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Numerical Solution of Schrödinger Equation by using Crank-Nicolson Method

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ABSTRACT

The Schrödinger equation is a fundamental equation in quantum mechanics that describes how wave functions evolve over time. The study explored specific focus on the Crank-Nicolson scheme, which is widely used and efficient method. By applying these methods to the one-dimensional Schrödinger equation, the work provided insights into the behavior of these systems. To confirm the accuracy and reliability of this method, a test problem is solved. The result obtained from numerical method is compared with analytical solution. The graph of compared result is shown with the help of computational software. The test demonstrates that the method is effective for solving the Schrödinger equation, even when an analytical solution is not possible or too difficult to obtain. Overall, the Crank-Nicolson difference scheme is a valuable tool for understanding the behavior of quantum systems and solving problems.

Keywords: Schrödinger equation; Wave function; Quantum systems; Crank-Nicolson difference scheme.

1 INTRODUCTION

The Schrödinger equation, proposed by Erwin Schrödinger in 1926, is a critical component of modern physics and the primary equation used in quantum mechanics [12]. It helps physicists understand the behavior of matter and energy at the atomic and subatomic scale, just as Newton's laws of motion are essential in classical mechanics [14]. By studying this equation, researchers have gained insights into the properties of matter and energy at the quantum level, leading to technological advancements in fields such as electronics and materials science [20]. The Schrödinger equation is also the basis for several critical concepts in quantum mechanics, including wave-particle duality, the uncertainty principle, and the superposition principle. The equation represents the wave function of a quantum mechanical system and provides probabilistic information about a particle's position and momentum [1, 17]. By modulating the wave function, the Schrödinger equation predicts the behavior and properties of quantum mechanical systems, enabling researchers to study the behavior of isolated physical systems at the quantum level [5, 7, 14, 15].

The Schrödinger equation is crucial in describing the behavior of quantum particles in a wide range of physical systems [11]. The wave function of a particle, represented by the symbol ψ, is used to calculate the probability density of its position and momentum [1, 14]. When studying quantum tunneling phenomena, the Schrödinger equation is used to determine the wave function of a particle encountering a potential barrier [14]. The shape of the barrier and the energy of the particle are used to calculate the probability of the particle passing through the barrier [15]. If the barrier is thin and the particle has enough energy, there is a non-zero probability of the particle tunneling through the barrier, despite not having enough energy classically [22, 25]. The Schrödinger equation is important in understanding the wave-like nature of particles, which is responsible for quantum tunneling. It predicts the probability of a particle being on one side of a barrier or another and how that probability changes over time [21]. The

Schrödinger equation also accounts for the time evolution of a particle's wave function, predicting how it changes over time [13]. The Crank-Nicolson scheme is used to numerically solve the Schrödinger equation, obtaining the time-dependent wave function of a quantum system. This method is useful for solving partial differential equations and provides a stable and accurate solution by combining forward-time and backward-time finite difference methods [3].

At a particular time, the probability amplitude of a particle being in a specific state can be represented by the time-dependent wave function obtained through the application of the Crank-Nicolson scheme [12]. This wave function can be used to calculate various properties of the quantum system, such as the probability density, expectation values of observables, and the energy spectrum of the system [14]. In comparison to other numerical methods such as the forward-time or backward-time finite difference methods, the Crank-Nicolson scheme generally yields a more precise and reliable solution to the Schrödinger equation [19]. The precision of the computed solution of the Schrödinger equation through numerical calculation is dependent on the chosen time step and spatial grid size [3]. Therefore, the Crank-Nicolson scheme can be a useful tool in simulating the behavior of quantum systems in various contexts, such as in quantum chemistry, condensed matter physics, and quantum computing [15].

After the development of Quantum Mechanics, physicists have conducted various studies and research in the field. These studies have utilized numerical simulations and various numerical approaches to solve the Schrödinger equation and investigate the behavior of particles at the quantum level [4]. Amin Khan (2022) [14] utilized the Crank-Nicolson scheme to solve the Schrödinger equation numerically. The goal was to assess the effectiveness of the method in obtaining accurate results. The results of the study showed that the Crank-Nicolson scheme was indeed appropriate for obtaining precise solutions to the Schrödinger equation. This study was significant in demonstrating the utility of the Crank-Nicolson scheme in physics research. In contrast, Documet (2006) [9] study focused on proposing a condition for unconditional stability and presenting an alternative approach to transparent boundary conditions for Crank-Nicolson finite-difference schemes. The goal was to address the challenges associated with transparent boundary conditions in numerical simulations. The research was crucial in providing an alternative solution to the problem of transparent boundary conditions and in improving the accuracy of numerical simulations.

Taha (1984) [23] approximated the nonlinear Schrödinger equation using various numerical approaches such as the classical explicit method, hopscotch method, implicit-explicit method, and Crank-Nicolson implicit scheme. Delfour *et al.* (1981) [8] described a finite-difference method for simulating the Schrödinger equation with power non-linearity. Erbe (1994) [12] investigated the existence of positive solutions to the equation w" + c(t)g(w) = 0 with linear boundary conditions by applying the Fixed Point Theorem in cones. To sum, these studies illustrate the importance of numerical methods and analytical techniques in advancing the understanding of complex equations and physical phenomena [8, 12, 23].

Katsunori (2021) [16] research in 2021 demonstrated a new formulation of Schrödinger's equation as two real equations, which can be rewritten in polar form. This approach reduced one equation to the continuity equation, and the other to a nonlinear dynamical equation for the probability density. This research was significant in providing a new understanding of Schrödinger's equation and its behavior, which could lead to new applications in various fields. Dongling (2013) [24] investigated the stability and convergence of the Crank-Nicolson difference technique for the coupled nonlinear Schrödinger equations with the Riesz space fractional derivative. The research aimed to determine the effectiveness of the Crank-Nicolson method in solving this type of equation. The study was significant in advancing the understanding of the behavior of the coupled nonlinear Schrödinger equations and in identifying a reliable numerical method for solving them. In Kalvin (2013) [21], the goal was to understand the timing effects of wave packet tunneling through a barrier. Non relativistic wave packets were used in numerical simulations to achieve this aim. The results of the study were significant in providing insights into the nature of wave packet tunneling and its timing effects.

Bernard (2014) [10] focused on practical error analysis in the context of tunnel effect in a rectangular barrier. The research involved numerical outcomes, which provided useful information on the nature of errors in tunneling experiments. This study was important in understanding the sources of error in tunneling experiments and how to mitigate them. Davies

(2005) [6] research indicated that signals faster than light have no significant use, as only transit duration is measurable. This statement implies that although faster-than-light signals may exist, their practical utility is limited due to measurement constraints. The study was important in understanding the limitations of faster-than-light signals and their potential usefulness. Mohandas (2012) [18] recommended the use of the software for the correct calculation and plotting of eigen values and eigenvectors in potential problems. The computational software has proven to be useful in solving complex problems in physics, including those involving potential problems.

2 CRANK-NICOLSON SCHEME FOR SCHRÖDINGER EQUATION

The mathematical expression of the time dependent Schrödinger equation in its standard form is given by [19],

$$\iota \frac{\partial \Psi}{\partial t} + k\frac{\delta^2 \Psi}{\partial x^2} + a|\Psi|^2 \Psi + b f(x,t) = 0;\ x \in [p,q],\ t \in [0,1] \quad \text{.....(1)}$$

Where, Ψ is a complex-valued function depending upon x, t and $\iota = \sqrt{-1}$.

With initial and boundary conditions,

$\Psi(p, t) = \zeta_0(x)$ .....(2)

$\Psi(q, t) = \zeta_1(x)$..... (3)

$\Psi(x,0) = \phi(x)$ .....(4)

Where, Ψ is a smooth function, $k \neq 0$ [7].

Since, we are considering linear Schrodinger equation, i.e , $\alpha = 0$. Therefore equation (1) reduces to,

$$\iota\frac{\partial \Psi}{\partial t} + k\frac{\delta^2 \Psi}{\partial x^2} + bf(x,t) = 0 \quad \text{.....(5)}$$

Where, b is the parameter whose value might be positive or negative [15].

A approach that decreases the overall amount of calculation and is acceptable (i.e., convergent and stable) for all finite values was originally proposed by Crank and Phyllis Nicolson in 1947 [25]. In case of finite difference approximations, document [9] declare the midpoint ($i(\Delta x^2$; $(j + \frac{1}{2}) \Delta t$) satisfied the partial differential equation and $\frac{\partial^2 \Psi}{\partial x^2}$ is substituted by average of midpoint at j^{th} and $(j + 1)^{th}$ time levels.

When $k = -1$ and $b = 0$ equation (5) takes the form,

$$\iota \frac{\partial \Psi}{\partial t} - \frac{\partial^2 \Psi}{\partial x^2} = 0 \quad \text{.....(6)}$$

$$\left(\iota \frac{\partial \Psi}{\partial t}\right)_{i,\ ,j+\frac{1}{2}} = \left(\frac{\partial^2 \Psi}{\partial x^2}\right)_{i,\ ,j+\frac{1}{2}}$$

Apply forward difference in time j and central difference scheme in space i, we get

$$\iota \frac{\Psi_{i,j+1} - \Psi_{i,j}}{\Delta t} = \frac{1}{2}\left(\frac{\Psi_{i-1,j} - 2\Psi_{i,j} + \Psi_{i+1,j}}{(\Delta x)^2} + \frac{\Psi_{i-1,\ j+1} - 2\Psi_{i,j+1} + \Psi_{i+1,\ j+1}}{(\Delta x)^2}\right)$$

After simplification,

$$2\iota(\Psi_{i,j+1} - \Psi_{i,j}) = \frac{\Delta t}{\Delta x^2}(\Psi_{i-1,j} - 2\Psi_{i,j} + \Psi_{i+1,j} + \Psi_{i-1,\ j+1} - 2\Psi_{i,j+1} + \Psi_{i+1,\ j+1})$$

Let $\frac{\Delta t}{(\Delta x)^2} = \alpha$

Then, equation (7) takes the form,

$$2\iota\Psi_{i,j+1} - 2\iota\Psi_{i,j} = \alpha\Psi_{i-1,j} - 2\alpha\Psi_{i,j} + \alpha\Psi_{i+1,j} + \alpha\Psi_{i-1,j+1} - 2\alpha\Psi_{i,j+1} + \alpha\Psi_{i+1,j+1}$$

Where, $i = 1, 2, ..., N - 1$ and $j = 0, 1, 2, ... , M$.....(8)

To solve above equation we use following constraints,

where, $i = 1, 2, ... , N$

$\Psi_{i,j} = \zeta_1(t_j)$

$\Psi_{N,j} = \zeta_2(t_j)$

where j = 0, 1, ... , M

Moreover, arranging equation (8)

$$-\alpha\Psi_{i+1,j+1} + 2\alpha\Psi_{i,j+1} + 2\iota\Psi_{i,j+1} - \alpha\Psi_{i+1,j+1} = \alpha\Psi_{i-1,j} - 2\alpha\Psi_{i,j} 2\iota\Psi_{i,j} + \alpha\Psi_{i+1,j}$$
$$-\alpha\Psi_{i-1,j+1} + 2(\iota+\alpha)\Psi_{i,j+1} - \alpha\Psi_{i+1,j+1} = \alpha\Psi_{i-1,j} + 2(\iota-\alpha)\Psi_{i,j} + \alpha\Psi_{i+1,j} \quad \text{..... (9)}$$

Suppose there are N internal mesh points along every row of time, i.e., j = 0 then i = 1,2, ..., N – 1. Thus we get N – 1 simultaneous equations for N–1 unknown values along the initial row, initial and boundary values are pre-defined.

For $i = 1$,

$$-\alpha\Psi_{0,1} + 2(\iota+\alpha)\Psi_{1,1} - \alpha\Psi_{2,1} = \alpha\Psi_{0,0} + 2(\iota-\alpha)\Psi_{1,0} + \alpha\Psi_{2,0}$$

In general, for i = N – 1,

$$-\alpha\Psi_{N-2,1} + + 2(\iota+\alpha)\Psi_{N-1,1} - \alpha\Psi_{N,1} = \alpha\Psi_{N-2,0} + 2(\iota-\alpha)\Psi_{N-1,0} + \alpha\Psi_{N,0}$$

All these simultaneous equations can be written in matrix form,

$$\begin{bmatrix} 2(\iota+\alpha) & -\alpha & 0 & . & . & . & 0 \\ -\alpha & 2(\iota+\alpha) & -\alpha & . & . & . & 0 \\ 0 & -\alpha & 2(\iota+\alpha) & -\alpha & . & . & 0 \\ 0 & . & . & . & 2(\iota+\alpha) & -\alpha & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 0 & . & . & . & . & -\alpha & 2(\iota+\alpha) \end{bmatrix} \begin{bmatrix} \Psi_{1,j+1} \\ \Psi_{2,j+1} \\ \Psi_{3,j+1} \\ . \\ . \\ \Psi_{N-2,j+1} \\ \Psi_{N-1,j+1} \end{bmatrix}$$

$$= \begin{bmatrix} 2(\iota-\alpha) & \alpha & 0 & . & . & . & 0 \\ \alpha & 2(\iota-\alpha) & \alpha & . & . & . & 0 \\ 0 & \alpha & 2(\iota-\alpha) & \alpha & . & . & 0 \\ 0 & . & . & . & 2(\iota-\alpha) & \alpha & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 0 & . & . & . & . & \alpha & 2(\iota-\alpha) \end{bmatrix} \begin{bmatrix} \Psi_{1,j} \\ \Psi_{2,j} \\ \Psi_{3,j} \\ . \\ . \\ \Psi_{N-2,j} \\ \Psi_{N-1,j} \end{bmatrix} + \begin{bmatrix} \alpha\Psi_{0,j} + \alpha\Psi_{0,j+1} \\ 0 \\ . \\ . \\ . \\ \alpha\Psi_{N,j} + \alpha\Psi_{N,j+1} \end{bmatrix} \quad \text{...(10)}$$

Above equation in simplified form is, $AV_{j+1} = NV_j + P_j$ ..... (11)

Where,

$$\begin{bmatrix} 2(\iota+\alpha) & -\alpha & 0 & . & . & . & 0 \\ -\alpha & 2(\iota+\alpha) & -\alpha & . & . & . & 0 \\ 0 & -\alpha & 2(\iota+\alpha) & -\alpha & . & . & 0 \\ 0 & . & . & . & 2(\iota+\alpha) & -\alpha & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 0 & . & . & . & . & -\alpha & 2(\iota+\alpha) \end{bmatrix}$$

$$N = \begin{bmatrix} 2(\iota-\alpha) & \alpha & 0 & . & . & . & 0 \\ \alpha & 2(\iota-\alpha) & \alpha & . & . & . & 0 \\ 0 & \alpha & 2(\iota-\alpha) & \alpha & . & . & 0 \\ 0 & . & . & . & 2(\iota-\alpha) & \alpha & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 0 & . & . & . & . & \alpha & 2(\iota-\alpha) \end{bmatrix}$$

$$P_j = \begin{bmatrix} \alpha\Psi_{0,j} + \alpha\Psi_{0,j+1} \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ \alpha\Psi_{N,j} + \alpha\Psi_{N,j+1} \end{bmatrix}, \; v_{j+1} = \begin{bmatrix} \Psi_{1,j+1} \\ \Psi_{2,j+1} \\ \Psi_{3,j+1} \\ \cdot \\ \cdot \\ \Psi_{N-2,j+1} \\ \Psi_{N-1,j+1} \end{bmatrix}, \; v_j = \begin{bmatrix} \Psi_{1,j} \\ \Psi_{2,j} \\ \Psi_{3,j} \\ \cdot \\ \cdot \\ \Psi_{N-2,j} \\ \Psi_{N-1,j} \end{bmatrix}$$

Equation (11) can be solved for V_j

$$V_{j+1} = A^{-1}N\,V_j + A^{-1}P_j$$

Therefore,

$$V_{j+1} = RV_j + S_j$$

where $R = A^{-1}\,N$ and $S_j = A^{-1}P_j$. Likewise we can find $V_1, V_2, V_3, \ldots, Vm$ and $M = j\Delta t$.

3 NUMERICAL SOLUTION OF SCHRÖDINGER EQUATION

We solve the following Schrödinger equation by Crank-Nicolson Method [14, 15]:

$$\iota \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \text{ subject to the boundary condition}$$

$u(x, 0) = \sin x, -2 \le x \le 2$, and $u(-2, t) = -e^{\iota t} \sin 2$ $u(2, t) = e^{\iota t} \sin(2)$

Let $h = 0.2$ and $l = 0.8$, so that

$$\lambda = \frac{\alpha^2 l}{h^2} = \frac{-\iota(0.04)}{(0.8)^2} = 0.3135\iota$$

For $\lambda = 1$, Crack-Nicolson Formula

$$-\lambda u_{i-1}^{k+1} + (2 + 2\lambda)u_i^{k+1} - \lambda u_{i+1}^{k+1} = \lambda u_{i-1}^{k} + (2 - 2\lambda)\,\lambda u_i^{k} + \lambda\, u_{i+1}^{k}$$

becomes

$$0.3125\iota\, u_{j-1}^{k+1} + (2 - 0.625\iota)\, u_j^{k+1} + 0.3135\iota\, u_{j+1}^{k+1} = -0.3135\iota\, u_{j-1}^{k} + (2 + 0.625\iota)\, u_i^{k} - 0.3135\iota\, u_{i+1}^{k} \quad \ldots(12)$$

Putting $k = 0$ in (12), we obtained

$$0.3125\, u_{j-1}^{1} + (2 - 0.625\iota)\, u_j^{1} + 0.3135\iota\, u_{j+1}^{1} = -0.3135\iota\, u_{j-1}^{0} + (2 + 0.625\iota)\, u_i^{0} - 0.3135\iota\, u_{i+1}^{0} \quad \ldots\ldots\ldots\ldots\ldots(13)$$

Corresponding to i = 1, 2, 3 and 4

$$0.3125\iota\, u_0^{1} + (2 - 0.625\iota)\, u_1^{1} + 0.3125\iota\, u_2^{1} = -0.3125\iota\, u_0^{0} + + (2 + 0.625\iota)\, u_1^{0} - 0.3125\iota\, u_2^{0}$$

$$0.3125\iota\, u_1^{1} + (2 - 0.625\iota)\, u_2^{1} + 0.3125\iota\, u_3^{1} = -0.3125\iota\, u_1^{0} + + (2 + 0.625\iota)\, u_2^{0} - 0.3125\iota\, u_3^{0}$$

$$0.3125\iota\, u_2^{1} + (2 - 0.625\iota)\, u_3^{1} + 0.3125\iota\, u_4^{1} = -0.3125\iota\, u_2^{0} + + (2 + 0.625\iota)\, u_3^{0} - 0.3125\iota\, u_4^{0}$$

$$0.3125\iota\, u_3^{1} + (2 - 0.625\iota)\, u_4^{1} + 0.3125\iota\, u_5^{1} = -0.3125\iota\, u_3^{0} + + (2 + 0.625\iota)\, u_4^{0} - 0.3125\iota\, u_5^{0}$$

We have

$$u(x,0) = \mathrm{Sin}x$$

But

$$u(jh,kl) = u_j^{k} \;\Rightarrow u_i^{0} = u(-2 + jh, 0) = \sin jh = \sin(-2 + 0.8j)$$

Putting $j = 0, 1, 2, 3, 4$. Therefore,

$u_0^0 = -0.9093,\ u_1^0 = -0.9320,\ u_2^0 = -0.3894,\ u_3^0 = 0.9320,\ u_4^0 = 0.9093$

$u(-2,t) = -e^{iotat} \sin 2 = -(\cos t + \iota \sin t)\sin 2$

$u_0^0 = u(-2,0) = -(\cos 0 + \iota \sin 0)\sin 2 = -0.9093$

$u_0^1 = u(-2,0.2) = -(\cos 0.2 + \iota \sin 0.2)\sin(2) = -0.8912 - 0.1807\iota$

and

$u(2,t) = e^{iotat} \sin 2 = (\cos t + \iota \sin t)\sin 2$

$u_0^1 = u(2,0) = (\cos 0 + \iota \sin 0)\sin 2 = 0.9093$

$u_0^1 = u(2,0.2) = (\cos 0.2 + \iota \sin 0.2)\sin(2) = 0.8912 + 0.1807\iota$

Therefore, above system become

$(2 + 0.625\iota)\, u_1^1 + 0.3125\iota\, u_2^1 = -1.9204 + 0.7098\iota$

$0.3125\iota\, u_2^1 + (2 - 0.625\iota)\, u_2^1 + 0.3125\iota\, u_3^1 = -0.7788 - 0.2434\iota$

$0.3125\iota\, u_3^1 + (2 - 0.625\iota)\, u_3^1 + 0.3125\iota\, u_4^1 = 1.5798 + 0.7042\iota$

$0.3125\iota\, u_3^1 + (2 - 0.625\iota)\, u_4^1 = 1.9204 - 0.2643\iota$

$$\begin{pmatrix} (2+0.625\iota) & 0.3125\iota & 0 & 0 \\ 0.3125\iota & (2-0.625\iota) & 0.3125\iota & 0 \\ 0 & 0.3125\iota & (2-0.625\iota) & 0.3125\iota \\ 0 & 0 & 0.3125\iota & (2-o.625\iota) \end{pmatrix} \begin{pmatrix} u_1^1 \\ u_2^1 \\ u_3^1 \\ u_4^1 \end{pmatrix} = \begin{pmatrix} -1.9204 + 0.7098\iota \\ -0.7788 - 0.2434\iota \\ 1.5798 + 0.7042\iota \\ 1.9204 - 0.2643\iota \end{pmatrix}$$

or, $Ax = B$.....(14)

Where

$$A = \begin{pmatrix} (2+0.625\iota) & 0.3125\iota & 0 & 0 \\ 0.3125\iota & (2-0.625\iota) & 0.3125\iota & 0 \\ 0 & 0.3125\iota & (2-0.625\iota) & +0.3125\iota \\ 0 & 0 & 0.3125\iota & (2-o.625\iota) \end{pmatrix} \quad x = \begin{pmatrix} u_1^1 \\ u_2^1 \\ u_3^1 \\ u_4^1 \end{pmatrix}$$

$$B = \begin{pmatrix} -1.9204 + 0.7098\iota \\ -0.7788 - 0.2434\iota \\ 1.5798 + 0.7042\iota \\ 1.9204 - 0.2643\iota \end{pmatrix}$$

And

$$A^{-1} = \begin{bmatrix} 0.4458 - 0.1239\iota & -0.008 - 0.0684\iota & -0.0096 - 0.0028\iota & -0.0008 + 0.0012\iota \\ 0.008 - 0.0684\iota & 0.4394 + 0.1317\iota & 0.0369 - 0.0561\iota & -0.0063 - 0.0078\iota \\ -0.0096 - 0.0028\iota & 0.0369 - 0.0561\iota & -0.4427 + 0.1267\iota & 0.0377 - 0.0574\iota \\ -0.008 + 0.0012\iota & 0.0063 - 0.0078\iota & 0.0377 - 0.0574\iota & 0.4490 + 0.1344\iota \end{bmatrix} \quad \text{.....(15)}$$

Using $X = A^{-1} B$ we get

$$\begin{pmatrix} u_1^1 \\ u_2^1 \\ u_3^1 \\ u_4^1 \end{pmatrix} = \begin{pmatrix} -0.7879 + 0.6287\iota \\ -0.1765 - 0.1546\iota \\ 0.6455 + 0.4249\iota \\ 1.0016 + 0.0799\iota \end{pmatrix} \quad \text{.....(16)}$$

Above example shows manual calculation of a Schrödinger equation by Crank-Nicolson method. This method is long, very difficult to solve if number of partitions is more. So, we solved similar problem by using computational software and the obtained result is shown below.

4 RESULT AND DISCUSSION

The Schrödinger equation in one-dimension is,

$$\iota \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

subject to the boundary condition.

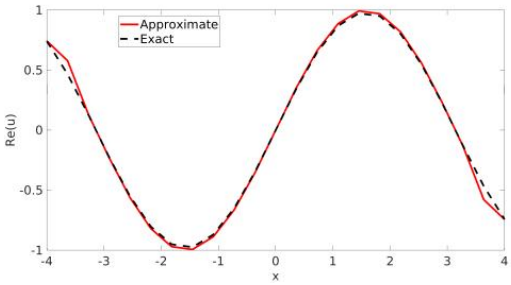
$u(x; 0) = \sin x$, $-4 \le x \le 4$, and $u(-4, t) = -e^{tt} \sin 2$ $u(4, t) = e^{tt} \sin(4)$.

We compare computational and analytical solutions with variation of length taking the value of each t fixed at t = 0.2. The 2D figure shows that computational solution obtained using Crank-Nicolson scheme is very close to analytical solution.

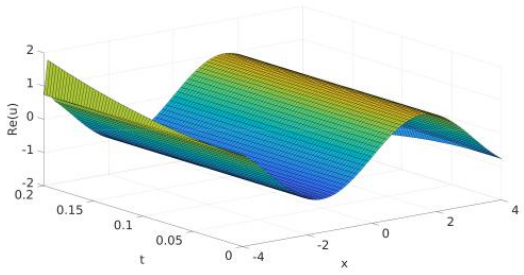
4.1 Real Part of the Solution

In Fig. 1A, x-axis represents x, y-axis represents real part of u and in Fig. 1B, x-axis represents x, y-axis represents time and z-axis represents real part solution. The graph Fig.1A between exact and approximate solution of a Schrödinger equation in real solution shows that applied method tends to the exact solution. The result obtained from Crank-Nicolson scheme is near and equals to exact solution.

The mesh plot can be visualized as a three-dimensional surface that evolves in time. The shape of the mesh plot can provide insights into the behavior of the particle. The x-axis represents x, the y-axis represents time, and the z-axis represents the real part of u. The Fig. 1B represents surface plot for the position of a particle in a one-dimensional Schrödinger equation. The amplitude of the wave function is displayed as a function of position and time, where higher amplitudes indicate a higher probability of finding the particle at that position. The peaks and troughs in the mesh plot represent regions where the particle is more or less likely to be found, respectively.



(a)



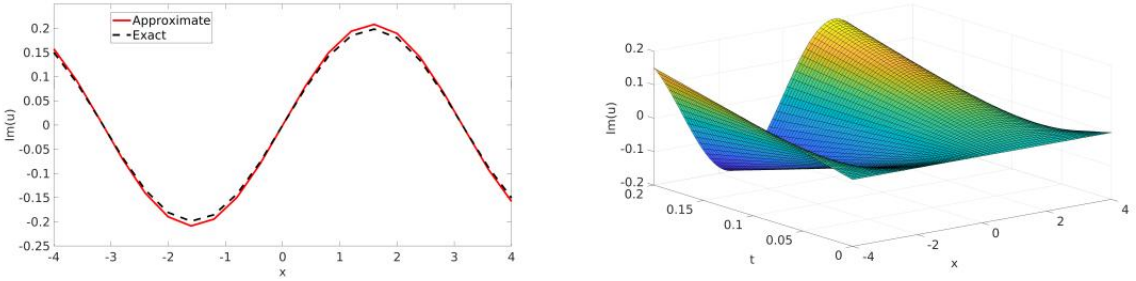
(b)

Fig. 1: (a) Comparison of approximate(red) and exact (dotted black) solution in case of real at h = 0,2,l = 0,8 and t = 0,2. and, **(b)** Surface plot of real part of the solution.

4.2 Imaginary Part of the Solution

In Fig. 2A, x-axis represents x, y-axis represents imaginary part of u and in Fig. 2B x-axis represents x, y-axis represents time and z-axis represents imaginary part of solution. By comparing imaginary part of the solution of Schrödinger equation we can conclude that exact and approximate imaginary solutions are about to coincide with evidence Fig. 2A. And analyzing the surface plot of the imaginary solution Fig. 2B, we

can gain information about the momentum of the particle at different positions and times. For example, if the mesh plot displays a region of high probability current density in one direction and a region of low probability current density in the opposite direction, this could indicate that the particle has a net momentum in the first direction. Furthermore, the mesh plot of the imaginary solution can also provide information about the energy of the particle. Similar to the mesh plot of the real solution, a periodic pattern in the mesh plot of the imaginary solution can indicate that the particle has a quantized energy.



(a) (b)

Fig. 2: (a) Comparison of approximate (red) and exact (dotted black) solution in case of imaginary at h = 0:2, l = 0:8 and t = 0:2. and, **(b)** Surface plot of imaginary part of the solution.

5 CONCLUSION

The work is detail about the application of Crank-Nicolson scheme in Schrödinger equation. The study explored the Crank-Nicolson scheme, which is a widely used and efficient method for solving the Schrödinger equation. By applying finite difference method to the one-dimensional Schrödinger equation the work provided insights into the behavior of these systems. The results obtained from the computational software were presented through graphs, which were clear and informative, highlighting the salient features of the solutions. The work mainly focuses on comparison of approximate and exact solution. The explanation was aided by the use of graphs, which helped to make the concept more accessible and the Crank-Nicolson method was shown to be effective. Overall, the work provided a thorough understanding of the Schrödinger equation and the Crank-Nicolson method, making both a valuable contribution to the field.

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