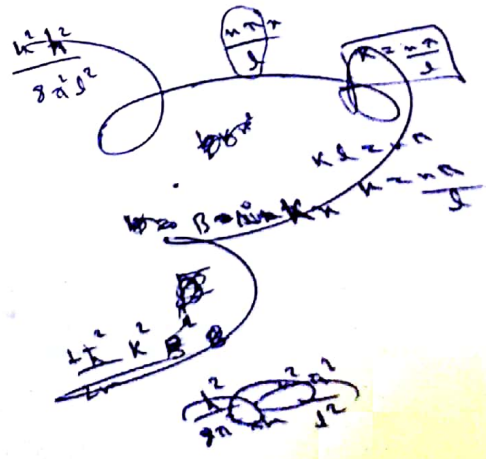
Answer all parts together.

1. A measurement on a particle in a 1D box shows it is 90% time in the ground state and 10% in the first excited state. What is the expectation value of the measured energy for a neutron in a cavity that is 10 nm long? [2]
2. Many proteins contain metal porphyrin molecules. These molecules are approximated as square planar and contain 26 π electrons.
   a. If the edge of the molecule is ~1000 pm, then what is the predicted lowest energy absorption of the porphyrin molecule? [1]
   b. Without the metals present, comment on the magnetic nature – whether these are diamagnetic or paramagnetic? [1]
3. This problem is on a 1-D quantum mechanical harmonic oscillator in a state with energy $\frac{7}{2}\hbar\sqrt{\frac{k}{\mu}}$.
   a. What is the normalized wavefunction describing this state? [2]
   b. A transition is seen at ~3000 cm^{-1} for $H^{35}Cl$ molecule when it is in the ground state. At what frequency, ν, does one expect to see the transition if the molecule is in the state whose energy is $\frac{7}{2}\hbar\sqrt{\frac{k}{\mu}}$? [1]
   c. Calculate the force constant k for the $H^{35}Cl$ bond. [2]
4. A H-atom is in the state given by,

$$\psi = \frac{1}{81\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2}\left(\frac{6r}{a_0}-\frac{r^2}{a_0^2}\right)e^{-r/3a_0}\sin\theta\,(\cos\phi + i\sin\phi)$$

   a. Write the values of n, l, m giving brief justifications. [1]
   b. What is the probability of finding the electron at $x = 0, y = 0, z = 2.6$? [1]
   c. Is ψ an eigenfunction of $\hat{L}_z$? If yes, determine the eigenvalue. [1]
   d. Determine the position of the radial nodes. [1]
   e. Where are the angular nodes? [1]
   f. To which of these states (*2s,2p,4d,4f*) would a transition occur from this state? [1]
   g. What is the ionization energy of this atom? [1]
   h. Plot the radial part as a function of z. [1]
5. Linear combination of two $1s$ A.O.s gives two M.O.s for H_2^+ denoted as ψ_+ and ψ_-.
   a. If the overlap integral at some internuclear distance R is 0.5, write the normalized form of ψ_+ and ψ_-. [2]
   b. What atomic system results when the internuclear distance in H_2^+ is zero? [1]
   c. To which atomic orbitals do ψ_+ and ψ_- *now* correspond to? Give a brief reason. [1]



Useful information

$m_n = m_p = 1.67 \times 10^{-27}\ kg;\ h = 6.626 \times 10 - 34\ \text{Js};\ c = 2.998 \times 108\ \text{ms}^{-1}$

Harmonic Oscillator

$$\psi_v(x) = N_v H_v(y) e^{-y^2/2} \qquad y = \frac{x}{\alpha} \qquad \alpha = \left(\frac{\hbar^2}{mk}\right)^{1/4}$$

v	$H_v(y)$
0	1
1	$2y$
2	$4y^2 - 2$
3	$8y^3 - 12y$
4	$16y^4 - 48y^2 + 12$
5	$32y^5 - 10y^3 + 120y$
6	$64y^6 - 480y^4 + 720y^2 - 120$

$$\int_{-\infty}^{\infty} H_v H_{v'} e^{-y^2}\, dy = \begin{cases} 0 & \text{if } v \neq v' \\ \alpha\sqrt{\pi}\, 2^v\, v! & \text{if } v = v' \end{cases}$$

Rigid rotor

$$Y_l^m(\theta,\phi) = \left[\frac{(2l+1)}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2} P_l^{|m|}(\cos\theta) e^{im\phi} \quad l = 0,1,2 \ldots \quad m = 0, \pm 1, \pm 2 \ldots$$

$P_0^0(x) = 1$

$P_1^0(x) = x = \cos\theta$

$P_1^1(x) = (1-x^2)^{1/2} = \sin\theta$

$P_2^0 = \frac{1}{2}(3x^2 - 1) = \frac{1}{2}(3\cos^2\theta - 1)$

$P_2^1(x) = 3x(1-x^2)^{1/2} = 3\cos\theta\sin\theta$

$P_2^2(x) = 3(1-x^2) = 3\sin^2\theta$

H-atom

$$E_n = -\frac{m_e e^4}{8\varepsilon_0^2 h^2 n^2} = -\frac{m_e e^4}{32\pi^2\varepsilon_0^2\hbar^2 n^2} \quad n = 1,2,3 \ldots$$