Chapter

Schrodinger Wave Equation for Simple Harmonic Oscillator

Noor-ul-ain, Sadaf Fatima, Mushtaq Ahmad, Muhammad Rizwan Khan and Muhammad Aslam

Abstract

In physics, harmonic motion is among the most representative types of motion. A simple harmonic oscillator is often the source of any vibration with a restoring force proportional to Hooke's law. Every minimum potential has a solution in the form of the harmonic oscillator potential. Little oscillations at the minimum are characteristic of almost all natural potentials and of many quanta mechanical systems. Harmonic motion is an essential building block for these more complex uses. The Schrödinger equation is a defining feature of the harmonic oscillator. Here, we demonstrate that the time-frequency plane is a useful tool for analyzing their dynamics. We numerically integrate several examples involving different input forces and demonstrate that the oscillations are clearly displayed and easily interpretable in the time-frequency plane.

Keywords: harmonic motion, frequency, pendulum, displacement, amplitude

1. Introduction

A system that uses simple harmonic motion (SHM) is known as a harmonic oscillator.

A physical system called a harmonic oscillator experiences a restoring force proportionate to the displacement when it is moved away from its mean position.

A wave equation that describes the behavior of quantum particles is the Schrödinger equation. A harmonic oscillator's energy levels can be demonstrated by the Schrödinger equation to be quantized, which means that they can only take on specific discrete values. The Schrödinger equation has the effect of restricting the possible energies that an oscillator that is harmonic can have [1, 2].

A physical system known as harmonic oscillator oscillates at a frequency proportional to the displacement from its equilibrium position and is governed by a restoring force F_r. The F_r is proportional to the displacement from its mean position. This means that the system tends to return to its equilibrium position when disturbed from it, and the rate at which it oscillates is determined by the strength of the restoring force and the mass of the system. An equation of simple harmonic motion which is sinusoidal function of time with constant amplitude and frequency can be used to describe the motion of harmonic oscillator [1, 3]. The two examples of harmonic oscillator are mass connected to the spring and a simple pendulum. Harmonic oscillators are important in physics and engineering because they provide a useful model for many physical systems and can be used to analyze and predict the behavior of those systems [3, 4].

2. Classical behavior of simple harmonic oscillator

The simple example of linear harmonic oscillator is a mass attached to a wall by means of a spring as illustrated in the following **Figure 1**.

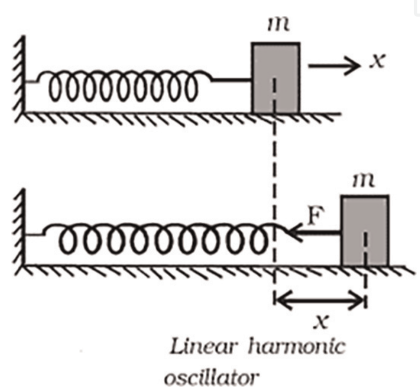

Figure 1.
Shows the experimental device for the study of the spring-mass system [1].

2.1 Expression for potential energy of simple harmonic oscillator

Hooke's law states that the force required to stretch or compress a spring is proportionate to the distance extended or compressed from its original length. Mathematically, this relation can be expressed as:

$$\begin{gathered} F \propto x \\ F \propto -x \\ F_r = -kx \end{gathered} \tag{1}$$

Where, F_r is the force applied to the spring, x is the displacement of the spring from the original length, and k is a constant which is known as spring constant and represents the stiffness of spring [5] .

Hooke's law applies to all elastic materials, not just springs. It is an important concept in physics and engineering because it helps to understand and predict the behavior of systems that involve elastic materials, such as springs, rubber bands, and other materials. Hooke's law is also the basis for the design of many mechanical systems, such as shock absorbers, suspension systems, and other devices that rely on the properties of elastic materials [6, 7].

When an object is displaced from its equilibrium position, a restoring force acts on it to push or pull it back toward that position. The $F_r$is directly proportional to the displacement from the equilibrium position and also acts in opposite direction [5]. This force is present in many physical systems, such as springs, pendulums, and mass-spring systems, and it plays a vital role in the behavior of these systems [3, 4].

$$F = -\frac{dv}{dx} \tag{2}$$

∵Force F can be expressed as negative derivative of potential energy V.

The work done in stretching spring to distance dx

$$W = F \times \text{distance}$$
$$P.E = F \times dx$$
$$-dv = F \times dx$$
$$dv = -F \times dx$$
$$dv = -F \times dx$$

From Eq. (1)

$$F = -kx$$
$$dv = kx \times dx \tag{3}$$

Integrate Eq. (3) within limits 0 → x

$$\int dv = + \int_0^x kxdx$$
$$V = k \int_0^x xdx$$
$$V = k \lim_{0 \to x} \frac{x^2}{2}$$
$$V = k \left(\frac{x^2}{2} - \frac{0}{2} \right)$$
$$V = k \frac{x^2}{2}$$
$$V = \frac{1}{2} kx^2 \tag{4}$$

Where x is the distance from equilibrium position [8, 9].

The plot of potential energy (V) of a particle executing simple harmonic motion against displacement from its equilibrium length is a parabola as illustrated in the following **Figure 2**.

2.2 Expression for frequency of linear harmonic oscillator

The frequency of a harmonic oscillator is the number of complete oscillations or cycles it completes per unit time. The frequency of a harmonic oscillator depends on the physical characteristics of the system, such as its mass and stiffness.

According to second law of motion

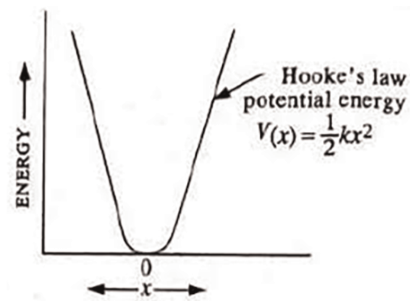

Figure 2.
The potential energy for a simple harmonic oscillator [6].

$$F = ma \tag{5}$$

Comparing Eqs. (1) and (5)

$$ma = -kx$$

$$m\frac{d^2x}{dt^2} = -kx \quad \because a = \frac{d^2x}{dt^2}$$

$$\frac{d^2x}{dt^2} + \frac{k}{m}x = 0 \tag{6}$$

Eq. (6) is a second-order differential equation. The general solution of this Eq. (6)

$$x = A\sin\omega t \tag{7}$$

We know $\omega = \sqrt{\frac{k}{m}}$

$$x = A\sin\sqrt{\frac{k}{m}}t \tag{8}$$

We know that

$$\omega = 2\pi\vartheta t$$

$$x = A\sin 2\pi\vartheta \tag{9}$$

Comparing Eqs. (8) and (9)

$$A\sin\sqrt{\frac{k}{m}}t = A\sin 2\pi\vartheta t$$

$$\sin\sqrt{\frac{k}{m}} = \sin 2\pi\vartheta$$

$$\sin^{-1}\sin\sqrt{\frac{k}{m}} = \sin^{-1}\sin 2\pi\vartheta$$

$$\because \sqrt{\frac{k}{m}} = 2\pi\vartheta$$

$$\vartheta = \frac{1}{2\pi}\sqrt{\frac{k}{m}} \tag{10}$$

Eq. (10) gives the frequency of the simple harmonic oscillator, where ϑ the frequency, k is the spring constant, and m is the mass of a linear harmonic oscillator. The above equation determines that the frequency of a harmonic oscillator is directly proportional to spring constant's square root and inversely proportional to mass's square root. This means that by increasing the stiffness of the spring or by decreasing the mass of the oscillator, the frequency of an oscillator will increase [8].

Generally, the frequency of harmonic oscillator is an important characteristic that determines its behavior and can be used to analyze and predict its motion. The frequency of a harmonic oscillator can be measured experimentally using various methods, such as by measuring the time period of its oscillations or by analyzing its response to external forces.

$$\because \vartheta = \frac{c}{\lambda} \nabla = \frac{1}{\lambda} \vartheta = c\nabla$$

$$2\pi c\nabla = \sqrt{\frac{k}{m}}$$

$$\nabla = \frac{1}{2\pi c}\sqrt{\frac{k}{m}}$$

∇ is wave number

For two particles connected to each other through a spring as in diatomic molecule, we use term reduced mass μ [10].

$$\nabla = \frac{1}{2\pi c}\sqrt{\frac{k}{\mu}} \tag{11}$$

3. Quantum mechanical treatment of simple harmonic oscillator

The wave function is a mathematical representation of a quantum system's state in quantum mechanics. All of the information about a particle or a group of particles, including their position, momentum, and energy, is contained in the wave function. It is a complex-valued function depends on position and time of particle. It is denoted by symbol Ψ [11].

Probability of finding the particle at a certain position is proportional to absolute square of wave function. It is also used to determine the probability density of finding a particle within a certain volume of space.

In quantum mechanics, wave function is a fundamental concept used to calculate many properties of quantum systems, such as energy levels, transition probabilities, and scattering cross-sections. The wave function is also used to describe the behavior of systems that exhibit wave-like properties, such as electrons, atoms, and molecules [12, 13].

The wave function follows the Schrödinger equation, which is a differential equation that determines how the wave function evolves over time. The Schrödinger equation is used to determine the temporal evolution of quantum systems and to predict particle and system behavior under different conditions [14].

3.1 Representation of wave function

In quantum mechanics, the wave function can be represented in several ways, depending on the context and the physical system being described. Here are three common representations [15]:

3.1.1 Position representation

In this position representation, Ψ(x,t) gives the probability amplitude of finding a particle at position x at time t. The position representation is used for systems with definite position, such as single particle in a box or a molecule. In this representation, a wave function is typically denoted as Ψ(x,t) i.e., function of position and time. Its mathematical form can be written as: Ψ(x,t) = A(x,t) * exp(iφ(x,t)) where A(x,t) is the amplitude of the wave function and φ(x,t) is its phase. The amplitude is a real-valued function that describes the intensity of the wave, while the phase is a real-valued function that describes the position of the wave in space and time [16, 17].

3.1.2 Momentum representation

In this representation, the wave function is function of momentum rather than the position. The wave function Ψ(p,t) gives the probability amplitude of finding a particle with momentum p at time t. The momentum representation is useful for systems with definite momentum, like a free particle. In this representation, wave function is typically denoted as Ψ(p,t) and is function of momentum and time. Its mathematical form can be written as: Ψ(p,t) = B(p,t) * exp(iχ(p,t)) where B(p,t) is the amplitude of the wave function in momentum space and χ(p,t) is its phase. This amplitude is real-valued function that determines the intensity of the wave in momentum space, while the phase is a real-valued function that describes the position of wave in momentum space [16–18].

3.1.3 Energy representation

In this representation, the wave function is a function of energy. The wave function Ψ(E) gives the probability amplitude of finding a system with energy E. The energy representation is useful for systems with definite energy, like a particle in the potential well. In the energy representation, wave function is typically denoted as Ψ(E) and is a function of energy. Mathematically, it can be written as

$$\Psi(\mathrm{E}) = \mathrm{C}(\mathrm{E}) * \exp(\mathrm{i}\psi(\mathrm{E})) \tag{12}$$

where C(E) is the amplitude of the wave function in energy space and ψ(E) is its phase. This amplitude is real-valued function that determines the intensity of wave in energy space, while the phase is a real-valued function that describes the position of the wave in energy space.

In each representation, Ψ is a complex-valued function satisfies the Schrödinger equation. It can be normalized, which means that the integral of the absolute square of the wave function over all space or momentum or energy is equal to one, ensuring that the probability of locating a particle in the system is one.

The mathematical form of wave function can be used to calculate various properties of the system, such as probabilities of finding the particle in a certain position, momentum, or energy state [19].

3.2. Boundaries conditions

For the harmonic oscillator, the two common boundary conditions are described as follows [20].

3.2.1 Normalizability condition

The wave function must be normalizable, which means that the integral of the absolute square of the wave function over all space must be finite. This assures that probability of locating a particle in the system is one [19].

3.2.2 Continuity condition

The wave function must be continuous and differentiable at the ends of the range. This ensures that the probability density and its first derivative are continuous and smooth throughout the range of motion.

For the harmonic oscillator, the boundary conditions are typically satisfied by using a particular type of wave function, called the Hermite polynomials. The Hermite polynomials are a set of orthogonal polynomials that satisfy both the normalizability and continuity conditions. They form a complete basis set for the wave function of the harmonic oscillator, allowing the solution to be expressed as a linear combination of these polynomials [6].

3.3 Schrodinger wave equation for harmonic oscillator

The mathematical form of the wave function in quantum mechanics depends on the physical system being described and the representation being used. However, in general, it is a complex-valued function that satisfies Schrödinger equation [8, 21].

In Quantum mechanics, the one-dimensional time-independent Schrödinger wave equation for harmonic oscillator follows as [22]:

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0 \tag{13}$$

But the potential energy of the simple harmonic oscillator is V=$\frac{1}{2}Kx^2$, therefore

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}Kx^2\right)\psi = 0 \tag{14}$$

Or

$$\frac{\partial^2\psi}{\partial x^2} + \frac{-mKx^2}{2}\psi = \frac{-2mE}{2}\psi$$
$$\frac{mK}{\hbar^2} = \alpha^2 \frac{2mE}{\hbar^2} = \varepsilon$$

Them

$$\frac{\partial^2\psi}{\partial x^2} - \alpha^2 x^2 \ \psi = -\varepsilon\psi \tag{15}$$

This is Schrodinger's equation for harmonic oscillator [23–25]. Here x^2 is the coefficient of ψ, so it is difficult to obtain its solution. Hence we will find its asymptotic solution

When $x \to \infty \ \alpha^2 x^2 >> \varepsilon$

So we can write:

$$\frac{\partial^2\psi}{\partial x^2} - \alpha^2 x^2 \ \psi = 0 \tag{16}$$

Its solution is $\psi = e^{\pm\alpha x^2/2}$

$$\frac{\partial\psi}{\sigma x} = \pm\alpha x e^{\pm\alpha x^2/2}$$

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\partial}{\sigma x}\left(\pm\alpha x e^{\pm\alpha x^2/2}\right) = \alpha^2 x^2 e^{\pm\alpha x^2/2} \pm \alpha e^{\pm\alpha x^2/2} = (\pm\alpha) e^{\pm\alpha x^2/2}\alpha^2 x^2$$

Value of αx is larger hence we take $(\alpha^2 x^2 \pm \alpha) \approx \alpha^2 x^2$

$$\frac{\partial^2\psi}{\partial x^2} = \alpha^2 x^2 e^{\pm\alpha x^2/2}$$

Or $\frac{\partial^2\psi}{\partial x^2} = \alpha^2 x^2 \ \psi$ or $\frac{\partial^2\psi}{\partial x^2} - \alpha^2 x^2 \ \psi = 0$

Now we take $\psi = e^{-\alpha x^2/2}$

Because it obeys the condition that $|\psi|^2$ decreases with increasing x

General solution:

$$\psi_{(x)=} f_{(x)} e^{-\alpha x^2/2}$$

Differentiating w.r.t x

$$\frac{\partial\psi}{\sigma x} = f_{(x)} e^{-\alpha x^2/2}(-\alpha x) + e^{-\alpha x^2/2}\frac{\partial f}{\partial x}$$

Again differentiating w.r.t x

$$\frac{\partial^2\psi}{\partial x^2} = f_{(x)}\left[e^{-\alpha x^2/2}(-\alpha) + (-\alpha x)(-\alpha x)e^{-\alpha x^2/2}\right]$$
$$+(-\alpha x)\ e^{-\alpha x^2/2}\frac{\partial f}{\partial x} + \frac{\partial f}{\partial x} e^{-\alpha x^2/2}\left(-\alpha x + e^{-\alpha x^2/2}\frac{\partial^2 f}{\partial x^2}\right.$$

$$\frac{\partial^2\psi}{\partial x^2} = e^{-\alpha x^2/2} f_{(x)}\left(-\alpha + \alpha^2 x^2\right) + \frac{\partial f}{\partial x} e^{-\alpha x^2/2}(-2\alpha x) + e^{-\alpha x^2/2}\frac{\partial^2 f}{\partial x^2}$$

$$\frac{\partial^2\psi}{\partial x^2} = e^{-\alpha x^2/2}\left[\frac{\partial^2 f}{\partial x^2} - 2\alpha x \ \frac{\partial f}{\partial x} + \left(\alpha^2 x^2 - \alpha\right)\mathrm{f}\right]$$

Substituting values of ψ and $\frac{\partial^2\psi}{\partial x^2}$ in Eq. (15)

$$e^{-\alpha x^2/2}\left[\frac{\partial^2 f}{\partial x^2} - 2\alpha x\ \frac{\partial f}{\partial x} + \left(\alpha^2 x^2 - \alpha\right)\mathrm{f}\right] - \alpha^2 x^2 f e^{-\alpha x^2/2} = -\varepsilon f e^{-\alpha x^2/2}$$

$$\text{Or } \frac{\partial^2 f}{\partial x^2} - 2\alpha x\ \frac{\partial f}{\partial x} + (\varepsilon - \alpha)f = 0 \tag{17}$$

Now substituting y = $\sqrt{\alpha}$ x and $f_{(x)} = H_{(y)}$ converting into standard Hermite polynomial equation

y = $\sqrt{\alpha}\,x$ then $\frac{dy}{dx} = \sqrt{\alpha}$

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y}.\frac{\partial y}{\partial x} = \sqrt{\alpha}\frac{\partial f}{\partial y}$$

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right) = \frac{\partial}{\partial x}\left(\sqrt{\alpha}\frac{\partial f}{\partial y}\right) = \frac{\partial}{\partial y}\left(\sqrt{\alpha}\frac{\partial f}{\partial y}\right)\frac{\partial y}{\partial x} = \alpha\frac{\partial^2 f}{\partial y^2}$$

Substituting values of $\frac{\partial f}{\partial x}$ and $\frac{\partial^2 f}{\partial x^2}$ in Eq. (17), we get

$$\alpha\frac{\partial^2 f}{\partial y^2} - 2\alpha\frac{y}{\sqrt{\alpha}}\sqrt{\alpha}\frac{\partial f}{\partial y} + (\varepsilon - \alpha)f = 0$$

$$\alpha\frac{\partial^2 f}{\partial y^2} - 2\alpha y\ \frac{\partial f}{\partial y} + (\varepsilon - \alpha)f = 0$$

$$\frac{\partial^2 f}{\partial y^2} - 2y\ \frac{\partial f}{\partial y} + \left(\frac{\varepsilon}{\alpha} - 1\right)f = 0$$

Now f(x) = H(y)

$$\frac{\partial^2 H}{\partial y^2} - 2y\ \frac{\partial H}{\partial y} + \left(\frac{\varepsilon}{\alpha} - 1\right)H = 0 \tag{18}$$

This is standard Hermite differential equation [22]. It can be expressed as

$$\mathrm{H}(\mathrm{y}) = \sum_{p=0}^{\infty} a_p y^p \tag{19}$$

$$\frac{\partial H}{\partial y} = \sum p a_p y^{p-1}$$

$$\frac{\partial^2 H}{\partial y^2} = \sum p(p-1)a_p y^{p-2}$$

From Eq. (18)

$$\sum p(p-1)a_p y^{p-2} - \sum\left[2p - \left(\frac{\varepsilon}{\alpha} - 1\right)\right]a_p y^p = 0$$

This expression is valid only when coefficient of each power of y is zero.

And p = p + 2

$$\sum(p+2)(p+2-1)a_{p+2}y^{p+2-2} - \sum\left[2p - \left(\frac{\varepsilon}{\alpha} - 1\right)\right]a_p y^p = 0$$

$$a_{p+2}(p+2)(p+1) = a_p\left[2p - \left(\frac{\varepsilon}{\alpha}\right) + 1\right]$$

$$a_{p+2} = \frac{\left[2p - \left(\frac{\varepsilon}{\alpha}\right) + 1\right]}{(p+2)(p+1)}a_p \tag{20}$$

We can determine values of all the coefficients in terms of two arbitrary constants a_0 and a_1

Thus, complete solution of Schrodinger's equation is [26]

$$\psi = e^{-\alpha x^2/2}H_{(y)}$$

$$\psi = e^{-y^2/2}H_{(y)}$$

3.4 Energy eigen values

$\psi = e^{-y^2/2}H_{(y)}$ of a simple harmonic oscillator will be physically accepted only when y→ ∞ , the increase in the value of Hermite Polynomial $H_{(y)}$ is more rapid than the decrease in the value of $e^{-y^2/2}$ value [27].

Value of $e^{-y^2/2}H_{(y)}$ can be zero only when power series for $H_{(y)}$ is finite series.

Let series be finite for p=n, the Eq. (20) becomes.

$$2\text{n} - \frac{\varepsilon}{\alpha} + 1 = 0$$

$$\text{N} = \frac{1}{2}\left(\frac{\varepsilon}{\alpha} - 1\right)\frac{\varepsilon}{\alpha} = 2n + 1\varepsilon = \frac{2mE}{\hbar^2}\alpha = \sqrt{\frac{mk}{\hbar^2}}$$

$$\frac{2mE}{\hbar^2}\Big/\sqrt{\frac{mk}{\hbar^2}} = 2\text{n} + 1\ \frac{2}{\hbar}\sqrt{\frac{m}{k}}E = 2n + 1$$

$$\text{E} = \frac{2n+1}{2}\hbar\sqrt{\frac{k}{m}}$$

But we know $\sqrt{\frac{k}{m}} = \omega$ (angular frequency)

$$\text{E} = \left(\frac{2n+1}{2}\right)\hbar\omega = \left(n + \frac{1}{2}\right)\hbar\nu \tag{21}$$

Where n = 0, 1, 2, 3, ...

The above equation gives the energy levels of a harmonic oscillator [28], where n is a non-negative integer, h is reduced Planck constant, ω is an angular frequency of the oscillator, and E_n is the energy of the oscillator in the nth energy level. In quantum mechanics, the energy levels of simple harmonic oscillator are quantized, which means they take on only certain discrete values.

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If n = 0 then $E_0 = \frac{1}{2}\,\nu$

n = 1 then $E_1 = \frac{3}{2}\,\nu$

n = 2 then $E_2 = \frac{5}{2}\,\nu$

The energy levels of a harmonic oscillator are equally spaced, with the energy of each level separated by an amount $h\,\omega$. The ground state of the oscillator, n=0, has the lowest energy level and corresponds to the oscillator's minimum energy state, where the particle is localized at the center of the potential well. As n increases, the energy levels increase and the wave function oscillates with more nodes [27].

The energy of the harmonic oscillator is always positive, and the oscillator can never reach the zero-point energy, which is the minimum possible energy that a quantum mechanical system can have [29].

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