1. (40 pts.) Hydrogen atom is prepared in the state described by the following wavefunction, where $N$ is the normalization constant.

$$\psi(r, \theta, \varphi) = N \{(i+1) | n = 4, l = 3, m_l = 3 \rangle - 3 | n = 1, l = 0, m_l = 0 \rangle\}$$

1.1 (20 pts) Calculate the normalization constant $N$.

Solution

$$\langle \psi(r, \theta, \varphi) | \psi(r, \theta, \varphi) \rangle = N^2 \left( |i - 1|^2 + (3)^2 \right) = 11N^2 = 1 \Rightarrow N = 1/\sqrt{11}.$$
1.2 (20 pts) What is the emission energy in [eV] in the transition from $|n = 4, l = 3, m_l = 3\rangle$ to $|n = 1, l = 0, m_l = 0\rangle$?

**Solution**
The emission energy $\Delta E = E_4 - E_1 = -Ry \left(1/4^2-1\right) = 15Ry/16 = 12.75$ eV
2. (40 pts.) Use the following $x$ and $p_x$ operators to calculate $\langle 4 | (p_x^2 \cdot x - 1/2) | 3 \rangle$ where $x$ and $p_x$ are the position and momentum operators of a particle in a harmonic oscillator system. $|3\rangle$ and $|2\rangle$ are the eigenfunctions of the 1D harmonic oscillator.

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^+), \quad p_x = i\sqrt{\frac{\hbar m\omega}{2}} (a^+ - a),$$

where $\hbar$ is the Planck constant, $\omega = \sqrt{\frac{k}{m}}$, $k$ is a string constant of the harmonic oscillator, $m$ is a mass of the particle. $a$ and $a^+$ are the annihilation and creation operators for the harmonic oscillator system.

**Solution**

$$p_x^2 x = -\sqrt{\frac{\hbar^3 m\omega}{8}} (a^+ - a)^2 (a + a^+)$$

$$= -\sqrt{\frac{\hbar^3 m\omega}{8}} (a^+ a^+ a + a^+ a^+ a^+ - a^+ a a - a^+ a a^+ - a a^+ a^+ + a a + a a a^+)$$

where $a^+ a^+ a, a^+ a a^+, a a^+ a^+$ terms are non-zero, thus,

$$\langle 4 | p_x^2 x | 3 \rangle = -\frac{1}{2} \sqrt{\frac{\hbar^3 m\omega}{2}} \langle 4 | a^+ a^+ a - a^+ a a^+ - a a^+ a^+ | 3 \rangle$$

$$= -\frac{1}{2} \sqrt{\frac{\hbar^3 m\omega}{2}} (3 \cdot 2 - 4 \cdot 2 - 5 \cdot 2) = 6 \sqrt{\frac{\hbar^3 m\omega}{2}}$$
3. (60 pts) Consider a particle of mass $1.00 \times 10^{-25}$ g moving freely in a three-dimensional cubic box of side 10.00 nm. The potential is zero inside the box and is infinite at the wall and outside the box.

(a) (20 pts) Calculate the ground state energy of the particle in [eV].

(b) (20 pts) Consider the energy level that has an energy 9 times greater than the ground state energy. What is the degeneracy of this level? Identify all sets of quantum numbers that correspond to this energy.

(c) (20 pts) Compute the wavelength of the photon responsible for the transition from the ground state of the particle to the energy level of part (b).

Solution

(a) 
$$E_0 = E_{n_x=1,n_y=1,n_z=1} = \frac{3h^2}{8ml^2} = 0.10276 \text{ meV}$$

(b) 
$$E = 9E_0 = \frac{27h^2}{8ml^2} = \frac{h^2}{8ml^2} (n_x^2 + n_y^2 + n_z^2).$$

- $n_x = 5$, $n_y = 1$ and $n_z = 1$.
- $n_x = 1$, $n_y = 5$ and $n_z = 1$.
- $n_x = 1$, $n_y = 1$ and $n_z = 5$.
- $n_x = 3$, $n_y = 3$ and $n_z = 3$.

(c) 
$$E = 8E_0 = 24 \frac{h^2}{(8ml^2)} = 1.3171 \times 10^{-22} \text{ [J]}.$$  
$$L = \frac{hc}{E} = 1.5 \text{ mm}$$
4. (60 pts) Harmonic oscillators. Consider coupled-Harmonic oscillators given by the following Hamiltonian,

\[ H = -\frac{\hbar^2}{2m} \left( \frac{d^2}{dx_1^2} + \frac{d^2}{dx_2^2} \right) + \frac{1}{2} k x_1^2 + \frac{1}{2} k x_2^2 + \frac{1}{2} k (x_2 - x_1)^2 \]

where \( m \) is the mass of harmonic oscillators and \( k \) is the spring constant.

4.1. (30 pts) Using the following,

\[ x_+ = \frac{1}{\sqrt{2}} (x_2 + x_1) \quad \text{and} \quad x_- = \frac{1}{\sqrt{2}} (x_2 - x_1) \]

Rewrite the Hamiltonian in the representation of \((x_+, x_-)\).

Solution

Using \( x_1 = \frac{1}{\sqrt{2}} (x_+ - x_-) \) and \( x_2 = \frac{1}{\sqrt{2}} (x_+ + x_-) \),

\[ x_1^2 + x_2^2 = x_+^2 + x_-^2 \]

\[ \frac{d}{dx_1} = \frac{\partial x_+}{\partial x_1} \frac{d}{dx_+} + \frac{\partial x_-}{\partial x_1} \frac{d}{dx_-} = \frac{1}{\sqrt{2}} \left( \frac{d}{dx_+} - \frac{d}{dx_-} \right) \]

\[ \frac{d}{dx_2} = \frac{1}{\sqrt{2}} \left( \frac{d}{dx_+} + \frac{d}{dx_-} \right) \]

\[ \rightarrow \frac{d^2}{dx_1^2} + \frac{d^2}{dx_2^2} = \frac{d^2}{dx_+^2} + \frac{d^2}{dx_-^2} \]

Thus, the Hamiltonian is given by

\[ H = -\frac{\hbar^2}{2m} \left( \frac{d^2}{dx_+^2} + \frac{d^2}{dx_-^2} \right) + \frac{1}{2} k_+ x_+^2 + \frac{1}{2} k_- x_-^2 \]

where \( k_+ = k \) and \( k_- = 3k \).
4.2. (30 pts) Show the energy of the Harmonic oscillators (indicates the quantum numbers and constants explicitly).

Solution

Using separation of variables, the energy of the coupled system (which is same as the uncoupled system) is obtained by,

$$E = \hbar \omega_1 (\nu_1 + \frac{1}{2}) + \hbar \omega_2 (\nu_2 + \frac{1}{2}), \; \nu_1, \nu_2 = 0, 1, 2\ldots$$

where $$\omega_1 = \sqrt{\frac{k}{m}}$$ and $$\omega_2 = \sqrt{\frac{3k}{m}}$$. 