The Quantum Harmonic Oscillator

Partial Differential Equations

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Objectives

In this lesson we will:

- review the classical harmonic oscillator and its properties,
- introduce the wave function and some axioms of quantum mechanics,
- present the Schrödinger equation, and
- solve the Schrödinger equation for the quantum analogue of the classical harmonic oscillator.

Classical Harmonic Oscillator

Ignoring damping, the initial value problem for the classical harmonic oscillator resembles,

$$
\begin{aligned}
m\,u'' + k\,u &= 0 \\
u(0) &= u_0 \\
u'(0) &= v_0.
\end{aligned}
$$

The displacement of the mass can be described by the function,

$$u(t) = u_0 \cos\left(\sqrt{\frac{k}{m}}t\right) + v_0\sqrt{\frac{m}{k}} \sin\left(\sqrt{\frac{k}{m}}t\right).$$

Properties of the Classical Harmonic Oscillator

- The period of the oscillation is $T = 2\pi/\omega$ and the frequency of the oscillation is $f = \omega/(2\pi) = 1/T$.
- The amplitude of the oscillation is $A = \sqrt{u_0^2 + v_0^2/\omega^2}$.
- The total energy of the spring-mass system is the sum of the kinetic and potential energies:

$$E = \frac{1}{2} m \left(u'(t)\right)^2 + \frac{1}{2} k \left(u(t)\right)^2 .$$

- Since there are no other forces present in the spring-mass system the total energy is constant, and thus

$$E = \frac{1}{2} k \left(u_0^2 + \frac{v_0^2}{\omega^2} \right) .$$

Location of the Mass

Suppose an observer examines a subinterval of $[-A, A]$ of length Δu. What is the probability of observing the mass in this subinterval?

- Let the probability distribution for the displacement u defined for $u \in [-A, A]$ be denoted as $P(u)$.
- For any fixed $u \in (-A, A)$, if Δu is small, the probability of observing the mass in the subinterval $[u, u + \Delta u]$ is $P(u)\Delta u$.
- Let Δt be the time required for the mass to travel distance Δu.
- During a complete period of oscillation the mass will traverse the subinterval of length Δu twice,

$$P(u)\Delta u = \frac{2\Delta t}{T} \implies P(u)\frac{\Delta u}{\Delta t} = \frac{2}{T}.$$

  As Δu and Δt approach zero, $P(u) = 2/(|u'(t)|T)$ where $|u'(t)| = \omega\sqrt{A^2 - (u(t))^2}$ is the speed of the mass.
- The probability density function for the displacement of the mass is

$$P(u) = \frac{2}{\omega\sqrt{A^2 - (u(t))^2}\,\frac{2\pi}{\omega}} = \frac{1}{\pi\sqrt{A^2 - u^2}}.$$

Background

- In 1926, Louis de Broglie stated that all matter has wave-like properties. This assertion has since become known as the **de Broglie hypothesis**.
- The fundamental property of an object is its **wave function** $\Psi(x, t)$, from which quantities such as the position and velocity of the object can be derived. The wave function is a complex-valued function.
- Max Born developed the statistical interpretation of the wave function which implies the probability of finding an object in the interval $[x, x + dx]$ at time t is $P(x, t)\, dx = \Psi(x, t)\overline{\Psi(x, t)}\, dx$ where $\overline{\Psi(x, t)}$ is the complex conjugate of the wave function.
- The wave function of an object solves the linear partial differential equation known as the linear **Schrödinger equation.** The one-dimensional version of the linear Schrödinger equation can be written as

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2\mu}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi(x, t).$$

Solving Schrödinger's Equation

Assume $V(x) = kx^2/2$ (the same as for the classical harmonic oscillator), Schrödinger's equation can be written as

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2\mu} \frac{\partial^2 \Psi}{\partial x^2} + \frac{1}{2} k x^2 \Psi(x, t).$$

Assume this equation is defined for $-\infty < x < \infty$ and the solutions asymptotically approach 0 as $|x| \to \infty$. Let the initial wave function be $\Psi(x, 0) = f(x)$.

Use separation of variables assuming $\Psi(x, t) = X(x)T(t)$.

$$\begin{aligned} i\hbar X(x)T'(t) &= -\frac{\hbar^2}{2\mu} X''(x)T(t) + \frac{1}{2} k x^2 X(x)T(t) \\ i\hbar \frac{T'(t)}{T(t)} &= -\frac{\hbar^2}{2\mu} \frac{X''(x)}{X(x)} + \frac{1}{2} k x^2. \end{aligned}$$

Energy

$$i\hbar\frac{T'(t)}{T(t)} = -\frac{\hbar^2}{2\mu}\frac{X''(x)}{X(x)} + \frac{1}{2}kx^2 = E$$

The induced ordinary differential equation involving x is

$$-\frac{\hbar^2}{2\mu}X''(x) + \left(\frac{1}{2}kx^2 - E\right)X(x) = 0.$$

Let ω be a constant such that $k = \mu\omega^2$ and make the substitution $x = \xi\sqrt{\hbar/(\mu\omega)}$.

$$\frac{d^2X}{d\xi^2} + \left(\frac{2E}{\hbar\omega} - \xi^2\right)X = 0$$

Hermite's Equation

$$y'' - 2xy' + \lambda y = 0 \text{ for } -\infty < x < \infty,$$

Let $\phi(x) = e^{-x^2/2} y(x)$ where $y(x)$ is a solution to Hermite's ordinary differential equation then

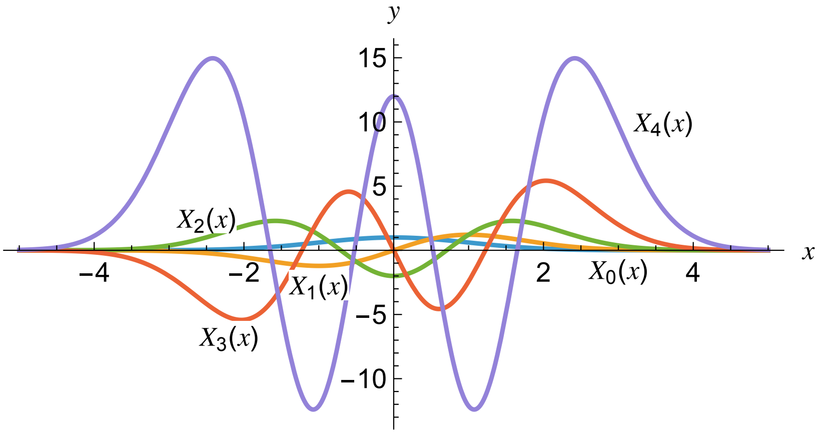
$$0 = \left[e^{x^2/2}\phi(x)\right]'' - 2x\left[e^{x^2/2}\phi(x)\right]' + \lambda e^{x^2/2}\phi(x)$$
$$0 = \left(\phi''(x) + (\lambda + 1 - x^2)\phi(x)\right) e^{x^2/2}.$$

Dividing both sides of by $e^{x^2/2}$ and note that this is of the form of the previous equation if $2E/(\hbar\omega) = \lambda + 1$. If $\lambda = 2n$ where $n = 0, 1, 2, \ldots$, then $y(x) = H_n(x)$, the nth Hermite polynomial. Thus for $E \equiv E_n = \hbar\omega(n + 1/2)$ the function $X_n(\xi) = e^{-\xi^2/2} H_n(\xi)$.

Hermite Functions

$$X_n(x) = e^{-\frac{\mu\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{\mu\omega}{\hbar}}x\right) \text{ for } n = 0, 1, 2, \ldots.$$

Functions of this form are non-normalized **Hermite functions**.



Product Solutions

Product solutions to the one-dimensional linear Schrödinger equation for the quantum harmonic oscillator have the form,

$$\Psi_n(x,t) = e^{-i\omega(n+\frac{1}{2})t} e^{-\frac{\mu\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{\mu\omega}{\hbar}}x\right) \text{ for } n = 0, 1, 2, \ldots.$$

The symbol E_n was chosen for the eigenvalues, since these are typically called **energy eigenvalues**. The implication is that energies of the product solutions for the quantum harmonic oscillator take on values from an infinite, but discrete set of values. The energy levels are separated by the finite positive quantity $\hbar\omega$. The least energy the quantum harmonic oscillator can possess is $E_0 = \hbar\omega/2 > 0$ which is sometimes called the **zero point energy**.

Series Solution

$$\Psi(x,t) = e^{-\frac{\mu\omega x^2}{2\hbar}} \sum_{n=0}^{\infty} A_n e^{-i\omega(n+1/2)t} H_n\left(\sqrt{\frac{\mu\omega}{\hbar}}x\right),$$

where the expressions A_n are constants. If the initial form of the wave function is $f(x)$, then

$$f(x) = e^{-\frac{\mu\omega x^2}{2\hbar}} \sum_{n=0}^{\infty} A_n H_n\left(\sqrt{\frac{\mu\omega}{\hbar}}x\right),$$

where

$$A_n = \frac{1}{2^n n!}\sqrt{\frac{\mu\omega}{\hbar\pi}} \int_{-\infty}^{\infty} f(x) H_n\left(\sqrt{\frac{\mu\omega}{\hbar}}x\right) e^{-\frac{\mu\omega x^2}{2\hbar}}\, dx.$$

Example

Suppose the probability distribution function for the position of the mass is initially Gaussian in shape with $f(x)\overline{f(x)} = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$. This implies $f(x) = \frac{1}{\sqrt[4]{2\pi}} e^{-x^2/4}$. The coefficients of the infinite series solution are then

$$A_n = \frac{1}{2^n n!} \sqrt{\frac{\mu\omega}{\hbar\pi}} \int_{-\infty}^{\infty} \frac{1}{\sqrt[4]{2\pi}} e^{-\frac{x^2}{4}} H_n\left(\sqrt{\frac{\mu\omega}{\hbar}} x\right) e^{-\frac{\mu\omega x^2}{2\hbar}} \, dx.$$

Since $H_n(x)$ is an odd function when n is odd, $A_n = 0$ for n odd. The calculation of the remaining coefficients is made easier if it is assumed that $\mu\omega/\hbar = 1$. In this case,

$$A_{2n} = \frac{1}{2^{2n+1/4}\pi^{3/4}(2n)!} \int_{-\infty}^{\infty} e^{-3x^2/4} H_{2n}(x) \, dx = \frac{2}{12^n (n!) \sqrt[4]{18\pi}}.$$

Comparison Between Classical and Quantum Solutions

As n increases the energy E_n increases and the relative change in energy vanishes,

$$\lim_{n\to\infty} \frac{\hbar\omega}{E_n} = \lim_{n\to\infty} \frac{\hbar\omega}{\left(n+\frac{1}{2}\right)\hbar\omega} = 0.$$

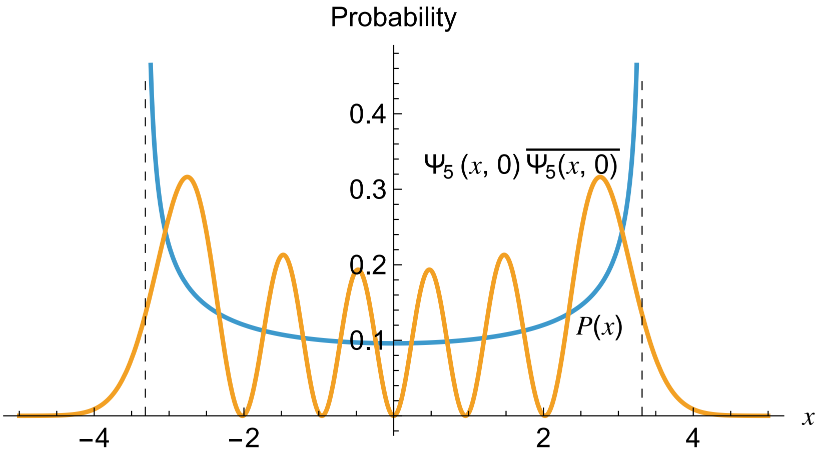
Thus for energetic oscillators the discrete differences between energy levels is less discrete and more continuous.

Let the amplitude of the classical harmonic oscillator be $A = \sqrt{2E/k}$. If the classical harmonic oscillator has energy equal to one of the discrete energy levels of the quantum harmonic oscillator, then

$$A = \sqrt{\frac{2(n+1/2)\hbar\omega}{k}} = \sqrt{\frac{(2n+1)\hbar}{\mu\omega}},$$

for some $n \in \mathbb{N}$.

Probability $n = 5$



Probability $n = 10$