Problems on Harmonic oscillator, Angular momentum and Hydrogen atom.

Problem. a) Find the amplitude *A* of oscillations for a classical oscillator with energy equal to the energy of a quantum oscillator in the quantum state *n*.

b) Consider a classical oscillator of mass $m = 1.0g$, it makes 20 oscillation in $10\ sec$. Find the values of quantum number *n* corresponding to this oscillation with maximum amplitude *1 cm*.

Solution

a) To determine the amplitude *A*, we set the classical energy $E = \frac{1}{2}m\omega^2 A^2$ equal to $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$

Then we obtain $A = \sqrt{(2n+1)\frac{\hbar}{m\omega}}$.

As the quantum number *n* increases, the energy of the oscillator and therefore the amplitude of oscillation increases (for a fixed natural angular frequency. For large *n*, the amplitude is approximately proportional to the square root of the quantum number.

b) Solving the equation $A = \sqrt{(2n+1)\frac{\hbar}{m\omega}}$ for *n* we obtain

$$n = 6 \times 10^{27}.$$

Problem. The vibrational frequency of the hydrogen iodide HI diatomic molecule is $6.69 \times 10^{13} Hz$. Iodine atom is 127 times more massive than hydrogen atom. $(m_H = 1.67 \times 0^{-27} kg, c = 3.0 \times 10^8 m/s)$

a) What is the force constant of the molecular bond between the hydrogen and the iodine atoms? (295 N/m)
b) What is the energy of the emitted photon when this molecule makes a transition between adjacent vibrational energy levels? (0.277 eV)
c) What is the wavelength of the emitted photon?
d) The possible wavelengths of photons emitted with the *HI* molecule decays from the third excited state eventually to the ground state.

Solution

a) Relation between the force constant and frequency is given by:

$$\omega = 2\pi f = \sqrt{\frac{k}{\mu}}$$

Since iodine is 127 times massive than hydrogen then the reduced mass μ is given by

$$\mu = \frac{m_H m_I}{m_H + m_I} \cong m_H$$

Substituting values of given quantities we obtain:

$$k = 295\ N/m$$

b) Adjent vibrational energy levels are the energy level between *n* and *n+1*

$$E_{n+1} - E_n = \Delta E = \left(n + 1 + \frac{1}{2}\right)\hbar\omega - \left(n + \frac{1}{2}\right)\hbar\omega = \hbar\omega$$
$$\Delta E = 4.4 \times 0^{-20} J = 0.277 eV$$

c) $\lambda = \frac{c}{f} = 4.48 \times 10^{-6} m = 4.48 \mu m$

d) Energy of molecule is given by

$$E_n = 0.277\left(n + \frac{1}{2}\right) eV$$

Then calculate the transitions between $n = \{3 \to 2, 3 \to 1, 3 \to 0, 2 \to 1, 2 \to 0\}$

Problem. For a harmonic oscillator, what is the number of degeneracy for the 3th and 4th energy levels,

Solution

In this case we assume that the particles are spinless, then:

	Energy	$n_x n_y n_z$	#degeneracy
0	3/2		
1	5/2		
2	7/2		
3	9/2	003(3), 012(6), 111(1)	10
4	11/2	004(3),013(6), 022(3), 112(3)	15
5	13/2		
6	15/2		

Problem. A particle in the harmonic oscillator potential and start out its motion with an initial wave function:

$$\Psi(x, 0) = A(\psi_0 - 2\psi_1)$$

a) Determine A.
b) Construct $\Psi(x, t)$.
c) Find $\langle x \rangle$ and $\langle p_x \rangle$.
d) Find $\Delta x \Delta p$.
e) Find commutation relations $[a, x]$ and $[p, a^+]$
f) Find $\langle n | \left(a^+ a + \frac{1}{2}\right) | n \rangle$.

Hint:
$a = \frac{1}{\sqrt{2\hbar\omega m}}(ip_x + m\omega x)$, $a^+ = \frac{1}{\sqrt{2\hbar\omega m}}(-ip_x + m\omega x)$.
$p = -i\hbar\frac{d}{dx}$; $a\psi_n = \sqrt{n}\psi_{n-1}$; $a^+\psi_n = \sqrt{n+1}\psi_{n+1}$.
Uncertainty of an operator is $\Delta O = \sqrt{\langle O^2 \rangle - \langle O \rangle^2}$

Solution:

a)Using the normalization conditions:

$$1 = A^2(\langle\psi_0|\psi_0\rangle + 4\langle\psi_1|\psi_1\rangle) = 5A^2, then\ A = \frac{1}{\sqrt{5}}.$$

b) It is easy to construct time dependent wave function:

$$\Psi(x,t) = \frac{1}{\sqrt{5}}\left(\psi_0 e^{-\frac{iE_0}{\hbar}t} - 2\psi_1 e^{-\frac{iE_1}{\hbar}t}\right) = \frac{1}{\sqrt{5}}\left(\psi_0 e^{-i\frac{\omega t}{2}} - 2\psi_1 e^{-i\frac{3\omega t}{2}}\right)$$

Using energy values $E_0 = \frac{1}{2}\hbar\omega\ and\ E_1 = \frac{3}{2}\hbar\omega$. Norm of the wave function is given by:

c) We can use integral relations or operators to obtain expectation values. Here let us use operators The ladder operators then we can obtain the relations

$$x = \frac{\sqrt{2\hbar\omega m}}{2m\omega}(a_+ + a)\ and\ p = \frac{\sqrt{2\hbar\omega m}}{2i}(a - a^+)$$

with the action of the operators $a^+\psi_n = \sqrt{n+1}\psi_{n+1}\ and\ a\psi_n = \sqrt{n}\psi_{n-1}$

See lecture notes

Problem. Calculate the energy eigenvalues of an axially symmetric rotator and find the degeneracy of each energy level (i.e., for each value of the azimuthal quantum number m, find how many states $|l,m\rangle$correspond to the same energy). We may recall that the Hamiltonian of an axially symmetric rotator is given by

$$H = \frac{L_x^2 + L_y^2}{2I_1} + \frac{L_z^2}{2I_2}$$

where I_1 and I_2 are the moments of inertia.

(b) From part (a) infer the energy eigenvalues for the various levels of $l = 3$.

(c) In the case of a rigid rotator (i.e., $I_1 = I_2 = I$), find the energy expression and the corresponding degeneracy relation.

(d) Calculate the orbital quantum number l and the corresponding energy degeneracy for a rigid rotator where the magnitude of the total angular momentum is $\sqrt{56}\hbar$.

Hint: Use $L^2|lm_l\rangle = l(l+1)\hbar^2|lm_l\rangle\ and\ L_z|lm_l\rangle = m\hbar|lm_l\rangle$.

Problem. Consider the wave function in the state ψ_{nlm} describing motion of an electron in the Hydrogen atom:

$$\psi = \frac{1}{6}\left(4\psi_{200} + 3\psi_{211} - c\psi_{210} + \sqrt{10}\,\psi_{21-1}\right)$$

a) Using normalization and orthogonalization conditions determine the constant c.

b) Calculate expectation values of the Energy, $L^2\ and\ L_z$.

c) Is ψ eigenfunction of L^2 or Energy?

Problem. Energy of the electron in a hydrogen atom depends on the principal quantum number n, and given by

$$E = -\frac{13.6}{n^2}eV.$$

a. Using the $\psi_{nlm_l m_s}$ notation for the wave function, list all the $n = 1, 2\ and\ 3$ hydrogen states.

b. Calculate wavelengths of the emitted photons in (nm) when the transitions occurs $3 \to 2; 4 \to 2\ and\ 5 \to 2$. $(1nm = 10^{-9}m)$.

Problem. A wavefunction ψ_{nlm_l} describe Hydrogen atom. Action of the operators, energy H, angular momentum L and magneti moment L_z on the wavefunction are given by:

$$H\psi_{nlm_l} = -\frac{13.6}{n^2}\psi_{nlm_l}$$
$$L\psi_{nlm_l} = \sqrt{l(l+1)}\,\hbar\psi_{nlm_l}$$
$$L_z\psi_{nlm_l} = m_l\,\hbar\psi_{nlm_l}$$

a) What is the relation between quantum numbers $n, l\ and\ m_l$ and explain physical meaning of each quantum number.
b) What is the commutation relations $[H, L]\ and\ [L, L_z]$.
c) Calculate $\Delta H \Delta L$ and $\Delta L \Delta L_z$.

Problem. An electron of a hydrogen atom is in the state described by the wave function:

$$\psi = N(\psi_{300} + i\psi_{311} - i\psi_{31-1} + \psi_{320})$$

a) Find normalization constant N.
b) Find the expected value of the Energy, E, $L^2\ and\ L_z$.
c) Is ψ eigenfunction of $L^2\ or\ E\ or\ L_z$?

Problem. A state vector $|nlm_l m_s\rangle$ describe an atom. Where n , l, m_l and m_s are principal quantum number, angular momentum quantum number, magnetic quantum number and spin quantum number of an electron in an atom, respectively.

a) What is the relation between the quantum numbers $n, l, and\ m_l$?
b) What is the values of m_s?
c) How many total number of electrons can exist in the $n = 6$ state?
d) If superposition of a wavefunction of an hydrogen atom is given by

$$|nlm_l m_s\rangle = A\left|210 - \frac{1}{2}\right\rangle + \frac{\sqrt{3}}{2}\left|210\frac{1}{2}\right\rangle$$

Find A.

Problem. Find degree of degeneracy of state of electron in hydrogen atom, for the principal quantum numbers, $n = 1, 2, 5, 8$.