SOME POSSIBLY USEFUL INFORMATION:

\[ N_A \text{ or } L = 6.022 \times 10^{23} \text{ mol}^{-1} \]

\[ k = 1.38 \times 10^{-23} \text{ J K}^{-1} \quad \text{and} \quad c = 2.998 \times 10^8 \text{ m s}^{-1} \]

\[ \text{H atom mass} = 1.66 \times 10^{-27} \text{ kg} \quad \text{and} \quad \text{electron mass} = 9.11 \times 10^{-31} \text{ kg} \]

\[ R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1} \]

Planck: \( E = hv \)

Schrodinger: \( \hat{H}\psi = E\psi \)

de Broglie: \( \lambda = h/p \)

Particle in 1-D box:

\[ \psi_n = \left(\frac{2}{a}\right)^{1/2} \sin(n\pi x/a), \]

\[ E_n = \frac{h^2 n^2}{8ma^2} \]

Harmonic oscillator:

\[ E_n = (n + 1/2) \hbar \omega \]

\[ \nu = k/\mu \]

Rigid rotor: \( |L_z|^2 = \hbar (l + 1) \hbar^2/(4\pi^2) \)

\[ L_z = m_l \hbar/(2\pi) \]

x operator is multiply by x

\( p \) operator is \( h/(2\pi) d/dx \)

\( E_k \) operator is \( -\hbar^2/(8\pi^2m) d^2/dx^2 \)

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} \text{ J} \)

\[ \sin^2 x = (1 - \cos 2x)/2 \]

\[ \cos^2 x = (1 + \cos 2x)/2 \]

\[ \int_0^\infty x^n \exp(-ax) = \frac{n!}{a^{n+1}} \]
1) 30 points
i) Draw (no work required) the electron configuration of a ground-state sulfur atom (Z=16) showing the arrangement of electrons among the orbitals and the electron spins. What is the spin multiplicity of a ground-state sulfur atom?

\[
\text{Spin multiplicity} = 2S + 1 = 2 \left( \frac{3}{2} + \frac{1}{2} \right) + 1 = \frac{3}{2}
\]

\[\text{3p}\ \uparrow \downarrow \uparrow \uparrow \]
\[\text{3s}\ \uparrow \]
\[\text{2p}\ \uparrow \downarrow \uparrow \uparrow \]
\[\text{2s}\ \uparrow \]
\[\text{1s}\ \uparrow \]

ii) List all possible values of the orbital angular momentum and its z-component for an electron in a d orbital. Leave h and \( \pi \) in your answers.

\[l = 2\]
\[
\text{magnitude of the angular momentum is}
\]
\[
\sqrt{\ell(\ell+1)} \cdot \frac{\hbar}{2\pi} = \sqrt{6} \cdot \frac{\hbar}{2\pi}
\]

Possible z-components are \( m_l \frac{\hbar}{2\pi} \), i.e.,

\[\frac{3}{2} \cdot \frac{\hbar}{2\pi}, \ \frac{1}{2} \cdot \frac{\hbar}{2\pi}, \ 0, \ -\frac{1}{2} \cdot \frac{\hbar}{2\pi}, \ -\frac{3}{2} \cdot \frac{\hbar}{2\pi} \]
iii) Why is it easier to remove an electron from the 2p orbital of a neon atom than from the 2s orbital? Give as much detail as possible.

See notes. Relevant topics are $Z_{eff}$, shielding, penetration and inter-electron repulsion.
2) 20 points

A quantized harmonic oscillator has a force constant \( k \) and a reduced mass of \( 3 \times 10^{-27} \) kg.

a) A photon whose energy matches the gap between \( \nu=0 \) and \( \nu=1 \) has a wavenumber of 2000 cm\(^{-1}\). Evaluate \( k \) in Nm\(^{-1}\).

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

\[
\nu = c/\lambda = 2.998 \times 10^3 \text{ cm}^{-1} \times 2000 \text{ cm}^{-1} = 5.996 \times 10^{13} \text{ Hz},
\]

\[
= \frac{1}{2\pi} \sqrt{\frac{k}{m}} \quad \therefore \quad k = 4\pi^2 \nu^2 m
\]

\[
= 4\pi^2 \times (5.996 \times 10^{13} \text{ Hz})^2 \times 3 \times 10^{-27} \text{ kg}
\]

\[
= 426 \text{ Nm}^{-1}
\]

b) The zero point energy is \( \frac{1}{2} \hbar \nu = \frac{1}{2} \times 6.626 \times 10^{-34} \text{ J s} \times 5.996 \times 10^{13} \text{ Hz} \)

\[
= 1.986 \times 10^{-20} \text{ J}
\]
3) 50 points
A spherically symmetrical orbital in a hypothetical atom is given by
\[ \psi = N r^{1.5} \exp(-0.5 r) \]
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) Find the average or expectation value of \( r \), i.e., \( \langle r \rangle \). The operator for \( r \) is multiply by \( r \).

i) RDF: \[ \rho = 4\pi r^2 \psi^2 = 4\pi r^2 N^2 r^3 e^{-r} = 4\pi N^2 r^5 e^{-r} \]

\[ \frac{d\rho}{dr} = 4\pi N^2 (r^5 e^{-r} + e^{-r}, 5r^4) = 4\pi N^2 r^4 e^{-r} (5-r) \]

so when \( r=0 \) or \( r=5 \),

The shape to \[ P \]

so \( r=0 \) is a minimum and \( r=5 \) is the maximum.

ii) \[ \langle r \rangle = \frac{\int_0^\infty r^2 |\psi|^2 dr}{\int_0^\infty r^2 |\psi|^2 dr} = \frac{\int_0^\infty r^2 N^2 e^{-0.5 r} r^3 e^{-0.5 r} dr}{\int_0^\infty N^2 r^2 e^{-r} r^2 dr} \]

\[ \int_0^\infty r^6 e^{-r} dr = \frac{6!}{5!} = 6 \]