

Formulas:

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

Electron rest mass : $m_e = 0.511 \text{ MeV}/c^2$; Proton : $m_p = 938.26 \text{ MeV}/c^2$; Neutron : $m_n = 939.55 \text{ MeV}/c^2$

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 : $\lambda_m T = \frac{hc}{4.96 k_B}$

Photons : $E = pc$; $E = hf$; $p = h/\lambda$; $f = c/\lambda$

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

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

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

Constants : $hc = 12,400 \text{ eV}\cdot\text{Å}$; $\hbar c = 1,973 \text{ eV}\cdot\text{Å}$; $k_B = 1/11,600 \text{ eV/K}$; $ke^2 = 14.4 \text{ eV}\cdot\text{Å}$

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

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

Bohr atom: $E_n = -\frac{ke^2 Z}{2r_n} = -\frac{Z^2 E_0}{n^2}$; $E_0 = \frac{ke^2}{2a_0} = \frac{mk^2 e^4}{2\hbar^2} = 13.6 \text{ eV}$; $E_n = E_{kin} + E_{pot}$, $E_{kin} = -E_{pot}/2 = -E_n$

$hf = E_i - E_f$; $r_n = r_0 n^2$; $r_0 = \frac{a_0}{Z}$; $a_0 = \frac{\hbar^2}{mke^2} = 0.529\text{Å}$; $L = mvr = n\hbar$ angular momentum

X - ray spectra: $f^{1/2} = A_n(Z - b)$; K : $b = 1$, L : $b = 7.4$

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

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

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

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

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

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

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

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

Ground state of hydrogen and hydrogen-like ions: $\Psi_{1,0,0} = \frac{1}{\pi^{1/2}} (\frac{Z}{a_0})^{3/2} e^{-Zr/a_0}$

Orbital magnetic moment: $\vec{\mu} = \frac{-e}{2m_e} \vec{L}$; $\mu_z = -\mu_B m_l$; $\mu_B = \frac{e\hbar}{2m_e} = 5.79 \times 10^{-5} eV/T$

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

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

Orbital ordering:

$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 4f < 5d < 6p < 7s < 6d \sim 5f$

Justify all your answers to all problems

Problem 1 (10 pts)

A two-dimensional infinite square well with side lengths $L_1=L_2=4A$ has 4 electrons.

Assume the electrons don't interact with each other.

(a) Find the ground state energy (in eV), taking into account that electrons are fermions with spin $\frac{1}{2}$.

(b) Give the degeneracy of the ground state (number of different states with the same energy).

(c) Taking into account now that electrons interact, do you expect the total spin of the ground state to be zero or nonzero? Justify.

(d) Answer the questions (b) and (c) for the case where $L_1=4A$, $L_2=4.2A$.

Use $\hbar^2/2m_e = 3.81 eV A^2$

Problem 2 (10 pts)

The $n=3$, $l=2$ radial wavefunction for an electron in a hydrogen-like ion is

$$R(r) = Cr^2 e^{-2r/a_0}$$

where a_0 is the Bohr radius and C is a constant.

- Find the most probable r for this electron, in terms of a_0 .
- Find the average r for this electron, in terms of a_0 .
- Give the value of the radius of this orbit within Bohr theory and compare with the results of (a) and (b). Discuss similarities and differences.

$$\text{Use } \int_0^{\infty} dr r^s e^{-\lambda r} = \frac{s!}{\lambda^{s+1}}$$

Problem 3 (10 pts)

Boron has atomic number $Z=5$, and electronic configuration $1s^2 2s^2 2p^1$.

- Give a qualitative explanation for why the ionization energy of boron, $I_B=8.3$ eV, is lower than both the ionization energy of Be ($Z=4$, $I_{Be}=9.3$ eV) and that of C ($Z=6$, $I_C=11.3$ eV).
- Calculate by how much (in eV) the energy of a Boron atom will change in an external magnetic field $B_{\text{ext}}=15\text{T}$, ignoring spin-orbit coupling. Will the energy increase or decrease if B_{ext} is (i) along the z direction, (ii) along the $-z$ direction, or (iii) along the x direction?
- Explain what are the consequences (if any) of spin-orbit coupling for the electronic states of the Boron atom in the absence of an external magnetic field.
- Give an example of an atom (other than hydrogen) for which spin-orbit coupling does not affect the ground state.

Justify all your answers to all problems