

**Formulas and constants:**

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

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

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

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

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

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

Stefan's law :  $R = \sigma T^4$  ;  $\sigma = 5.67 \times 10^{-8} \text{ W/m}^2 \text{K}^4$  ;  $R = cU/4$  ,  $U = \int_0^\infty u(\lambda) d\lambda$

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

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

Rutherford scattering:  $b = \frac{kq_1 q_2}{m_\alpha v^2} \cot(\theta/2)$  ;  $\Delta N \propto \frac{1}{\sin^4(\theta/2)}$

Electrostatics:  $F = \frac{kq_1 q_2}{r^2}$  (force) ;  $U = q_0 V$  (potential energy) ;  $V = \frac{kq}{r}$  (potential)

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

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

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

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

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

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

$\infty$  square well:  $\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$  ;  $E_n = \frac{\pi^2 \hbar^2 n^2}{2mL^2}$  ;  $x_{op} = x$  ,  $p_{op} = \frac{\hbar}{i} \frac{\partial}{\partial x}$  ;  $\langle A \rangle = \int_{-\infty}^{\infty} dx \psi^* A_{op} \psi$

Eigenvalues and eigenfunctions:  $A_{op} \Psi = a \Psi$  ( $a$  is a constant) ; uncertainty:  $\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$

Harmonic oscillator:  $\Psi_n(x) = C_n H_n(x) e^{-\frac{m\omega}{2\hbar} x^2}$  ;  $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$  ;  $E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 = \frac{1}{2}m\omega^2 A^2$  ;  $\Delta n = \pm 1$

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

3D square well:  $\Psi(x,y,z) = \Psi_1(x)\Psi_2(y)\Psi_3(z)$  ;  $E = \frac{\pi^2 \hbar^2}{2m} \left( \frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2} \right)$

Spherically symmetric potential:  $\Psi_{n,\ell,m}(r,\theta,\phi) = R_{n\ell}(r)Y_{\ell m}(\theta,\phi)$  ;  $Y_{\ell m}(\theta,\phi) = f_{\ell m}(\theta)e^{im\phi}$

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

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

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

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:  $Z \rightarrow Z_{\text{eff}}$ ,  $1 < Z_{\text{eff}} < Z$

Orbital ordering:

1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 4f < 5d < 6p < 7s < 6d ~ 5f

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

$f_B(E) = C e^{-E/kT}$  ;  $f_{BE}(E) = \frac{1}{e^\alpha e^{E/kT} - 1}$  ;  $f_{FD}(E) = \frac{1}{e^\alpha e^{E/kT} + 1}$  ;  $n(E) = g(E)f(E)$

Rotation:  $E_R = \frac{L^2}{2I}$ ,  $I = \mu R^2$ , vibration:  $E_v = \hbar \omega (v + \frac{1}{2})$ ,  $\omega = \sqrt{k/\mu}$ ,  $\mu = m_1 m_2 / (m_1 + m_2)$

$g(E) = [2\pi(2m)^{3/2} V / h^3] E^{1/2}$  (translation, per spin) ; Equipartition:  $\langle E \rangle = k_B T / 2$  per degree of freedom

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

**Problem 1** (10 pts)

Consider a system of one-dimensional harmonic oscillators, each with angular frequency  $\omega$ , with  $\hbar\omega = 0.01\text{eV}$ . Ignore the zero-point energy  $1/2 \hbar\omega$ .

- (a) Find the average energy per oscillator at temperature  $T=100\text{K}$ . Express your answer as  $\langle E \rangle = C(k_B T)$  with  $C$  a dimensionless constant and  $k_B$  Boltzmann's constant. Find the value of  $C$ .
- (b) Find a range of temperatures where  $\langle E \rangle > 0.9 k_B T$ .
- (c) Find a range of temperatures where  $\langle E \rangle < 0.01 k_B T$ .
- The ranges asked for in (b) and (c) don't have to be the largest possible ranges.

**Problem 2** (10 pts)

The electron affinity of Cl is 3.62 eV. It forms an ionic bond with an unknown atom X from the first column of the periodic table. The distance between ions in this XCl molecule is 2.5Å.

- (a) What is the maximum possible value of the ionization energy of X so that this molecule would still form, assuming there is no repulsion due to the exclusion principle? In other words, the maximum ionization energy of X so that the energy of the molecule is lower than the energy of the separated atoms.
- (b) The dissociation energy of this molecule is measured to be 2eV. Find what the ionization energy of X would be, assuming there is no repulsion due to the exclusion principle. Give your answer in eV.
- (c) The ionization energy of X is measured to be 5eV. Find the energy of repulsion due to the exclusion principle for this molecule.

**Problem 3** (10 pts)

A diatomic molecule is composed of two atoms of mass  $M$  at distance  $R$ , and has vibrational frequency  $\omega$ . The specific heat of a gas of such molecules at temperature  $T_1$  is measured to be approximately  $5/2 k_B$  per molecule and at another temperature  $T_2$  it is measured to be approximately  $7/2 k_B$  per molecule.

- (a) Explain what this result implies for the relative magnitudes of  $k_B T_1$ ,  $k_B T_2$ , and  $\hbar\omega$ , and why.
- (b) Assume a molecule in this gas is in its lowest vibrational state and is in a rotational state with quantum number  $\ell = 3$ . Give expressions for the energies of the photons that this molecule can absorb without changing its electronic energy state. Your answers should be in terms of  $\hbar\omega$ ,  $M$  and  $R$ .
- (c) Find numerical values for the answers in (b) assuming  $M=938\text{MeV}/c^2$ ,  $R=1\text{Å}$ ,  $\hbar\omega=0.05\text{eV}$ . Use that  $\hbar^2/M=0.0042\text{eVÅ}^2$  for that value of  $M$ .

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