A_n(Z-b)$ ; K: b = 1, L: b = 7.4

de Broglie :  $\lambda = \frac{h}{p}$ ;  $f = \frac{E}{h}$ ;  $\omega = 2\pi f$ ;  $k = \frac{2\pi}{\lambda}$ ;  $E = \hbar \omega$ ;  $p = \hbar k$ ;  $E = \frac{p^2}{2m}$ ;  $\hbar c = 1973 \ eV \ A$ 

group and phase velocity:  $v_g = \frac{d\omega}{dk}$ ;  $v_p = \frac{\omega}{k}$ ; Heisenberg:  $\Delta x \Delta p \sim \hbar$ ;  $\Delta t \Delta E \sim \hbar$ 

Wave function  $\Psi(x,t) = |\Psi(x,t)| e^{i\theta(x,t)}$ ;  $P(x,t) dx = |\Psi(x,t)|^2 dx$  = probability

Schrodinger equation:  $-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi(x,t) = i\hbar \frac{\partial \Psi}{\partial t}$ ;  $\Psi(x,t) = \psi(x)e^{-i\frac{E}{\hbar}t}$ 

Time – independent Schrodinger equation:  $-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi(x) = E\psi(x)$ ;  $\int_{-\infty}^{\infty} dx \ \psi^* \psi = 1$ 

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: 
$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}$$
,  $T = 1 - R$ ;  $k = \sqrt{\frac{2m}{\hbar^2}(E - V)}$ 

Tunneling: 
$$\psi(x) \sim e^{-\alpha x}$$
;  $T \sim e^{-2\alpha \Delta x}$ ;  $T \sim e^{-\frac{2}{2}\int_{a}^{b}\alpha(x)dx}$ ;  $\alpha(x) = \sqrt{\frac{2m[V(x)-E]}{\hbar^2}}$ 

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:  $E_n = -13.6eV \frac{Z^2}{r^2}$ 

Spin 1/2: 
$$s = \frac{1}{2}$$
,  $|S| = \sqrt{s(s+1)}\hbar$ ;  $S_z = m_s \hbar$ ;  $m_s = \pm 1/2$ ;  $\vec{\mu}_s = \frac{-e}{2m_s} g\vec{S}$ 

$$\text{Total angular momentum}: \vec{J} = \vec{L} + \vec{S} \; \; ; \quad |J| = \sqrt{j(j+1)}\hbar \quad \; ; \quad |l-s| \leq j \leq l+s \quad ; \quad -j \leq m_j \leq j$$

Orbital + spin mag moment: 
$$\vec{\mu} = \frac{-e}{2m}(\vec{L} + g\vec{S})$$
; Energy in mag. field:  $U = -\vec{\mu} \cdot \vec{B}$ 

Two particles : 
$$\Psi(x_1, x_2) = +/-\Psi(x_2, x_1)$$
 ; symmetric/antisymmetric Screening in multielectron atoms :  $Z \to Z_{\text{eff}}$  ,  $1 < Z_{\text{eff}} < Z$ 

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 problems. Write clearly.

## **Problem 1** (10 pts)

- 5 electrons are put in a two-dimensional infinite well of side lengths  $L_1=2A$ ,  $L_2=3A$ . Assume the electrons don't interact via the Coulomb interaction but they obey Pauli's exclusion principle.
- (a) Make an energy level diagram showing the quantum numbers of the occupied states and of the lowest unoccupied state and the occupation of each state with the electron spin orientation for the lowest possible energy state of the system (ground state).
- (b) Find the ground state energy of this system in eV.
- (c) Find the wavelength of the lowest energy photon that this system will absorbe, in A. Assume there are no selection rules.

## **Problem 2** (10 pts)

An electron in a hydrogen-like ion is described by the wavefunction

$$\Psi(r,\vartheta,\phi) = Cr^3 e^{-r/2a_0} \sin^3 \vartheta e^{-i\phi}$$

with C a constant and a<sub>0</sub> the Bohr radius.

- (a) Give the values of the quantum numbers  $n,\,\ell$ , m and of the ionic charge Z. Justify your answers.
- (b) Calculate the average value of 1/r for an electron described by this wavefunction. Hint: you need to normalize the probability distribution.

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

(c) Show that your result in (b) agrees with the prediction of the Bohr atom for this n and Z. Alternatively, if you didn't find n and Z in (a), use the fact that your result in (b) should agree with the Bohr atom prediction to deduce the values of n and Z.

## **Problem 3** (10 pts)

- (a) Sodium has atomic number Z=11 and ionization energy 5.14 eV. The two lowest energy photons that can be absorbed by a sodium atom in its ground state have wavelengths 5890A and 5896A.
- (a) Give the ground state electronic configuration of sodium.
- (b) Assume a sodium atom is in an excited state where the outer electron occupies a 3p orbital. Estimate the energy required to remove this electron from the sodium atom, in eV.
- (c) Assume a sodium atom is in an excited state where the outer electron occupies a 3d orbital. Give the possible values for the magnitude of the total angular momentum for this atom and state which state has higher energy, and explain clearly why. What can you say about the energy required to remove this electron from the sodium atom? Explain.

Justify all your answers to all problems. Write clearly.