#### **Formulas and constants:**

*hc* = 12,400 *eVA* ;  $k_B = 1/11,600$  *eV/K* ;  $ke^2 = 14.4eVA$  ;  $m_e c^2 = 0.511 \times 10^6 eV$  ;  $m_p/m_e = 1836$ 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: Integrals:  $I_n = \int_a^{\infty} x^n e^{-\lambda x^2} dx$ ;  $\frac{dI_n}{d\lambda} = -I_{n+2}$ ;  $I_0 = \frac{1}{2} \sqrt{\frac{\pi}{\lambda}}$  $\vec{r}$ *F* = *q*  $\vec{r}$  $\vec{E} + q\vec{v} \times \vec{B}$ Photoelectric effect :  $eV_0 = (\frac{1}{2})$ 2  $mv^2$ <sub>max</sub> =  $hf - \phi$ ,  $\phi$  = work function  $\int_0^1$  *d* $\lambda$  $\int_{0}^{\infty} x^{n} e^{-\lambda x^{2}} dx$  ;  $\frac{dI_{n}}{d\lambda} = -I_{n+2}$  ;  $I_{0} = \frac{1}{2}$  $\pi$  $\frac{\pi}{\lambda}$  ;  $I_1 = \frac{1}{2\lambda}$  $\int \frac{x^3}{1+x^3}$  $\int_{0}^{1} e^{x} - 1$  $\int_{0}^{\infty} \frac{x^3}{e^x - 1} dx = \frac{\pi^4}{15}$ Planck's law:  $u(\lambda) = n(\lambda) \bar{E}(\lambda)$ ;  $n(\lambda) = \frac{8\pi}{\lambda^4}$ ;  $\bar{E}(\lambda) = \frac{hc}{\lambda}$ 1  $e^{hc/\lambda k_B T} - 1$ Energy in a mode/oscillator:  $E_f = nhf$ ; probability  $P(E) \propto e^{-E/k_B T}$ Stefan's law :  $R = \sigma T^4$ ;  $\sigma = 5.67 \times 10^{-8} W / m^2 K^4$ ;  $R = cU/4$ ,  $U = \int u(\lambda) d\lambda$ 0  $\mathring{\int}$ Wien's displacement law :  $\lambda_m T = hc/4.96k_B$ Compton scattering :  $\frac{h}{m_e c} (1 - \cos \theta)$  ;  $\lambda_c = \frac{h}{m_e c} = 0.0243 A$ Rutherford scattering: Hydrogen spectrum:  $\frac{1}{2} = R(\frac{1}{m^2} - \frac{1}{n^2})$  $b = \frac{kq_a Q}{2}$  $\frac{kq_{\alpha}Q}{m_{\alpha}v^2}$  cot( $\theta$ /2) ;  $\Delta N \propto \frac{1}{\sin^4(t)}$  $\sin^4(\theta/2)$ Electrostatics:  $F = \frac{kq_1q_2}{r^2}$  (force) ;  $U = q_0V$  (potential energy) ;  $V = \frac{kq}{r}$  (potential)  $\frac{1}{\lambda}$  =  $R(\frac{1}{m})$  $\frac{1}{m^2} - \frac{1}{n^2}$  ;  $R = 1.097 \times 10^7$   $m^{-1} = \frac{1}{911}$ . 911.3*A* Bohr atom:  $r_n = r_0 n^2$ ;  $r_0 = \frac{a_0}{Z}$ ;  $E_n = -E_0 \frac{Z^2}{n^2}$ ;  $a_0 = \frac{\hbar^2}{mke^2} = 0.529A$ ;  $E_0 = \frac{ke^2}{2a_0}$ =13.6*eV* ; *L* = *mvr* = *n*h  $E_k = \frac{1}{2}$  $mv^2$ ;  $E_p = -\frac{ke^2Z}{r^2}$  $\frac{r^2Z}{r}$  ;  $E = E_k + E_p$  ;  $F = \frac{ke^2Z}{r^2}$  $\frac{e^2Z}{r^2} = m\frac{v^2}{r}$  $\frac{1}{r}$  ; *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 :  $\lambda = \frac{h}{h}$ *p* ;  $f = \frac{E}{h}$ ;  $\omega = 2\pi f$ ;  $k = \frac{2\pi}{\lambda}$ ;  $E = \hbar \omega$ ;  $p = \hbar k$ ;  $E = \frac{p^2}{2m}$  $\frac{P}{2m}$ ;  $\hbar c = 1973 \, eV A$  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 :  $-\frac{\hbar^2}{2}$ 2m  $\partial^2 \Psi$  $\frac{\partial^2 \Psi}{\partial x^2}$  + V(x) $\Psi(x,t)$  = i $\hbar \frac{\partial \Psi}{\partial t}$  $\therefore \Psi(x,t) = \psi(x)e$  $-i\frac{E}{\hbar}t$ Time – independent Schrodinger equation :  $-\frac{\hbar^2}{2}$ 2m  $\partial^2\!\psi$  $\frac{\partial^2 \psi}{\partial x^2}$  + V(x) $\psi(x)$  = E $\psi(x)$ ;  $\int_{-\infty}^{x} dx$  $-\infty$  $\int d x \psi^* \psi = 1$  $\sqrt{L}$   $\sqrt{L$  $\infty$  square well:  $\psi_n(x) = \sqrt{\frac{2}{L}} \sin(\frac{n\pi x}{L})$ ;  $E_n = \frac{\pi^2 \hbar^2 n^2}{2mL^2}$ ;  $x_{op} = x$ ,  $p_{op} = \frac{\hbar^2 n}{2mL^2}$  $\partial$  $\frac{\partial}{\partial x}$  ; < A > =  $\int_{-\infty}^{\infty} dx \psi^* A_{op} \psi$ Eigenvalues and eigenfunctions:  $A_{op} \Psi = a \Psi$  (*a* is a constant) ; uncertainty:  $\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$ Harmonic oscillator :  $\Psi_n(x) = C_n H_n(x)e$  $-\frac{m\omega}{2\hbar}x^2$ ;  $E_n = (n + \frac{1}{2})$  $\frac{1}{2}$ ) $\hbar \omega$ ;  $E = \frac{p^2}{2m} + \frac{1}{2}$  $\frac{1}{2} m \omega^2 x^2 = \frac{1}{2} m \omega^2 A^2$  ;  $\Delta n = \pm 1$ 

Step potential: 
$$
R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}
$$
,  $T = 1 - R$ ;  $k = \sqrt{\frac{2m}{\hbar^2}} (E - V)$   
\nTunneling:  $\psi(x) \sim e^{-\alpha x}$ ;  $T \sim e^{-2\alpha \Delta x}$ ;  $T \sim e^{-\frac{2}{\alpha}} \frac{1}{\alpha} (\cos \alpha x) = \sqrt{\frac{2m[V(x) - E]}{\hbar^2}}$ 

 $\overline{a}$ 3D square well:  $\Psi(x,y,z) = \Psi_1(x)\Psi_2(y)\Psi_3(z)$ ;  $E = \frac{\pi^2 h^2}{2m}$ 2*m*  $\left(\frac{n_1^2}{r^2}\right)$  $L_1^2$  $rac{1}{2}$  +  $n_2^2$  $L^2_2$  $rac{2}{2}$  +  $n_3^2$  $L^2_3$  $\frac{3}{2}$ 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 :  $E_n = -13.6eV$  $Z^2$ *n* 2 Ground state of hydrogen and hydrogen - like ions:  $\Psi_{1,0,0} = \frac{1}{\pi^{1/2}} \left( \frac{Z}{a_0} \right)$  $a<sub>0</sub>$  $)^{3/2}e^{-Zr/a_0}$ Orbital magnetic moment:  $\vec{\mu} = \frac{-e}{2}$ 2*me*  $\vec{L}$  ;  $\mu_z = -\mu_B m_l$  ;  $\mu_B = \frac{e\hbar}{2m}$ 2*me*  $= 5.79 \times 10^{-5} eV/T$ Spin  $1/2$ :  $s = \frac{1}{2}$  $\frac{1}{2}$ ,  $|S| = \sqrt{s(s+1)}\hbar$ ;  $S_z = m_s\hbar$ ;  $m_s = \pm 1/2$ ;  $\vec{\mu}_s = \frac{-e}{2m}$ 2*me g*  $\vec{r}$ *S*  Total angular momentum:  $\vec{J} = \vec{L} +$  $\vec{r}$  $S$ ;  $|J| = \sqrt{j(j+1)}\hbar$ ;  $|l-s| \le j \le l+s$ ;  $-j \le m_j \le j$  $\overline{a}$ Orbital + spin mag moment :  $\vec{\mu} = \frac{-e}{2}$ 2*m* ( r *L* + *g*  $\vec{r}$  $\vec{S}$  ; Energy in mag. field :  $U = -\vec{\mu}$ .  $\vec{r}$ *B*  Two particles :  $\Psi(x_1, x_2) = +/- \Psi(x_2, x_1)$  ; symmetric/antisymmetric Screening in multielectron atoms:  $Z \rightarrow Z_{\text{eff}}$ ,  $1 < Z_{\text{eff}} < Z$ Orbital ordering:  $1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 4f < 5d < 6p < 7s < 6d \sim 5f$ 

Boltzmann constant :  $k_B = 1/11,600 \text{ eV/K}$ 

$$
f_B(E) = Ce^{-E/kT} \quad ; \quad f_{BE}(E) = \frac{1}{e^{\alpha}e^{E/kT} - 1} \quad ; \quad f_{FD}(E) = \frac{1}{e^{\alpha}e^{E/kT} + 1} \quad ; \quad n(E) = g(E)f(E)
$$
\nRotation: \n
$$
E_R = \frac{L^2}{2I}, \quad I = \mu R^2, \quad \text{vibration:} \quad E_{\nu} = \hbar \omega(\nu + \frac{1}{2}), \quad \omega = \sqrt{k/\mu}, \quad \mu = m_1 m_2 / (m_1 + m_2)
$$
\n
$$
g(E) = \left[2\pi (2m)^{3/2} V / h^3\right] E^{1/2} \text{ (translation, per spin)} \quad ; \quad \text{Equipartition:} \quad \langle E \rangle = k_B T / 2 \text{ per degree of freedom}
$$
\n

**Justify all your answers to all problems. Write clearly.**

**Problem 1** (10 pts)



Consider an electron in an infinite square well potential and an electron in a harmonic oscillator potential, both in 1 dimension. Both electrons are in the lowest energy state. The longest wavelength photons that these electrons can absorb has wavelength 1000A. (a) Find the width of the square well, in A.

(b) Find the classical amplitude of oscillation for the electron in the ground state of this harmonic oscillator potential, in A.

(c) Compare the probabilities that the electron is at the center of the well in both cases. Which one is larger?

(d) Draw the wavefunctions for both cases and point out their similarities and differences.

Hints: 
$$
\int_{-\infty}^{\infty} e^{-\lambda x^2} dx = \sqrt{\frac{\pi}{\lambda}} \quad ; \quad \hbar^2 / m_e = 7.62 \ eVA^2
$$

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

! A particle moving in one dimension is described by the wavefunction

 $\Psi(x) = Cxe^{-x^2/(2x_0^2)}$ 

with C and  $x_0$  constants.

(a) Calculate the uncertainty in the position of this particle,  $\Delta x$ . Give your answer in terms of  $x_0$ .

(b) At what value of x is this particle most likely to be found? Give your answer in terms of  $x_0$ .

(c) Approximately how much more or less likely is it to find this particle at position  $0.02x_0$  than it is to find it at position  $0.01x_0$ ?

$$
\underline{\text{Hint:}} \int_{-\infty}^{\infty} x^2 e^{-\lambda x^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{\lambda^3}} \quad ; \quad \int_{-\infty}^{\infty} x^4 e^{-\lambda x^2} dx = \frac{3}{4} \sqrt{\frac{\pi}{\lambda^5}}
$$

# **Problem 3** (10 pts)

An electron moves in the one-dimensional potential

$$
V(x) = V_0 \left[ \frac{1 - \cos(x/a)}{1 + \cos(x/a)} \right]
$$

for  $-\pi a < x < \pi a$ ,  $V(x) = \infty$  otherwise. a=1A. The electron is described by the wavefunction:

 $\Psi(x) = C(1 + \cos(x/a))$  for  $-\pi a < x < \pi a$ ,  $\Psi(x) = 0$  otherwise. C is a constant.

Schrodinger equation for this potential. Give your answers in eV. (a) Find the values of  $V_0$  and of the energy E so that this wavefunction is a solution of the

(b) I has the enassionary and wearlington for this electron. I.e., and potential energy of the electron is smaller than its total energy. (b) Find the classically allowed region for this electron. I.e., the region where the

(c) Make a graph of the potential versus x and of the wavefunction versus x, showing in particular where the classical turning points are, where the second derivative of the wavefunction is negative and where it is positive, where the wavefunction goes to zero and where the potential goes to  $\infty$ .

# **Problem 4** (10 pts)

Consider a solid as a system of N three-dimensional harmonic oscillators, each of them has frequency  $\omega = 0.02$ eV/ $\hbar$ . As you know, its heat capacity  $C_V$  at high temperatures is  $3Nk_B$ , with k<sub>B</sub>=Boltzmann's constant (Doulong-Petit law).

Find the energy of this system at temperatures

- (a) 100K
- (b)  $1000K$
- (c) 10000K

Give your answers as  $CNk_B T$ , with C a numerical coefficient.

# **Problem 5** (10 pts)

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

 $\Psi(r, \vartheta, \phi) = Cre^{-r/a_0} \cos \theta$ 

with C a constant and  $a_0$  the Bohr radius.

(a) Give the values of the quantum numbers n,  $\ell$ , m and of the ionic charge Z. Justify your answers.

(b) Find the most probable r value for this electron.

(c) Calculate the average value of 1/r for this electron.

! (d) Compare your results in (b) and (c) with the predictions of the Bohr atom.

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

Hint: you need to normalize the probability distribution.

### **Problem 6** (10 pts)



An electron is in the ground state of the one-dimensional potential well shown. Estimate how long it will take it to escape, in seconds.

Hint: compute the tunneling probability and the number of attempts per second using the velocity and width of the well.

## **Problem 7** (10 pts)

Consider a gas of hydrogen atoms where all the electrons are initially in the  $n=3$ ,  $\ell = 1$ state.

(a) What are the wavelengths of the photons emitted when these electrons make transitions to lower energy states? Ignore spin-orbit coupling.

(b) Assume all the electrons are in the  $n=3$ ,  $\ell = 1$  state, and a magnetic field of magnitude 100T is turned on. Ignore spin-orbit coupling. What are the wavelengths of the photons emitted when these electrons make a transition to the ground state?

account spin-orbit coupling. Assume the effective magnetic field seen by the electron is (c) Assume all the electrons are in the  $n=3$ ,  $\ell = 1$  state, no magnetic field, but take into ...<br>.  $B<sub>eff</sub>=0.5T$ . Give the possible values of the quantum number J, the change in energy for each J due to spin-orbit coupling, and indicate which J gives the higher energy and why.

#### **Problem 8** (10 pts)

Consider a two-dimensional harmonic oscillator potential

$$
V(x, y) = \frac{1}{2}K(x^2 + y^2)
$$

The Schrodinger equation for a particle of mass m moving in two dimensions in this potential is separable into one-dimensional equations, just like the Schrodinger equation for a two-dimensional infinite well is separable into one-dimensional equations.

(a) Work out the math to show that the above statement is true, and explain.

(b) Give the expression for the ground state wavefunction of a particle in this potential,  $\Psi(x, y)$ , in terms of m and  $\omega = \sqrt{K/m}$ .

(c) Give the expression for the energy of the first excited state of this particle. What is its degeneracy? What are the possible quantum numbers?

harmonic oscillator potential, what is the total energy of the system? Give your answer in (d) If there are 4 identical fermions of mass m and the same spin in this two-dimensional terms of ω.

### **Justify all your answers to all problems. Write clearly.**