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An Overview of the Time Independent Schrödinger Wave Equation with Applications

Dilruba Akter *[1], *Malati Mazumder*[1], *Kanak Chandra Roy*[1],*M Shakawat Hossain Shaon*[1]

Abstract

In this paper, the Schrödinger equation is investigated, and the mathematical used ideas are analyzed related to various fields of knowledge. In order to answer problems concerning the atomic structure of matter, this equation is extensively used in physics and chemistry. This wave equation predicts how a dynamic system will behave in the future by describing how a particle will behave in a field of force or how a physical quantity will change over time. In terms of the wave function, it is a wave equation that precisely and analytically forecasts the likelihood of events or outcomes. In this paper, we use the equation's time-independent part, and this will be the focus of this work. For many real-world issues, this equation is applied like Barrier penetration which is significant in radioactive decay, systems with bound states are related to the quantum mechanical especially particle inscribed by a box, and the quantum mechanical oscillator is applicable to molecular vibrational modes. By determining the Schrödinger equation's solution in a certain circumstance, it is also possible to understand problems with particles whose motion is constrained by some type of interaction. The Schrödinger equation is solved in this instance for particles interacting in a uniform potential well. In this paper, finding the wave function that just depends on location and not time is necessary. Here, we demonstrate the application of the time-independent component to the potential well and the hydrogen atom, as well as some graphs that represent the numerical outcomes of the aforementioned examples.

Keywords: *Schrödinger equation, Wave equation, Potential Equation .Time dependent and time-independent part of equation*

1. Introduction:

Schrödinger's equation, defining how a physical model, such as a collection of particles responding to specific forces, would change over time, equivalent to Classical mechanics' second equation of motion as applied to quantum physics. In classical physics, the locations and moments of all particles at each instant are what you're chasing because they provide a complete description of the system. [1,2] This equation offers a detailed probabilistic account of the real

[1] Department of Applied Mathematics, Gono Bishwabidyalay, Savar, Dhaka-1344.
*Corresponding Author: email: 416pansi@gmail.com, Phone: +8801516763192.

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nature of the microscopic universe and is essential for many non-relativistic problems. In many different branches of science, including quantum theory, nuclear physics, conceptual physics and chemistry, material science, biochemical physics, and many more, a well-defined wave function computed by an appropriate mathematical or computational method is employed to characterize the quantum system. [3,4,5,8]. Initially Wave-particle dualism was introduced mathematically by Joseph Alexander Schrödinger. In 1926, he believed that electrons exhibit standing waves similar to those of a stretched string. In order to address issues molecular and nuclear physics, as well as chemistry, wave mechanics was developed as a result of this novel theory at the time. Partial differential equations were used by Schrodinger to describe how the quantum state of a physical system evolves over time. “The Schrodinger wave equation” is the name given to this equation which is equivalent of Newton's law of motion because every Newtonian variable has an alternate value. This equation, which describes the temporal evolution of a system's wave function, is generally a linear partial differential equation and is not a straightforward algebraic equation. The Schrodinger wave equation mathematically describes how resources appear as the wave function under various physical circumstances [6]. We cannot perceive the wave-like behavior of minuscule particles in any way. But Schrödinger deserves credit for creating an equation that makes all of our misunderstandings clear. The key ideas presented by Schrödinger are the electronic mobility of the atomic model, the definition of an atom's resource levels using harmonic oscillators, and the definition of a diatomic molecule using its vibrational and rotational levels of energy [7]. Before publishing the non-relativistic one, Schrödinger did come across an wave function equation that obeyed relativistic energy conservation, but he rejected due to its negative prediction for probabilities and energies. It was also discovered in 1927 by Fock, Kleinand Gordon, and, but they added the electromagnetism and demonstrated that it was Lorentz invariant. In 1928, De Broglie reached the same conclusion. The Klein-Gordon equation is the name; most people now use to refer to this relativistic wave equation. [9] In this case the electron’s wave function or any other system that doesn't depend on time may occasionally be helpful to describe. We need a version of the Schrodinger equation that doesn't depend on time to figure out the wave function, which only depends on location and is independent of time. The time-independent part of Schrödinger equation will be the subject of this discussion. In this paper, we explore the Schrödinger wave equation used to describe a quantum particle in a stationary state, not over a change in time, and which describes a particle only based on its

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position (spatial data). [7] In quantum physics, the wave function ψ that results from solving Schrödinger's equation contains information about the system. The wave function's squared absolute value $|\psi|^2$ can be thought of as a probability density. For instance, with our particle in a box density of possibilities for locating our particle at x (position) is $|\psi(x)|^2$. However, it is also possible to find ψ for other considerable values, such as the moment of the nanoparticles, and to derive Schrödinger's equation for multi-particle systems. [11]

2. Derivation of wave equation in 3D space:

Consider a particle is in motion with mass m, along any direction referred to three dimensional space with the force $F(x, y, z)$ which is a function of the space coordinates (x, y, z) .For a particle in such a field of action the potential energy V is a function of the spatial coordinates rather than directly depending on time [2,12,14]. A conservative force is one such force.

Assume that $\vec{r}$ is the particle's momentum and that is the direction vector of the particle at the considering point in time t.

Then energy required for the particle is provided by $\frac{p^2}{2m} + V(\vec{r}) = E$, where the speed is less than that of light.

Since $p^2 = \vec{p}.\vec{p} = p_x{}^2 + p_y{}^2 + p_z{}^2$,

We have $\frac{1}{2m}\left(p_x{}^2 + p_y{}^2 + p_z{}^2\right) + V(\vec{r}) = E$

Multiplying both sides of this equation by the wave function ϕ

$$\frac{1}{2m}\left(p_x{}^2 + p_y{}^2 + p_z{}^2\right)\varphi + V\varphi = E\varphi \qquad (1)$$

Now $\psi\left(\vec{r}, t\right) = \mathrm{A}_e{}^{\frac{i}{h}\left(\vec{p}, \vec{r} - \mathrm{E}t\right)}$

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Since $\vec{p}.\vec{r} = p_x X + p_y Y + p_z Z$, we have $\psi(\vec{r},t) = Ae^{ih(p_x x+p_y y+p_z z-Et)}$ (2)

Differentiating equation (2) with respect to x

$$\frac{\partial \Psi}{\partial x} = A\left(\frac{i}{h}\right) p_x e^{\frac{i}{h}\left(p_x X + p_y Y + p_z Z - Et\right)} = \left(\frac{i}{h}\right) p_x \Psi \quad (3)$$

And $\frac{\partial^2 \psi}{\partial x^2} = \left(\frac{i}{h}\right) p_x \psi \frac{\partial \psi}{\partial x} = \left(\frac{i}{h}\right) p_x \left(\frac{i}{h}\right) p_x \psi = -\frac{i}{h^2} p^2{}_x \psi$

From this equation we have

$$p_x^2 \psi = -h^2 \frac{\partial^2 \psi}{\partial x^2} \quad (4a)$$

Similarly, we get $p_y^2 \psi = -h^2 \frac{\partial^2 \psi}{\partial y^2}$ (4b)

$$p_z^2 \psi = -h^2 \frac{\partial^2 \psi}{\partial z^2} \quad (4c)$$

Differentiating equation (2) with respect to t

$$\frac{\partial \psi}{\partial t} = A\left(\frac{i}{h}\right)(-E) e^{\frac{i}{h}\left(p_x X + p_y Y + p_z Z - Et\right)} = \left(-\frac{i}{h}\right) E\psi.$$

Therefore, $E\psi = -\frac{i}{h}\frac{\partial \psi}{\partial t} = ih\frac{\partial \psi}{\partial t}$ (5)

Substituting these expressions for $p_x{}^2\psi, p_y{}^2\psi, p_z{}^2\psi$ and $E\psi$ in equation(1),

$$-\frac{h^2}{2m}\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2}\right) + V\psi = ih\frac{\partial \psi}{\partial t} \quad (6)$$

$$-\frac{h^2}{2m}\nabla^2 \psi + V\psi = ih\frac{\partial \psi}{\partial t} \quad (7)$$

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This is the Schrödinger wave equation for the motion of a single particle in three dimensions and with time dependence. Schrödinger derived the wave equation in the form of Eq. (7) in 1926.This equation only has first-order time but second-order spatial coordinates. The wave equations with which we work in classical physics, such as the ones for sound waves or electromagnetic waves, are of second order in terms of both space coordinates and time.

3. Derivation of time-dependent and time-independent components of 3D wave equation:

Eq. (6) is separable under the consideration of time dependency if the potential energy is not a response to time. [11], [14], [16]

Let the time-independent part = $u(\vec{r})$ and time-dependent part= $f(t)$ respectively.

Then $\Psi\left(\vec{r},t\right)=u\left(\vec{r}\right)f(t)$ (8)

Substituting this equation in Eq. (6), we get

$$-\frac{h^2}{2m}f\left[\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right]=Vuf=ihu\frac{\partial f}{\partial t}$$

$$-\frac{h^2}{2m}\frac{1}{u}\left[\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right]=V=ih\frac{1}{f}\frac{\partial f}{\partial t} \quad (9)$$

4.1.Time-dependent part: Using $E\psi=ih\frac{\partial\psi}{\partial t}$

Substituting eq. (9) in this equation, we get $E\psi=ih\frac{\partial\psi}{\partial t}$

$$ihu\frac{df}{dt}=Euf$$

Dividing both the sides by uf, we get

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$$ih\frac{1}{f}\frac{df}{dt} = E \quad \ldots\ldots\ldots\ldots(10)$$

Thus the time-dependent part of the equation is equal to the total energy E of the particle, and so the time-independent part.

To solve this equation, we separate the variables, and we obtain

$$\frac{df}{f} = E\frac{1}{ih}dt$$

$$\frac{df}{f} = -\frac{-iE}{h}dt$$

Integrating, we get

$$f = Ce^{-\frac{iE}{h}} \quad \ldots\ldots\ldots\ldots(11)$$

Where C is a constant.

4.2Time –independent part: From Eqns. (9) and (10), we get

$$-\frac{h^2}{2m}.\frac{1}{u}\left[\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right]+V = E$$

$$-\frac{h^2}{2m}\left[\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right]+Vu = Eu \qquad (12a)$$

Or $-\frac{h^2}{2m}.\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right]u+Vu = Eu$

Or $-\frac{h^2}{2m}\nabla^2 u+Vu = Eu$

or $\left[-\frac{h^2}{2m}\nabla^2+V\right]u = Eu \qquad (12b)$

Where ∇^2 the Cartesian **Laplacian** operator in its coordinates; it is defined by

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$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

A convenient form of Eq. (12a) is

$$\left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right] + \frac{h^2}{2m}(E - V)u = 0 \qquad (12c)$$

5. Applications:

5.1 Schrödinger equation for one dimensional harmonic oscillator

Equations. (12a) or (12b) or (12c) is 3D time-independent part of the wave equation for a single particle.It is also called three-dimensional steady state Schrödinger equation, and its solutions are called time –independent or steady state wave function.

Consider the harmonic oscillator of a m-mass particle in 1-D space, bound to the origin by a restoring force $F = -kx$. The force can be represented by the potential energy,

$$V(x) = \frac{1}{2}kx^2 \qquad (13)$$

The Schrödinger wave equation in one dimension is

$$-\frac{i\hbar}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}kx^2\psi(x) = E\psi(x) \qquad (14)$$

To convert equation (14) in dimensionless from, we introduce a dimensionless variable $\xi = \alpha x$ and a dimensionless eigenvalue λ , so that

$$\frac{d\psi}{dx} = \frac{d\psi}{d\xi}.\frac{d\xi}{dx} = \alpha\frac{d\psi}{d\xi}$$

and $$\frac{d^2\psi}{dx^2} = \alpha\frac{d^2\psi}{d\xi^2}.\frac{d\xi}{dx} = \alpha^2\frac{d^2\psi}{d\xi^2}$$

Equation becomes,

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$$-\frac{\hbar^2}{2m}\alpha^2\frac{d^2\psi}{d\xi^2}+\frac{1}{2}k\frac{\xi^2}{\alpha^2}\psi=E\psi$$

$$\Rightarrow\frac{d^2\psi}{d\xi^2}+\left(\lambda-\xi^2\right)\psi=0 \qquad (15)$$

$$\text{Where, }\alpha=\left(\frac{mk}{\hbar^2}\right)^{1/4} \qquad (16)$$

$$\text{and} \quad \lambda=\frac{2mE}{\hbar^2\alpha^2}=\frac{2mE\hbar}{\hbar^2\sqrt{mk}}=\frac{2E}{\hbar}\sqrt{\frac{m}{k}}=\frac{2E}{\hbar w_c} \qquad (17)$$

with, $w_c=\sqrt{\frac{k}{m}}$ as the angular frequency of the oscillator.

Now we proceed to obtain the solution of the wave equation (15) through configuration space $-\infty<\xi<+\infty$ depending on the asymptotic solution which is of the form

$$\psi(\xi)=H(\xi)e^{-\xi^2/2} \qquad (18)$$

Where $H(\xi)$ is a finite order polynomial in ξ.

We obtain by adding +ve to the exponent, ψ will diverge since $\xi\rightarrow\infty$,

Now using(18), we have

$$\frac{d\psi}{d\xi}=H'(\xi)e^{-\xi^2/2}-\xi H(\xi)e^{-\xi^2/2}$$

$$=[H'(\xi)-\xi H(\xi)]e^{-\xi^2/2}$$

$$\text{and} \quad \frac{d^2\psi}{d\ \xi}=[H''(\xi)-\xi H'(\xi)-H(\xi)]e^{-\xi^2/2}-\xi[H'(\xi)-\xi H(\xi)]e^{-\xi^2/2}$$

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$$= \left[H''(\xi) - 2\xi H'(\xi) + \left(\xi^2 - 1\right)H(\xi)\right]e^{-\xi^2/2}$$

Hence using this value in (15), we get

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

$$\Rightarrow H''(\xi) - 2\xi H'(\xi) + \left(\xi^2 - 1\right)H(\xi) + \lambda H(\xi) - \xi^2 H(\xi) = 0$$

$$\Rightarrow H''(\xi) - 2\xi H'(\xi) + (\lambda - 1)H(\xi) = 0$$

5.2 Schrödinger equation for Infinite potential well

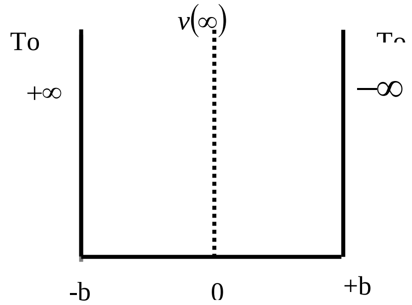

Fig 5.2: potential well **w**ith perfectly stiff walls in single dimensional space

We consider a particle's mobility in one dimension while it is constrained by reflective barriers. Here, as seen in the illustration Fig 5.2, we study a potential well with square shape andinfinite edge. This corresponds a particle enclosed by walls of thickness 2b that are impermeable. As shown in figure $v(x) = 0$ for $-b < x < b$ and $v(x) = \pm\infty$ for $|x| > b$ and on walls at $x = \pm b$. The necessary condition to be impose so that the function ψ vanish at the walls i.e, $(\psi)_{x=b} = 0$ and $(\psi)_{x=-b} = 0$.

The equation for $|x| < b$ is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$$

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$$\Rightarrow \frac{d^2\psi}{dx^2} + \alpha^2\psi = 0 \ , \qquad \text{where } \alpha^2 = \frac{2mE}{\hbar^2}$$

Which has the general solution

$$\psi = C_1 \cos\alpha x + C_2 \sin\alpha x \qquad (19)$$

Applying the conditions at $x = \pm b$

$$\psi = 0 \qquad \text{at } x = b$$

$$\psi = 0 \qquad \text{at } x = -b$$

i.e,

$$C_1 \cos\alpha b + C_2 \sin\alpha b = 0 \qquad (20)$$

$$C_1 \cos\alpha b - C_2 \sin\alpha b = 0 \qquad (21)$$

Adding and subtracting equation (20) & (21), we have

$$2C_1 \cos\alpha b = 0 \text{ and } 2C_2 \sin\alpha b = 0$$

This means either $C_1 = 0$ or $\cos\alpha b = 0$ and either $C_2 = 0$ or $\sin\alpha b = 0$.

Now we don't want both C_1 and C_2 to be zero. Since this would give thesolution $\psi = 0$. Alsoit's not possible to make both $\sin\alpha b$ and $\cos\alpha b$ zero for a given value of α and E . There are two possible classes of solution:

- $C_1 = 0$ and $\sin\alpha b = 0$
- $C_2 = 0$ and $\cos\alpha b = 0$

For $(\sin\alpha b = 0), \alpha b = \pi, 2\pi, \frac{n\pi}{2}$ (where n is even integer)

For $(\cos\alpha b = 0)$; $\alpha b = \frac{\pi}{2}, \frac{3\pi}{2}, \ldots\ldots\ldots\ldots \frac{n\pi}{2}$ (Where n is an odd integer)

Thus,

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$$\psi = C_1 \cos\frac{n\pi x}{-2b} \ , \quad \text{n odd}$$

$$\psi = C_2 \sin\frac{n\pi x}{2b} \ , \quad \text{n even}$$

$$\text{and} \quad \alpha^2 = \frac{2mE}{\hbar^2} \quad \text{or,} \ E = \frac{\alpha^2\hbar^2}{2m}$$

$$E_n = \frac{n^2\pi^2\hbar^2}{8mb^2} Joules$$

There is thus infinite sequence discrete energy levels that corresponds to all positive integral values of n.

5.2.1 In a one-dimensional potential well, a particle with mass m can be found, where

$$v = -v_0 \qquad |x| < b$$

$$v = 0 \qquad |x| > b$$

Solution: When w is positive, the particle's total energy is $E = -w$. Presuming the particle's wave function in its lowest state $(w_0)$is an even function of x .Demonstrate that

$$\tan \beta\alpha = \left[\frac{w_0}{v_0 - w_0}\right]^{1/2}$$

$$\beta^2 = \frac{8\pi^2 m}{\hbar^2}(v_0 - w_0)$$

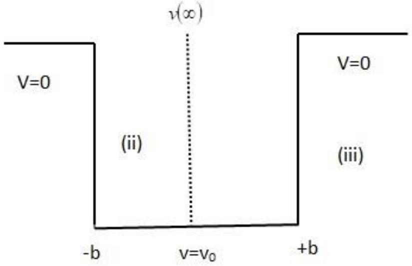

Fig 5.2.1

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where the situation is shown in Fig 5.2.1

Consider the particle in the lowest state, the wave equation in the 1st region is

$$\frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2} w_0 \psi_1 = 0$$

$$\text{Or, } \frac{d^2\psi_1}{dx^2} - \alpha^2\psi_1 = 0$$

$$\text{Where, } \alpha^2 = \frac{2mw_0}{\hbar^2}$$

The wave equation for the 2nd region is $\frac{d^2\psi_2}{dx^2} - \beta^2\psi_2 = 0$;Where, $\beta^2 = \frac{2m(v_0 = w_0)}{\hbar^2}$

The wave equation for the 3rd region is $\frac{d^2\psi_3}{dx^2} - \alpha^2\psi_3 = 0$

Wave functions for different regions are

$$\psi_1 = Ae^{+\alpha x}$$
$$\psi_2 = Be^{i\beta x} + Ce^{-i\beta x}$$
$$\psi_3 = De^{-\alpha x}$$

An even function of α is provided to the wave function at the lowest state. i.e;

$$\psi(x) = \psi(-x)$$

Hence, $A = D$; $B = C$

$$\psi_2 = 2B\cos\beta x$$

Now we apply the following boundary conditions

$$(\psi_1)_{x=-b} = (\psi_2)_{x=-b} \text{ and } (\psi_2)_{x=b} = (\psi_3)_{x=b}$$

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$$\left(\frac{d\psi_1}{dx}\right)_{x=-b}=\left(\frac{d\psi_2}{dx}\right)_{x=-b} \text{ and } \left(\frac{d\psi_2}{dx}\right)_{x=b}=\left(\frac{d\psi_3}{dx}\right)_{x=b}$$

Thus , $Ae^{-\alpha b}=2B\cos\beta b$ and $Ae^{-\alpha b}=2B\cos\beta b$

$$A\alpha e^{-\alpha b}=2B\beta\sin\beta b \text{ and } A\alpha e^{-\alpha b}=2B\beta\sin\beta b$$

From these equations, we have

$$\tan\beta\alpha=\frac{\alpha}{\beta}=\left(\frac{w_0}{v_0-w_0}\right)^{1/2}$$

5.2.2 Solve the Schrödinger wave equation for the potential defined by

$$V(x)=0 \qquad |x|<b$$
$$=\infty \qquad |x|>b$$

Solution **:**The potential energy distribution for this problem is

$$V(x)=0 \qquad |x|<b$$

$$=\infty \qquad |x|>b$$

where the region is enclosed by thick, impassable walls.. Let the region of the x-axis be chosen to be the centre of the wall. As the potential energy is infinite at $x=\pm b$, and since the wave function vanishes for $|x|>b$, Just within the wall, the wave equation has to be solved.

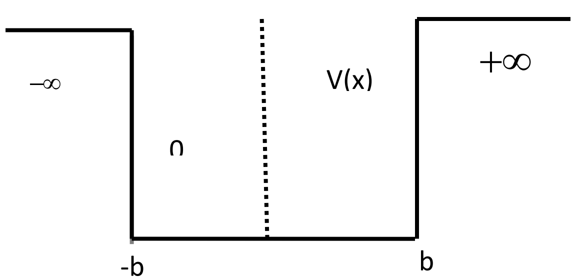

Fig 5.2.2

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The Schrödinger wave equation in one – dimensional is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{(x)}}{dx^2}+v(x)\psi(x)=E\psi(x) \qquad (22)$$

For $|x|<b$; The wave equation is $\frac{d^2\psi}{dx^2}+k\psi=0$, $k=\sqrt{\frac{2mE}{\hbar^2}}$ (23)

Which has the solution

$$\psi(x)=A\sin kx+B\cos kx \qquad (24)$$

Under the conditions: $\psi(x)|_{x=b}=0$ $\psi(x)|_{x=-b}=0$

The equation (24) gives

$$A\sin kb+B\cos kb=0$$

And $-A\sin kb+B\cos kb=0$

Solving we get, $A\sin kb=0$, $B\cos kb=0$

We consider two classes of solutions:

$$A=0,\ \cos kb=0$$
$$B=0,\ \sin kb=0$$

Then $ka=\frac{n\pi}{2b}$, when n is -ve integer for 1 and n is +ve integer for (n) . The two classes of solutions and the eigen values are:

$$\psi(x)=B\cos\frac{n\pi x}{2b} \text{ , n is odd}$$

and $\psi(x)=A\cos\frac{n\pi x}{2b}$, n is even

In both cases, $k^2=\frac{2mE}{\hbar^2}$ [by 23]

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$$\Rightarrow E = \frac{k^2\hbar^2}{2m} = \frac{n^2\pi^2\hbar^2}{8mb^2} \qquad \left[\mathrm{k} = \frac{\mathrm{n}\pi}{2}\right]$$

Now by normalization condition, $\int_{-b}^{b} \psi^* \psi dx = 1$

$$\Rightarrow B^2 \int_{-b}^{b} \cos^2 \frac{n\pi x}{2b} dx = 1$$

$$\text{for(22)} \Rightarrow 1 = \frac{B^2}{2} \int_{-b}^{b} \left(1 + \cos\frac{n\pi x}{b}\right) dx = \frac{B^2}{2}\left[x + \frac{b}{n\pi}\sin\frac{n\pi x}{b}\right]_{-b}^{b}$$

$$= \frac{B^2}{2}(b+b) = B^2 b$$

$$\therefore B = \sqrt{\frac{1}{b}}$$

So equation for class (22) is

$$\psi(x) = \frac{1}{\sqrt{b}} \cos\frac{n\pi x}{2b}, n = 1,3,5\ldots\ldots\ldots$$

Similarly for class (23) , we get

$$\psi(x) = \frac{1}{\sqrt{b}} \sin\frac{n\pi x}{2b}, n = 2,4,6\ldots\ldots\ldots$$

5.3 The hydrogen atom

We assume a hydrogonic atom with a charge Ze atomic nucleus and a $-e$charged electron that interact via the Coulomb potential $-Ze^2/r$.. Let's assume that the masses m_1, m_2 and locations of the two particles (nucleus and electron) are $x_1, y_1, z_1$and x_2, y_2, z_2 respectively. It is the wave equation.

$$i\hbar\frac{\partial}{\partial t}\psi(x_1,y_1,z_1,x_2,y_2,z_2,t) = \left[\frac{-\hbar^2}{2m_1}\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial y_1^2}+\frac{\partial^2}{\partial z_1^2}\right) - \frac{-\hbar^2}{2m_2}\left(\frac{\partial^2}{\partial x_2^2}+\frac{\partial^2}{\partial y_2^2}+\frac{\partial^2}{\partial z_2^2}\right) + (Vx_1,y_1,z_1,x_2,y_2,z_2,t)\right]\psi(x_1,y_1,z_1,x_2,y_2,z_2,t) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

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The potential energy depends only on the relative coordinates $V=V(x_1-x_2,y_1-y_2,z_1-z_2)=V(x,y,z)$ and if X,Y,Z be the coordinates of the center of mass, then $x=x_1-x_2, y=y_1-y_2, z=z_1-z_2$.................(2) and $MX=m_1x_1+m_2x_2, MY=m_1y_1+m_2y_2, MZ=m_1z_1+m_2z_2$ Where M= m_1+m_2 is the total mass of the system. Now we get

$$f=f(X,x)$$
$$\Rightarrow \frac{\partial f}{\partial x_1}=\frac{\partial f}{\partial x}\frac{\partial X}{\partial x_1}+\frac{\partial f}{\partial x}\frac{\partial x}{\partial x_1}=\frac{m_1}{M}\frac{\partial f}{\partial X}+\frac{\partial f}{\partial x}, by(2)$$
$$\Rightarrow \frac{\partial^2 f}{\partial x_1^2}=\frac{\partial}{\partial x_1}\left(\frac{\partial f}{\partial x_1}\right)=\frac{\partial}{\partial X}\left(\frac{\partial f}{\partial x_1}\right)\frac{\partial X}{\partial x_1}+\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x_1}\right)\frac{\partial x}{\partial x_1}$$

$$=\frac{\partial}{\partial X}\left(\frac{m_1}{M}\frac{\partial f}{\partial X}+\frac{\partial f}{\partial x}\right)\frac{m_1}{M}+\frac{\partial}{\partial x}\left(\frac{m_1}{M}\frac{\partial f}{\partial X}+\frac{\partial f}{\partial x}\right)$$
$$=\frac{m_1^2}{M^2}\frac{\partial^2 f}{\partial X^2}+\frac{m_1}{M}\frac{\partial^2 f}{\partial X\partial x}+\frac{m_1}{M}\frac{\partial^2 f}{\partial x\partial X}+\frac{\partial^2 f}{\partial x^2}$$
$$=\frac{m_1^2}{M^2}\frac{\partial^2 f}{\partial X^2}+\frac{2m_1}{M}\frac{\partial^2 f}{\partial X\partial x}+\frac{\partial^2 f}{\partial x^2}$$
$$\Rightarrow \frac{\partial^2}{\partial x_1^2}=\frac{m_1^2}{M^2}\frac{\partial^2}{\partial X^2}+\frac{2m_1}{M}\frac{\partial^2}{\partial X\partial x}+\frac{\partial^2}{\partial x^2}$$

and similarly for, $\frac{\partial^2}{\partial y_1^2}$ and $\frac{\partial^2}{\partial z_1^2}$,Also in the same way $\frac{\partial^2}{\partial x_2^2}=\frac{m_2^2}{M^2}\frac{\partial^2}{\partial X^2}-\frac{2m_2}{M}\frac{\partial^2}{\partial X\partial x}+\frac{\partial^2}{\partial x^2}$ and similarly for, $\frac{\partial^2}{\partial y_2^2}$ and $\frac{\partial^2}{\partial z_2^2}$. Now we write

$$\left[-\frac{\hbar^2}{2m_1}\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial y_1^2}+\frac{\partial^2}{\partial z_1^2}\right)-\frac{\hbar^2}{2m_2}\left(\frac{\partial^2}{\partial x_2^2}+\frac{\partial^2}{\partial y_2^2}+\frac{\partial^2}{\partial z_2^2}\right)\right]$$
$$=-\frac{\hbar^2}{2m_1}\left[\frac{m_1}{M^2}\left(\frac{\partial^2}{\partial X^2}+\frac{\partial^2}{\partial Y^2}+\frac{\partial^2}{\partial Z^2}\right)+\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\right]-\frac{\hbar^2}{2m_2}\left[\frac{m_2^2}{M^2}\left(\frac{\partial^2}{\partial X^2}+\frac{\partial^2}{\partial Y^2}+\frac{\partial^2}{\partial Z^2}\right)+\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\right] \text{Where}$$
$$=-\frac{\hbar^2}{2M^2}(m_1-m_2)\left(\frac{\partial^2}{\partial X^2}+\frac{\partial^2}{\partial Y^2}+\frac{\partial^2}{\partial Z^2}\right)-\frac{\hbar^2}{2}.\frac{m_1+m_2}{m_1m_2}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)$$
$$=-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial X^2}+\frac{\partial^2}{\partial Y^2}+\frac{\partial^2}{\partial Z^2}\right)-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)$$

$\mu=\frac{m_1+m_2}{m_1+m_2}$ is called the reduced mass. Using the above value in (1)

$$i\hbar\frac{\partial\Psi}{\partial t}=\left[-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial X^2}+\frac{\partial^2}{\partial Y^2}+\frac{\partial^2}{\partial Z^2}\right)-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V(x,y,z)\right]\Psi..........(3)$$

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we make the following separation

$$\Psi(x,y,z,X,Y,Z,t)=u(x,y,z)U(X,Y,Z)e^{-i(E+E')t/h}$$

in equation (3),then

$$(E+E')u(x,y,z)U(X,Y,Z)e^{-i(E+E')t/h}$$
$$=\left(-\frac{\hbar^2}{2M}\nabla U(X,Y,Z)\right)u(x,y,z)+\left(\frac{\hbar^2}{2\mu}\nabla^2 u(x,y,z)U(X,Y,Z)+[Vu(x,y,z)U(X,Y,Z)]e^{-i(E+E')t/h}\right)$$

Which is equivalent to the following two equations $-\frac{\hbar^2}{2\mu}\nabla^2 u+Vu=Eu.........(4)$ and

$$-\frac{\hbar^2}{2M}\nabla^2 U=E'u.........(5)$$

The relative movement of the two particles is defined by Equation (5); where an object with mass μ moving in a field of potential energy V is demonstrated. According to Eq. (5), the mass center of the pair behaves asa solitary particle with M mass.

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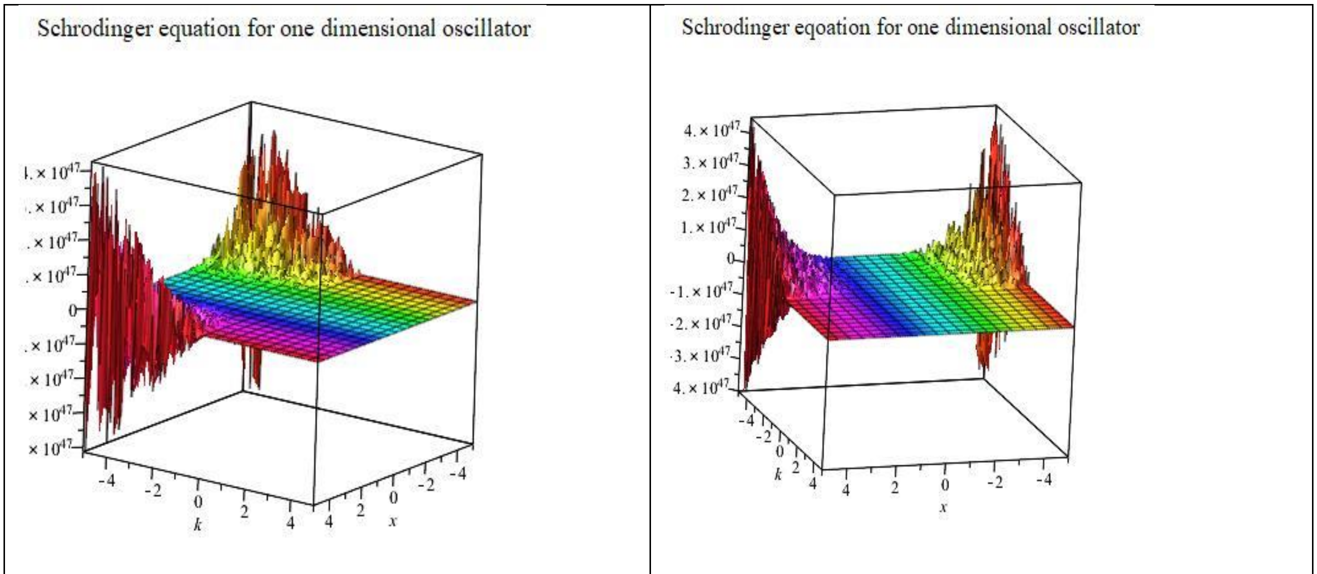
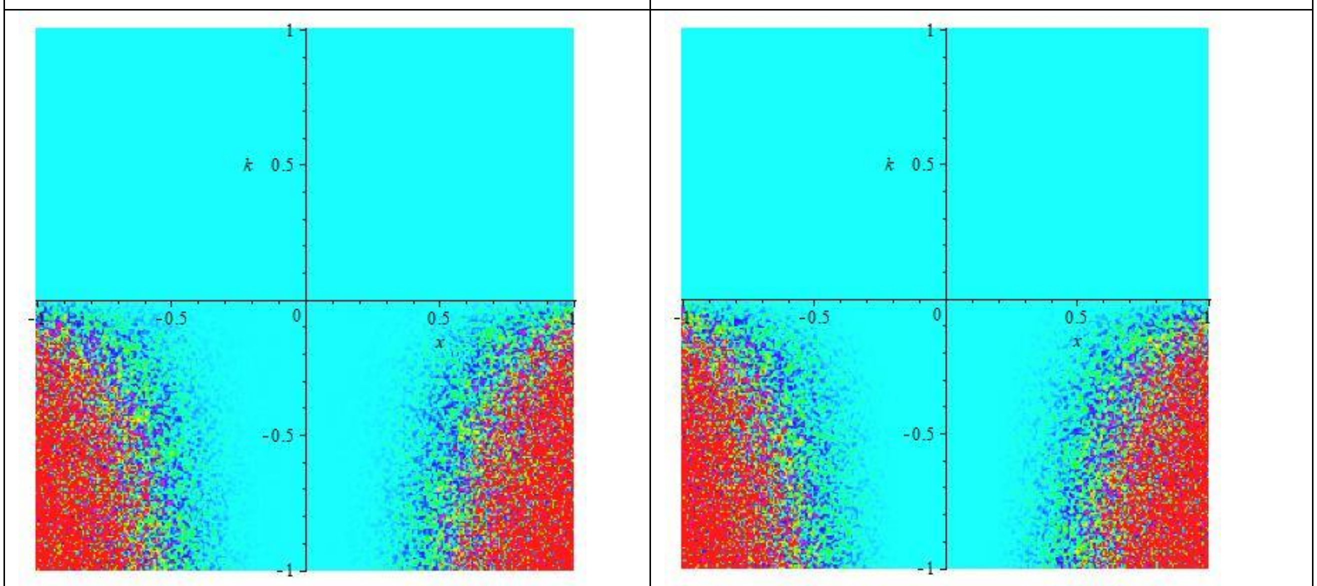


a) Real 3D plot

(b)imaginary 3D plot



(c)Real density plot

(d)imaginary density plot

Fig 5.3: The graphical representation of Schrödinger equation for 1-D harmonic oscillator

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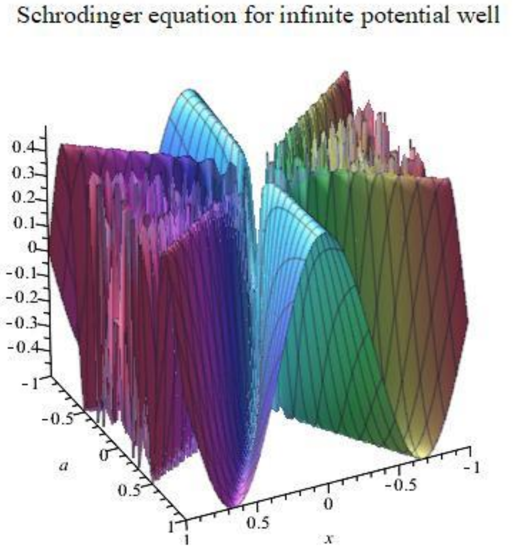
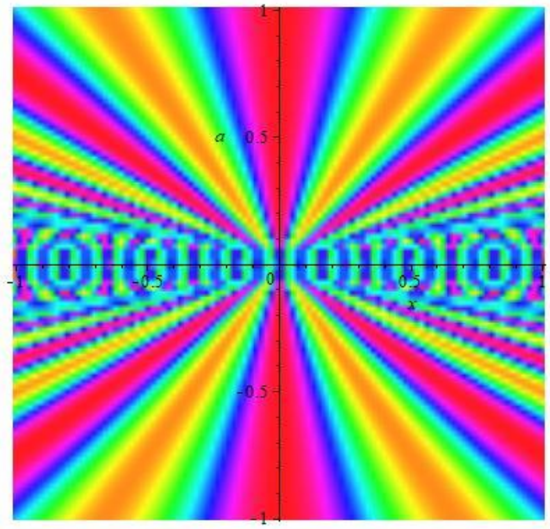
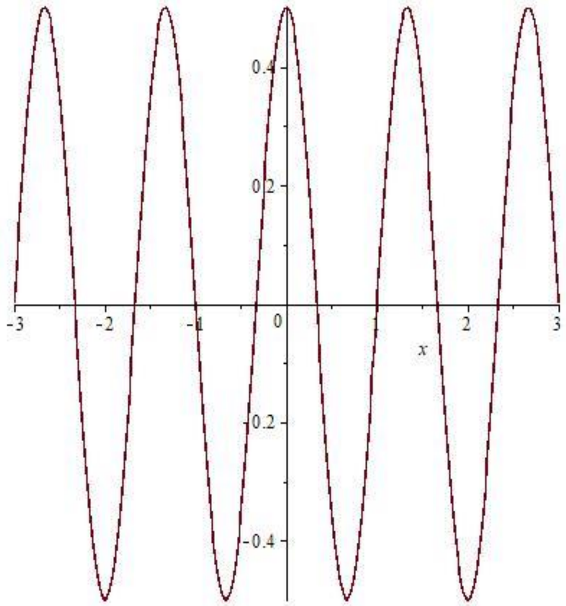


a) Real 3D plot



b) Real density plot



C) 2D plot

Fig 5.4: The graphical representation of $\psi = C_1 \cos\frac{n\pi x}{-2b}$ **when nis odd**

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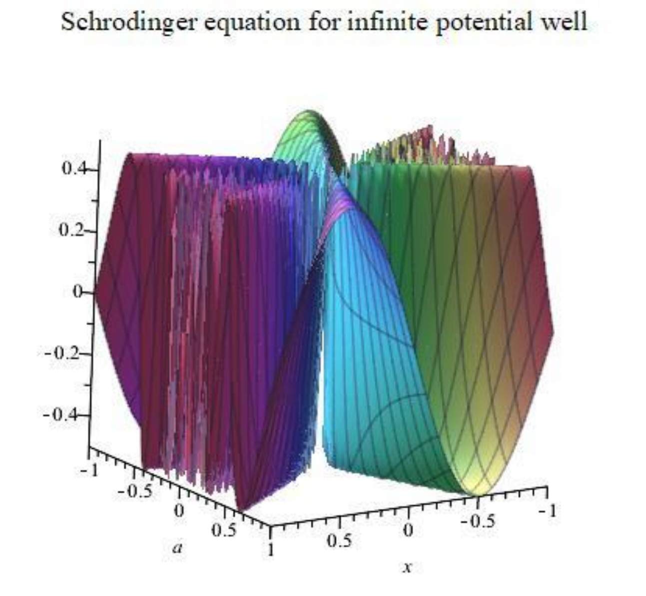
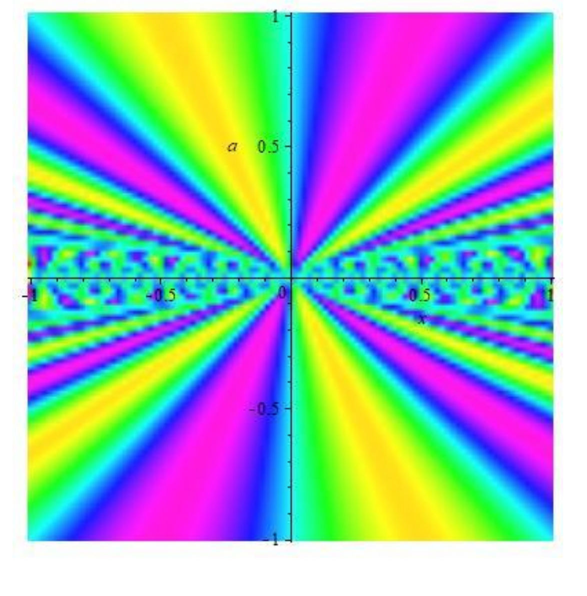
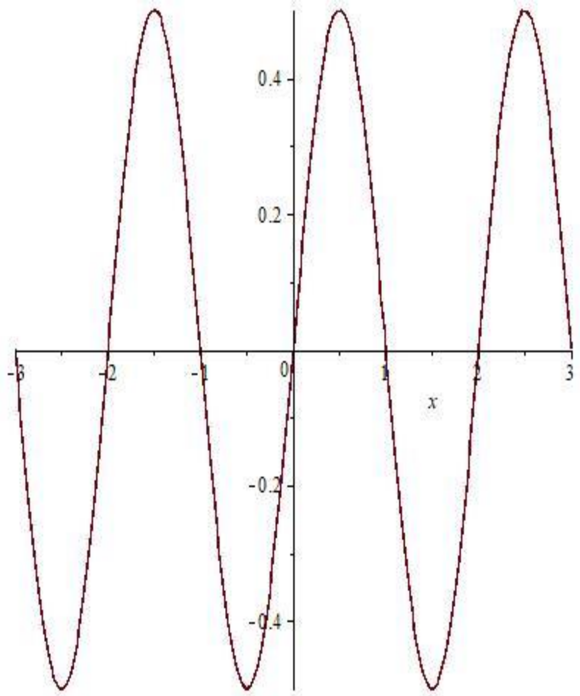


a) Real 3d plot



b) Real density plot



c) 2D plot

Fig 5.5: The graphical representation of $\psi = C_2 \sin\frac{n\pi x}{2b}$ **when n is even**

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Gono Bishwabidyalay

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6. Numerical Results:

In this portion using Maple software we got some computational graphs for Schrödinger equation for 1-D harmonic oscillator and Schrödinger equation for infinite potential well perspective to n odd and even. Fig 5.3 shows the 3D form in real and imaginary part, and density form of Schrödinger equation for 1-D harmonic oscillator using a finite order polynomial in ξ .this shape addresses a multiple soliton. The nature of the result for infinite potential well are shown in Fig 5.4 and 5.5 for n is odd and even respectively. This shape represent Cos wave function in 3D & 2D for n=3, C_1=0.5; and Sin wave function for n=2 ,C_2=0.5 for *x,b* defined on[-1,1].

7. CONCLUSION

This article explains how to solve Schrödinger's time-independent part and provides an illustration of its derivation. Additionally, a few examples of the Schrodinger wave equation with time independence are shown. Here 5.1 implements the equation for a one-dimensional harmonic oscillator, 5.2 illustrates the time-independent part of the potential well in various examples, and 5.3 illustrates the implementation of Schrödinger's time-independent part. Then, using Maple, we add some numerical graphs for the equation. In addition to its significance in physics, chemistry, and engineering, the time-independent Schrödinger wave equation is a key tool in these disciplines. It is specifically used to describe how electrons behave in atoms and molecules. In addition to semiconductors and other solid-state materials, the equation can also be used in cosmology and nuclear physics. In general, the Schrödinger wave equation is an effective tool for comprehending how particles behave in a variety of contexts.

Author Contribution:

Author **DilrubaAkter** planned and designed the manuscript, **DilrubaAkter**, **MalatiMazumder**and**M Shakawat Hossain Shaon** collected the literature, **DilrubaAkter** prepared the manuscript, **Malati Mazumder**, and **Kanak Chandra Roy** revised the manuscript. All authors read and approved the final manuscript.

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