Quantum harmonic Oscillator

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Learning objectives

By the end of this part, you will be able to:

1. Describe the model of the quantum harmonic oscillator
2. Identify differences between the classical and quantum models of the harmonic oscillator
3. Explain physical situations where the classical and the quantum models coincide

Classical Harmonic Oscillator

Simple Harmonic Oscillator (SHO)

- SHO is a system or a particle that under goes harmonic motion about an equilibrium point.
  Example: Mass-spring system
- The restoring force is

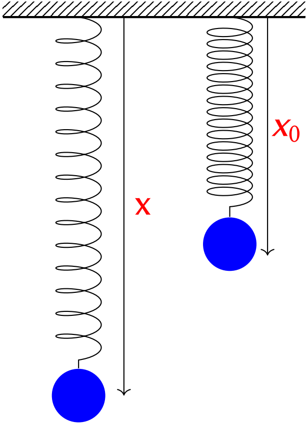
$$m\frac{d^2x}{dt^2} = F = -k\,x$$

- Solution to Newton's equation is

$$x(t) = A\sin(\omega t + \phi_0) \qquad \omega^2 = \frac{k}{m}$$

- Work done by the restoring force is

$$\Delta W = \int_x^{x_0} F \cdot x = -\frac{1}{2}k\left(x^2 - x_0^2\right)$$



k is spring constant
m is mass of the ball
spring is massless

Simple Harmonic Oscillator (SHO)

- Solution to Newton's equation is

$$x(t) = A\sin(\omega t + \phi_0) \qquad \omega^2 = \frac{k}{m}$$

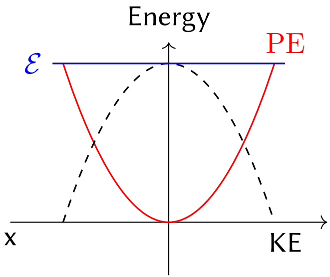
- The potential energy of the oscillator is

$$V(x) = -\Delta W = \frac{1}{2}k\left(x^2 - x_0^2\right)$$

- The total energy of the oscillator is:

$$\mathcal{E} = \underbrace{\frac{1}{2}mv^2(t)}_{\text{KE}} + \underbrace{\frac{1}{2}kx^2(t)}_{\text{PE}} = \frac{1}{2}kA^2 \qquad (1)$$

a constant.



Velocity any time is

$$v(t) = A\omega\cos\left(\omega t + \phi_0\right)$$

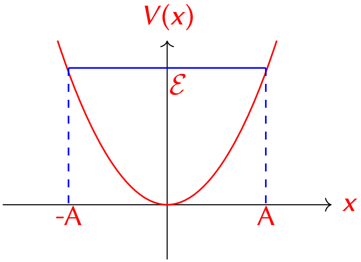
Time period is

$$T = \frac{2\pi}{\omega}$$

Classical HO: Properties

Quantum

- $v_{\pm A} = 0$ and Potential Energy $PE_{\pm A} = \mathcal{E}$.
- The motion of the HO is confined to the region where $KE \geq 0$. CHO can never be found beyond the turning points.
- The energy of the CHO changes in a continuous way.
- HO is at rest in its equilibrium position: $PE = 0$



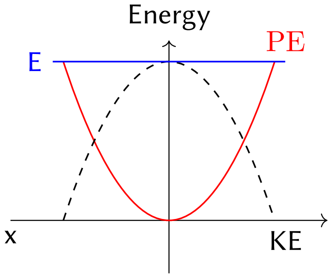
$x = 0$ is equilibrium point;
$x = \pm A$ are turning points

Classical HO: Properties

▸ Quantum

- When an object oscillates, with any value E, it spends the longest time near $x = \pm A$.
- At $x = \pm A$, object slows down and reverses its direction of motion. Hence, the probability to find CHO is largest at $x = \pm A$ and lowest at $x = 0$.
- To see this, let us calculate the classical probability to find the object in the internal x and $x + dx$:

$$\begin{aligned} P_{\mathrm{Cl}}(x)dx &= 2 \times \frac{dt}{T} = \frac{\omega}{\pi}\frac{dx}{v(t)} \\ &= \frac{1}{\pi}\frac{1}{\sqrt{A^2 - x^2(t)}}dx \end{aligned} \tag{2}$$



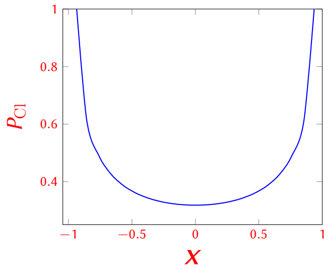
$$\begin{aligned} v(t) &= A\omega \cos(\omega t + \phi_0) \\ &= A\omega\sqrt{1 - \sin^2(\omega t + \phi_0)} \\ &= \omega\sqrt{A^2 - x^2(t)} \end{aligned}$$

Classical HO: Properties

▸ Quantum

- To see this, let us calculate the classical probability to find the object in the internal x and $x + dx$:

$$\begin{aligned} P_{\text{Cl}}(x)dx &= 2 \times \frac{dt}{T} = \frac{\omega}{\pi}\frac{dx}{v(t)} \\ &= \frac{1}{\pi}\frac{1}{\sqrt{A^2 - x^2(t)}}dx \end{aligned} \tag{2}$$



- Factor 2 appears above because HO is in the region x and $x + dx$ twice in one time-period T.

Importance of HO in Physics

Harmonic oscillator in Physics

Harmonic oscillator is one of the favourite systems a physicist uses to understand many complex phenomenon. There are very good reasons for this:

1. Oscillations are found throughout in the nature. Examples: Water waves, Vibration of a string, Vibrations of crystals, Light.

   HO serves as a prototype in the mathematical treatment of such diverse systems.

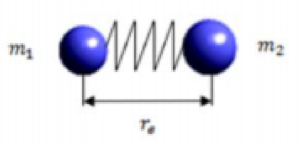
2. Close to the equilibrium point, most potentials look like HO:

$$V(x) = V(x_0) + \cancel{\left.\frac{dV(x)}{dx}\right|_{x_0}}^{\,0} (x - x_0) + \frac{1}{2}\left.\frac{d^2V(x)}{dx^2}\right|_{x_0} (x - x_0)^2 + \ldots$$

$$\Longrightarrow \quad V(x) - V(x_0) = \frac{1}{2} k\,(x - x_0)^2$$

Example 1: Vibrations of a diatomic molecule

- Consider a molecule consisting of two atoms.



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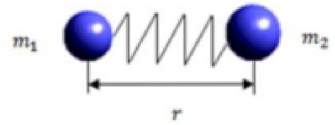

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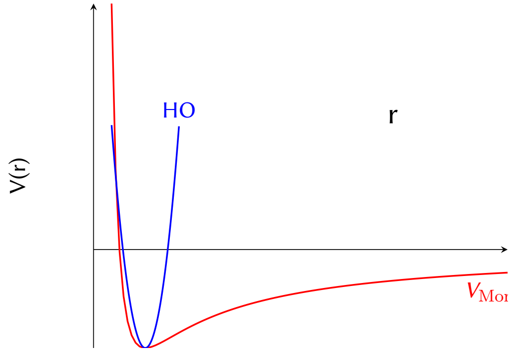
Example 1: Vibrations of a diatomic molecule

- Atoms attract each other via a potential — Morse potential

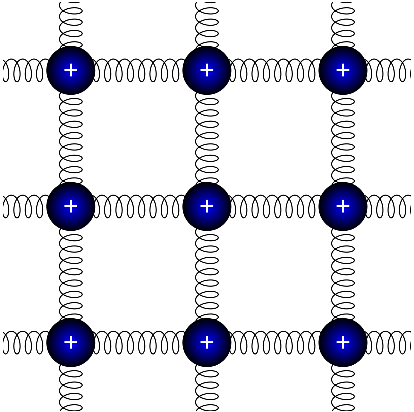
$$V(r) = D_e \left([1 - e^{-a(r-r_e)}]^2 - 1 \right)$$

- Atoms stay close to the equilibrium. Can be approximated by HO potential.



Example 2: Vibrations in solids

- A solid can be thought of a spheres connected by springs in all the 3 directions.
- Along each direction, motion can be analyzed in terms normal modes
- Each mode can be treated as a set of independent oscillator.
- Quantization of the crystal oscillators leads to the concept of phonons (sound quanta), which are analogous to photons.



Quantum Harmonic Oscillator

Hamiltonian and Schroedinger equation

- Hamiltonian operator is
$$\hat{H} = \underbrace{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}}_{\hat{T}(x)} + \underbrace{\frac{1}{2}m\omega^2 x^2}_{V(x)}$$

- Two important features about the potential:
  1. $V(x)$ increases without limit as $x \to \pm\infty$
  2. $V(x)$ is a symmetric potential.
- Time-independent Schroedinger equation (E are energy eigenvalues)

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi \tag{3}$$

- Divide the above equation by $\hbar\omega/2$ and define:

$$\epsilon = \frac{2E}{\hbar\omega}; \quad \beta^2 = \frac{m\omega}{\hbar}; \quad y = x\beta \quad \Longrightarrow \quad \frac{d^2\psi}{dy^2} + \left(\epsilon - y^2\right)\psi = 0 \tag{4}$$

(Check the dimensions of ϵ and y)

Hamiltonian and Schroedinger equation

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Strategy is to solve $\psi(y)$ and then replace $y \to x\beta$.

Heuristic way to find ψ

$$\frac{d^2\psi}{dy^2} + \epsilon\psi - \underbrace{y^2\psi}_{\text{need to keep } y^2\psi \text{ finite}} = 0 \tag{5}$$

- $e^{\pm iy}$: Do not fall off for large $|y|$.

  Need a function that falls off faster than $1/y^2$

- e^{-y}: Only works for positive y (or x).
- $e^{-|y|}$: Derivative is not smooth at 0. However, ψ and its derivative should be smooth everywhere in x.

Heuristic way to find ψ

$$\frac{d^2\psi}{dy^2} + \epsilon\psi - \underbrace{y^2\psi}_{\text{need to keep } y^2\psi \text{ finite}} = 0 \tag{5}$$

- Gaussian: It is valid for all values of y and is localised near $y = 0$.

$$\psi(y) = Ae^{-\alpha y^2} \; ; \; \frac{d\psi}{dy} = -2A\alpha y e^{-\alpha y^2} \; ; \; \frac{d^2\psi}{dy^2} = A\left(4\alpha^2 y^2 - 2\alpha\right) e^{-\alpha y^2} \tag{6}$$

- Substituting in Eq. (5), we have:

$$A\left[4\alpha^2 y^2 - 2\alpha + \epsilon_0 - y^2\right] e^{-\alpha y^2} = 0 \implies \alpha = \frac{1}{2}; \; \epsilon_0 = 1 \tag{7}$$

Heuristic way to find ψ

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- Solution is

$$\psi_0(x) = C_0 \exp\left(-\frac{\beta^2 x^2}{2}\right) \; ; \; E_0 = \frac{1}{2}\hbar\omega \tag{8}$$

- Normalization condition fixes C_0.

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1 \implies C_0 = \sqrt[4]{\frac{\beta^2}{\pi}} \tag{9}$$

Gaussian wavepacket centred at $x = 0$, but no motion

Properties of the solution

CHO

- Energy of the oscillator is not zero. It is a positive and depends on frequency of the oscillator.

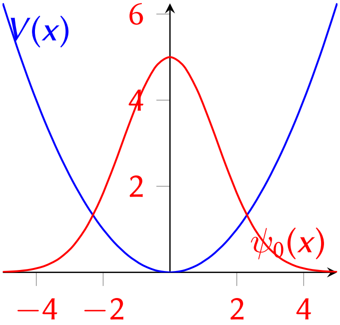
- From Eq. 1, classical turning points are

$$\mathcal{E} = \frac{1}{2}kx_{\max}^2 \implies x_{\max} = \sqrt{\frac{2\mathcal{E}}{k}} = \sqrt{\frac{2\mathcal{E}}{m\omega^2}}$$

- Substituting E_0 from Eq. (8), we have:

$$x_{\max} = \sqrt{\frac{\hbar}{m\omega}} = \frac{1}{\beta}$$

- However, for $x > x_{\max}$, $\psi_0(x) \neq 0$!



Properties of the solution

◂ CHO

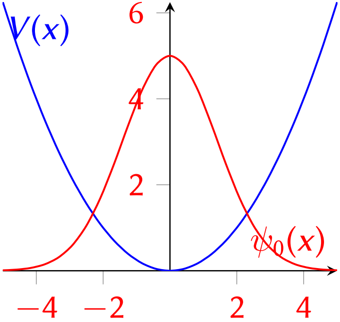
Key differences between CHO and QHO are:

1. CHO can not penetrate into the forbidden region $x > x_{\mathrm{max}}$.

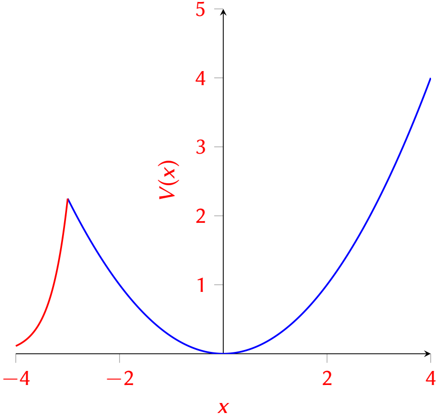
   QHO does penetrate into the classically forbidden regions.

2. In CHO, P_{Cl} was maximum at turning points.

   Quantum physics predicts that the particle is most likely to be found in the center.



Interesting consequence



- Consider a potential like in the figure. Potential stops rising and falls back to zero at some finite distance $A > x_{\text{max}}$. Assume $x_{\text{max}} = 2$
- CHO will never "know" and stay confined in the region $-x_{\text{max}} \leq x \leq x_{\text{max}}$ forever!
- QHO can "leak out" or tunnel through and can become a free particle within a finite time.

Example: $\alpha-$decay and Fission process

Are there more eigenstates and eigenvalues?

- $\psi_0(x)$ in Eq. (8) is one eigenstate and E_0 is corresponding eigenvalue.
- Let us try

$$\psi_1(y) = y\,\psi_0(y)\,;\;\frac{d\psi_1}{dy} = \psi_0(y) + y\,\frac{d\psi_0}{dy}\,;\;\frac{d^2\psi_1}{dy^2} = 2\frac{d\psi_0}{dy} + y\frac{d^2\psi_0}{dy^2}$$

- Substituting these in Eq. (5), we get:

$$2\frac{d\psi_0}{dy} + y\left(\frac{d^2}{dy^2} - y^2\right)\psi_0 = -y\epsilon_1\psi_0 \Longrightarrow -y\psi_0 - \frac{1}{2}\hbar\omega\,y\,\psi_0 = -y\epsilon_1\psi_0 \tag{10}$$

where we have used Eq. (6) to substitute $d\psi_0/dy$ and used (7) to replace the term in the bracket.

- Simplifying the above expression, we have

$$E_1 = \frac{3}{2}\hbar\omega\,;\;\psi_1(x) = \sqrt[4]{\frac{4\beta^2}{\pi}}(\beta\,x)\,\exp\left(-\frac{\beta^2x^2}{2}\right) \tag{11}$$

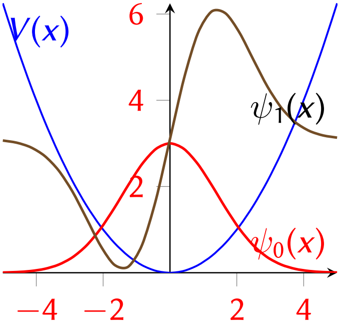
Difference between ψ_0 and ψ_1

Energy eigenvalues are

$$E_0 = \frac{1}{2}\hbar\omega; \quad E_1 = \frac{3}{2}\hbar\omega \tag{12}$$

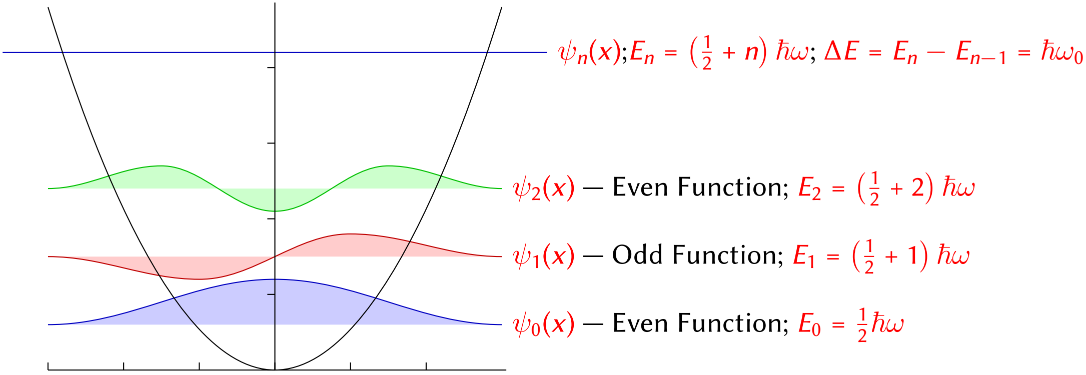
Eigen functions are

$$\psi_0(x) = C_0 \exp\left(-\frac{m\omega}{2\hbar}x^2\right); \psi_1(x) = C_1 x \exp\left(-\frac{m\omega}{2\hbar}x^2\right) \tag{13}$$



1. $\psi_0(-x) = \psi_0(x)$ (symmetric w.r.t x)
   $\psi_1(-x) = -\psi_1(x)$ (anti-symmetric w.r.t x)
2. $\epsilon_1 > \epsilon_0$
3. In ψ_0, the particle is most likely to be found in the center.
   In ψ_1, the particle is most likely to be found away from the center

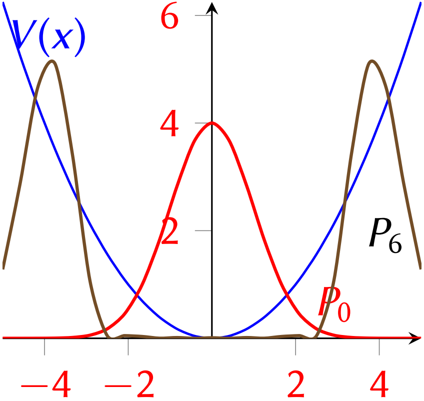
Other eigenfunctions



Other eigenfunctions

$$
\begin{array}{lll}
n & E_n & \psi_n(x) \\
0 & \frac{1}{2}\hbar\omega_0 & \left(\frac{\beta^2}{\pi}\right)^{1/4} e^{-\beta^2x^2/2} \\
1 & \frac{3}{2}\hbar\omega_0 & \left(\frac{\beta^2}{\pi}\right)^{1/4} \sqrt{\frac{1}{2}} 2\beta x e^{-\beta^2x^2/2} \\
2 & \frac{5}{2}\hbar\omega_0 & \left(\frac{\beta^2}{\pi}\right)^{1/4} \sqrt{\frac{1}{8}} \left(4\beta^2x^2 - 2\right) e^{-\beta^2x^2/2} \\
3 & \frac{7}{2}\hbar\omega_0 & \left(\frac{\beta^2}{\pi}\right)^{1/4} \sqrt{\frac{1}{48}} \left(8\beta^3x^3 - 12\beta x\right) e^{-\beta^2x^2/2} \\
4 & \frac{9}{2}\hbar\omega_0 & \left(\frac{\beta^2}{\pi}\right)^{1/4} \sqrt{\frac{1}{384}} \left(16\beta^4x^4 - 48\beta^2x^2 + 12\right) e^{-\beta^2x^2/2}
\end{array}
\tag{14}
$$

Comparison with CHO



- Quantum probability density distributions change in character for excited states, becoming more like the classical distribution for higher n.

- The classical probability density distribution corresponding to $n = 6$ quantum state is a reasonably good approximation of the quantum probability distribution for a quantum oscillator in this excited state. This agreement becomes increasingly better for highly excited states

$$\frac{\Delta E}{E_n} = \frac{\hbar\omega_0}{(n + 1/2)\hbar\omega_0} \to 0 \qquad n \to \infty$$

For large quantum numbers, energy levels become so close that it can be treated as continuum.

Δx and Δp for the Ground state

- GS wavefunction of HO is $\psi_0(x) = C_0 e^{-\beta^2 x^2/2}$

- Uncertainty in position and momentum are given by:

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \qquad \Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$$

- The expectation in position and momentum vanishes!

$$\begin{aligned} \langle x \rangle &= \int_{-\infty}^{+\infty} x |\psi_0(x)|^2 dx = C_0^2 \int_{-\infty}^{+\infty} x e^{-\beta^2 x^2} dx = 0 \\ \langle p \rangle &= -i\hbar \int_{-\infty}^{+\infty} \psi_0^*(x) \frac{d\psi_0(x)}{dx} dx \propto C_0^2 \int_{-\infty}^{+\infty} x e^{-\beta^2 x^2} dx = 0 \end{aligned}$$

- $\langle x^2 \rangle$ and $\langle p^2 \rangle$ are

$$\langle x^2 \rangle = \int_{-\infty}^{+\infty} x^2 |\psi(x)|^2 dx = \frac{\hbar}{2m\omega} \qquad \langle p^2 \rangle = -\hbar^2 \int_{-\infty}^{+\infty} \psi^*(x) = \frac{m\hbar\omega}{2} \qquad \Delta x \Delta p = \hbar/2$$

Why tunneling phenomena can occur?

- Due to the continuity requirement of the wave function at the boundaries when solving time-independent Schroedinger equation.

- The wave function cannot die off suddenly at the boundaries of a finite potential well or HO

  The wave function can only diminish in an exponential manner which then allow the wave function to extends slightly beyond the boundaries.

- The quantum tunneling effect is a manifestation of the wave nature of particle, which is governed by the Schroedinger equation.

- In classical physics, particles are just particles, hence never display tunneling effect.

Key Take-aways

- QHO is a model built in analogy with the model of a CHO. It models the behavior of many physical systems, such as molecular vibrations or Lattice vibrations.
- The allowed energies of a quantum oscillator are discrete and evenly spaced. The energy spacing is equal to Planck's energy quantum.
- The ground state energy is larger than zero. Unlike CHO, QHO is never at rest, even at the bottom of a potential well, and undergoes quantum fluctuations.
- The stationary states (states of definite energy) have non-zero values also in regions beyond classical turning points.
- When in the ground state, QHO is most likely to be found around the position of the minimum of the potential well, which is the least-likely position for CHO. For high quantum numbers, the motion of QHO becomes more similar to the motion of CHO.