Tut 5 - Part 2
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Simple Harmonic oscillator

Q1

1. Using the uncertainty principle, show that the lowest energy of an oscillator is $\hbar\omega/2$.

Min energy of harmonic oscillator:

$$\langle E\rangle = \underbrace{\frac{1}{2}m\omega^2\langle x^2\rangle}_{PE} + \underbrace{\frac{1}{2m}\langle p^2\rangle}_{KE}$$

$$= \frac{1}{2}m\omega^2\left[\Delta x^2 + \langle x\rangle^2\right] + \frac{1}{2m}\left[(\Delta p_x)^2 + \langle p_x\rangle^2\right]$$

[neglect $\Delta x\langle x\rangle$ and $\Delta p_x\langle p_x\rangle$ terms]

Now $\langle x\rangle = 0$, $\langle p_x\rangle = 0$ [oscillating about $x=0$]

$$\langle E\rangle = \frac{1}{2}m\omega^2(\Delta x)^2 + \frac{1}{2m}(\Delta p_x)^2$$

$$= \frac{1}{2}m\omega^2(\Delta x)^2 + \frac{1}{2m}\left[\frac{\hbar^2}{4\Delta x^2}\right]$$

using AM, GM, min energy avg $= \frac{\hbar\omega}{2}$

Hence, proved

Q2

2. Determine the expectation value of the potential energy for a quantum harmonic oscillator (with mass m and frequency ω) in the ground state. Use this to calculate the expectation value of the kinetic energy. The ground state wavefunction of quantum harmonic oscillator is:

$$\psi_0(x) = C_0\exp\left(-\frac{m\omega}{2\hbar}x^2\right) \quad C_0 \text{ is constant;} \qquad (1)$$

$\langle PE\rangle = \frac{1}{2}m\omega^2\langle x^2\rangle$ $\int \psi^* x^2\psi$ integral

$\langle KE\rangle = \hbar\omega/2 - \langle PE\rangle$

Q3

3. A diatomic molecule behaves like a quantum harmonic oscillator with the force constant $k = 12Nm^{-1}$ and mass $m = 5.6 * 10^{-26}kg$

(a) What is the wavelength of the emitted photon when the molecule makes the transition from the third excited state to the second excited state ?

(b) Find the ground state energy of vibrations for this diatomic molecule.

a) $\Delta E_{4-3} = \hbar\omega$, $\omega = \sqrt{\frac{k}{m}}$

$\hbar\omega = \frac{hc}{\lambda} \Rightarrow \sqrt{\frac{k}{m}} \times \frac{1}{2\pi} = \frac{c}{\lambda} = 128.8\,\mu m$

b) Ground state energy $= \hbar\omega/2 = 7.7\times10^{-22}J$

Q4

4. Vibrations of the hydrogen molecule (H_2) can be modeled as a simple harmonic oscillator with the spring constant $k = 1.13 * 10^3 Nm^{-2}$ and mass $m = 1.67 * 10^{27}$ kg.

(a) What is the vibrational frequency of this molecule ?

(b) What are the energy and the wavelength of the emitted photon when the molecule makes transition between its third and second excited states ?

a) Effective mass of diatomic molecule $= m/2$

$\omega = \sqrt{k/\mu} \Rightarrow 1.16\times10^{15}$ Hz

b) $\Delta E = \hbar\omega$, $\lambda = \frac{2\pi c}{\omega} = 1.625\,\mu m$

Q5

5. * A two-dimensional isotropic harmonic oscillator has the Hamiltonian

same prop in all direcns (k)

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{1}{2}k(x^2+y^2)$$

(a) Show that the energy levels are given by

$$E_{n_x,n_y} = \hbar\omega(n_x+n_y+1) \quad \text{where} \quad n_x, n_y \in (0,1,2...) \quad \omega = \sqrt{\frac{k}{m}}$$

(b) What is the degeneracy of each level?

2 D Harmonic oscillator

Using separatn of variables:

$\Psi(x,y) = \psi_x(x)\psi_y(y)$

$H\Psi(x,y) = E\Psi(x,y)$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_x(x)}{\partial x^2}\times\psi_y(y) - \frac{\hbar^2}{2m}\frac{\partial^2\psi_y(y)}{\partial y^2} + \frac{k}{2}(x^2+y^2)\psi_x(x)\psi_y(y) = E\psi_x(x)\psi_y(y)$$

Divide overall by $\psi_x(x)\psi_y(y)$

$$\underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2\psi_x(x)}{\partial x^2}\times\frac{1}{\psi_x(x)}}_{\text{funcn of } x} - \underbrace{\frac{\hbar^2}{2m}\frac{\partial^2\psi_y(y)}{\partial y^2}}_{\text{funcn of } y} + \underbrace{\frac{1}{2}k(x^2+y^2)}_{\text{Separate}} = \overbrace{E}^{E_x+E_y}$$

$$\therefore -\frac{\hbar^2}{2m}\frac{\partial^2\psi_x(x)}{\partial x^2} + \frac{1}{2}kx^2\psi_x(x) = E_x\psi_x(x)$$

$E_x = \left(n_x+\frac{1}{2}\right)\hbar\omega$, |||ly $E_y = \left(n_y+\frac{1}{2}\right)\hbar\omega$

Total Energy, $E_x + E_y = (n_x+n_y+1)\hbar\omega$, $\omega = \sqrt{k/m}$

b) Degeneracy of each level

E	n_x	n_y	degeneracy
$\hbar\omega$	0	0	1
$2\hbar\omega$	0	1	2
	1	0	
$3\hbar\omega$	2	0	
	0	2	3
	1	1	

and so on...

Q6

6. Consider the Hamiltonian of a two-dimensional anisotropic harmonic oscillator ($\omega_1 \neq \omega_2$)

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2}m\omega_1^2q_1^2 + \frac{1}{2}m\omega_2^2q_2^2$$

3

$q_1, q_2 \Rightarrow$ generalised coordinates
$[(x,y)(y,z)(z,x)]$

→ Done above in Q5

(a) Exploit the fact that the Schrödinger eigenvalue equation can be solved by separating the variables and find a complete set of eigenfunctions of H and the corresponding eigenvalues.

(b) Assume that $\frac{\omega_1}{\omega_2} = \frac{3}{4}$ .Find the first two degenerate energy levels. What can one say about the degeneracy of energy levels when the ratio between ω_1 and ω_2 is not a rational number.

Potentials are additive.

a) $\Psi(q_1,q_2) = \psi_{q_1}(q_1)\psi_{q_2}(q_2)$

$$\psi_{q_1}(q_1)_{n_1} = \left(\frac{m\omega_1}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^{n_1}(n_1)!}}H_{n_1}\left(\sqrt{\frac{m\omega}{\hbar}}q_1\right)e^{-\frac{m\omega_1 q_1^2}{2\hbar^2}}$$

||| for $\psi_{q_2}(q_2)_{n_2}$

and $E_{q_1} = \left(n_1+\frac{1}{2}\right)\hbar\omega_1$, $E_{q_2} = \left(n_2+\frac{1}{2}\right)\hbar\omega_2$

Eigenstate $\Rightarrow \psi(q_1,q_2) = \psi_{q_1}(q_1)_{n_1}\psi_{q_2}(q_2)_{n_2}$

with $E = \left(n_1\omega_1 + n_2\omega_2 + \frac{\omega_1+\omega_2}{2}\right)\hbar$

b) $\frac{\omega_1}{\omega_2} = \frac{3}{4}$

$3n_1 + 4n_2 = n$

Degeneracy at $(0,3)$ $(4,0)$, $E = \frac{31\hbar\omega_2}{8}$

when not a rational no, wont get integer values of $n \Rightarrow \therefore$ degeneracy not possible.

Q7 (Imp)

7. A particle of mass m is confined to move in the potential $(m\omega^2x^2)/2$. Its normalized wave function is

$$\psi(x) = \left(\frac{2\beta}{\sqrt{3}}\right)\left(\frac{\beta}{\pi}\right)^{1/4}x^2e^{-(\beta x^2/2)}$$

where β is a constant of appropriate dimension.
(a) Obtain a dimensional expression for β in terms of m, ω and $\hbar$.
(b) It can be shown that the above wave function is the linear combination

$$\psi(x) = a\psi_0(x) + b\psi_2(x)$$

where $\psi_0(x)$ is the normalized ground state wave function and $\psi_2(x)$ is the normalized second excited state wave function of the potential. Evaluate b and hence calculate the expectation value of the energy of the particle in this state $\psi(x)$.
Given: $I_0(\beta) = \int_{-\infty}^{+\infty}e^{-\beta x^2}dx = \sqrt{\frac{\pi}{\beta}}$, $I_n(\beta) = \int_{-\infty}^{+\infty}(x^2)^n e^{-\beta x^2}dx = (-1)^n\frac{\partial^n}{\partial\beta^n}(I_0(\beta))$,
$\psi_0(x) = \left(\frac{\beta}{\pi}\right)^{1/4}e^{\frac{-\beta x^2}{2}}$

a) $[\beta] = L^{-2}$ [dimensionless power of e]

$[m] = M$, $[\omega] = T^{-1}$, $[\hbar] = ML^2T^{-1}$

$\therefore \beta = m\omega/\hbar$

b) $\psi(x) = \left(\frac{2\beta}{\sqrt{3}}\right)\left(\frac{\beta}{\pi}\right)^{1/4}x^2e^{-(\beta x^2/2)}$

$\psi_0(x) = \left(\frac{\beta}{\pi}\right)^{1/4}e^{-\beta x^2/2}$

Extra info: $H_0(x) = 1$, $H_1(x) = x$, $H_2(x) = x^2-1$

$H_n(x) = (-1)^n e^{x^2}\frac{\partial^n}{\partial x^n}(e^{-x^2})$

Now, $a = \int\psi_0^*(x)\Psi(x)$, $b = \int\psi_2^*(x)\Psi(x)$

and $\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\hbar\pi}\right)^{1/4}e^{-\frac{m\omega x^2}{2\hbar}}H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)$

$= \frac{1}{\sqrt{2^n n!}}\left(\frac{\beta}{\pi}\right)^{1/4}e^{-\beta x^2/2}H_n(\sqrt{\beta}x)$

Also, $\Psi(x)$ can be written as:

$$\Psi(x) = \frac{2}{\sqrt{3}}\left(\left(\frac{\beta}{\pi}\right)^{1/4}\left((\sqrt{\beta}x)^2-1\right)e^{-\beta x^2/2} + \left(\frac{\beta}{\pi}\right)^{1/4}e^{-\beta x^2/2}\right)$$

$$= \frac{2}{\sqrt{3}}\left(\sqrt{2^2 2!}\,\psi_2(x) + \sqrt{2^0 0!}\,\psi_0(x)\right)$$

$$= \frac{4\sqrt{2}}{\sqrt{3}}\psi_2(x) + \frac{2}{\sqrt{3}}\psi_0(x)$$

After normalisation:

$a = 1/3$, $b = \frac{2\sqrt{2}}{3}$ $\left[\frac{4\sqrt{2}/\sqrt{3}}{\left[(4\sqrt{2}/\sqrt{3})^2 + (2/\sqrt{3})^2\right]^{1/2}}\right]$

$$\langle E\rangle = \frac{1}{9}\frac{\hbar\omega}{2} + \frac{8}{9}\left(\frac{5\hbar\omega}{2}\right)$$

$$= \frac{41\hbar\omega}{18}$$

Q8

8. Consider an 3D isotropic harmonic oscillator show that the degeneracy g_n of the nth excited state, which is equal the number of ways the non negative integers n_x, n_y, n_z may be chosen to total to n, is given by

$$g_n = \frac{1}{2}(n+1)(n+2)$$

$n_x + n_y + n_z = n$, just show by cases for now

Q9

9. * A charged particle of mass ' m ' and charge ' q ' is bound in a 1-dimensional simple harmonic oscillator potential of angular frequency ' ω '. An electric field E_0 is turned on.
(a) What is the total potential V(x) experienced by the charge ?
(b) Express the total potential in the form of an effective harmonic oscillator potential.
(c) Sketch V (x) versus x.
(d) What is the ground state energy of the particle in this potential?
(e) What is the expectation value of the position (x) if the charge is in its ground state ?

(a) Total potential $\Rightarrow \frac{1}{2}kx^2 - qE_0x$

(b) Effective harmonic oscillator $\Rightarrow$ quadratic

$$V(x) = \frac{1}{2}\left(m\omega^2x^2 - 2E_0qx + \frac{E_0^2q^2}{m\omega^2}\right) - \frac{1}{2}\frac{E_0^2q^2}{m\omega^2}$$

$$V(x) = \frac{1}{2}m\omega^2\left(x - \underbrace{\frac{E_0q}{m\omega^2}}_{\text{mean posn shift}}\right)^2 - \frac{E_0^2q^2}{2m\omega^2}$$

(c) TISE: $a = \frac{E_0q}{m\omega^2}$, $V_0 = \frac{E_0^2q^2}{2m\omega^2}$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + \frac{1}{2}m\omega^2(x-a)^2\Psi(x) = (E+V_0)\Psi(x)$$

$x - a = x'$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x')}{\partial x'^2} + \frac{1}{2}m\omega^2x'^2\psi(x') = (E+V_0)\phi(x')$$

$E + V_0 = \left(n+\frac{1}{2}\right)\hbar\omega$, $n = 0, 1, ..$

d) $\therefore$ stationary state energies

$$E = \left(n+\frac{1}{2}\right)\hbar\omega - \frac{E_0^2q_0^2}{2m\omega^2}$$

$$E_0 = \frac{\hbar\omega}{2} - \frac{E_0^2q^2}{2m\omega^2}$$

e) $\langle x\rangle =$ Mean posn for harmonic oscillator

$$= \frac{E_0q}{m\omega^2}$$