Your name: Solutions

SOME POSSIBLY USEFUL INFORMATION:

\( N_A \) or \( L = 6.022 \times 10^{23} \) mol\(^{-1} \) \hspace{2cm} \( h = 6.626 \times 10^{-34} \) J s

\( k = 1.38 \times 10^{-23} \) J K\(^{-1} \) \hspace{2cm} \( c = 2.998 \times 10^8 \) m s\(^{-1} \)

H atom mass = \( 1.66 \times 10^{-27} \) kg \hspace{2cm} electron mass = \( 9.11 \times 10^{-31} \) kg

\( R = 8.314 \) J K\(^{-1} \) mol\(^{-1} \)

Planck: \( E = h \nu \) \hspace{2cm} Schrodinger: \( \hat{H}\psi = E\psi \) \hspace{2cm} de Broglie: \( \lambda = h/\pi \)

Particle in 1-D box: \( \psi_n = (2/a)^{1/2} \sin(n\pi x/a), \) \hspace{2cm} \( E_n = h^2 n^2/(8ma^2) \)

Harmonic oscillator: \( E_v = (\nu + 1/2) h \nu; \) \hspace{2cm} \( \nu = (k/\mu)^{1/2}/(2\pi) \)

Rigid rotor \( |L|^2 = l(l+1) h^2/(4\pi^2) \) \hspace{2cm} \( L_z = m_l h/(2\pi) \) \hspace{2cm} \( E = L^2/(2I) \)

x operator is multiply by x \hspace{2cm} p operator is \( h/(2\pi) \) d/dx

\( E_k \) operator is \( -h^2/(8\pi^2 m) \) d\(^2\)/dx\(^2\) \hspace{2cm} V \) operator is multiply by V

radial distance r operator is multiply by r

IP of 1-electron atom proportional to \( Z^2/n^2 \). IP of H = 13.6 eV = \( 2.18 \times 10^{-18} \) J

\( \sin^2 x = (1 - \cos 2x)/2 \) \hspace{2cm} \( \cos^2 x = (1 + \cos 2x)/2 \)

\( \int_0^\infty x^n \exp(-ax) = \frac{n!}{a^{n+1}} \)
1) **30 points**

i) List all possible values of the orbital angular momentum and its z-component for an electron in an $f$ orbital. Leave $\hbar$ and $\pi$ in your answers.

ii) List all possible values of the spin angular momentum and its z-component for an electron in an $f$ orbital. Leave $\hbar$ and $\pi$ in your answers.

iii) Sketch the radial distribution function vs distance from the nucleus $r$ for a 3s electron.

\[ L^2 = \frac{L(L+1)\hbar^2}{4\pi^2} = \frac{3(4)\hbar^2}{4\pi^2} = \frac{3\hbar^2}{\pi^2} \]

so magnitude $= \sqrt{3} \frac{\hbar}{\pi}$

$m_L = -3, -2, -1, 0, 1, 2, 3$

\[ L_z = \frac{m_e \hbar}{2\pi} \]

so $L_z = -\frac{3\hbar}{2\pi}, -\frac{\hbar}{2\pi}, 0, \frac{\hbar}{2\pi}, \frac{3\hbar}{2\pi}$

ii) $S_z = m_s \frac{\hbar}{2\pi}$

$m_s = \pm \frac{1}{2}$

so $S_z = \frac{\hbar}{4\pi}, -\frac{\hbar}{4\pi}$

iii) 

![RDF Diagram](image)
2) 20 points
A quantized rigid rotor has a moment of inertia of $1.00 \times 10^{-46}$ kg m$^2$ and a rotational quantum number $l$.

a) What is the frequency (Hz) and wavenumber (cm$^{-1}$) of a photon whose energy matches the gap between $l=1$ and $l=2$?

b) What is the lowest possible value of the rotor's total energy, in J?

\[ E = \frac{L^2}{2I} = \frac{\ell(\ell+1)\hbar^2}{4\pi^22I} \]

For $\ell = 1$, $\ell(\ell+1) = 2$

$\ell = 2$, $\ell(\ell+1) = 6$

\[ E = \frac{\hbar^2}{4\pi^22I} (6-2) = \frac{4 \left( 6.626 \times 10^{-34} J_s \right)^2}{4 \pi^2 2 \left( 1 \times 10^{-46} \text{ kg m}^2 \right)} \]

\[ = 2.22 \times 10^{-22} J = h\nu \]

\[ \nu = \frac{2.22 \times 10^{-22} J}{6.626 \times 10^{-34} J_s} = 3.36 \times 10^7 \text{ s}^{-1} \]

b) $\ell = 0$, so

\[ E = \frac{0(0+1)\hbar^2}{4\pi^22I} = 0 \]
3) 50 points
A spherically symmetrical orbital in a hypothetical atom is given by
\[ \psi = N r^2 \exp(-0.3 r) \]
where \( r \) is the radial distance from the nucleus and \( N \) is the normalization constant.

i) Where are any local maxima in the radial distribution function?

ii) What is the value of \( N \)?

i) RDF is
\[ 4\pi r^2 \psi^2 = 4\pi r^2 N^2 r^4 e^{-0.6r} = P \]

\[ \frac{dP}{dr} = 4\pi N^2 r^6 e^{-0.6r} (-0.6) + 4\pi N^2 6r^5 e^{-0.6r} \]
\[ = 4\pi N^2 e^{-0.6r} [-0.6r^6 + 6r^5] \]
\[ = 4\pi N^2 e^{-0.6r} r^5 (6 - 0.6r) \]
\[ = 0 \quad \text{so} \quad r = \frac{6}{0.6} = 10 \]

ii) \[ \int_0^\infty 4\pi r^2 \psi^2 \psi \, dr = 1 \]

\[ 4\pi N^2 \int_0^\infty r^6 e^{-0.6r} \, dr = 4\pi N^2 \left( \frac{6^!}{0.6^4} \right) = 1 \]

\[ \implies N = 1.76 \times 10^{-3} \]