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A Modified Crank-Nicolson Method for Numerical Solution of the Linear Time-Dependent Schrodinger Equation

Bukar Hassan[a*] **and Ademola M. Badmus**[b]
[a]*Department of Mathematics, Nigerian Army University Biu, Borno State, Nigeria*
[b]*Department of Mathematics, Nigerian Defence Academy, Kaduna Nigeria*

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ABSTRACT

This paper presents the effectiveness of the solution of the time-dependent Schrodinger equation using the modified Crank-Nicolson Method (MCNM). The method was developed through finite difference approximation. To demonstrate the effectiveness of this approach, three different problems were tested with these approaches by using MATLAB soft code. Also, this research verifies that, in the presence or absence of potential energy, the modified Crank-Nicolson method for solving the time-dependent Schrödinger equation is accurate, convergent, and computationally efficient.

1. Introduction

Differential equations are indispensable mathematical tools used to model dynamic processes across multiple domains, representing phenomena such as current flow, population growth, and celestial gravitational fields. The Schrodinger's Equation (SE), a key equation in quantum mechanics, describes the behaviour of quantum systems over time. Quantum mechanics incorporates wave functions, which exhibit both wave-like and particle-like properties, and are crucial in determining the characteristics and probabilities of particles in quantum systems. The SE has both time-dependent and time-independent forms, with various methods used to solve it. Numerical methods are necessary for solving complex PDEs that lack analytical solutions due to nonlinearity or complex boundary conditions. This paper developed the Modified Crank-Nicolson Method (MCNM) for numerical solutions of the time-dependent Schrödinger equation. While Khan *et al*. (2022) and Kafle *et al*. (2023) worked on the Schrödinger equation, where the potential energy was neglected, resulting in the loss of the equation's physical meaning, this paper aims to address this issue by utilizing the derived (MCNM) to obtain their numerical solutions. The research conducted by Cari and Suparmi (2013) investigated energy eigenvalues and eigenfunctions within the Schrödinger equation.

This study was further conducted by Mao and Nakamura (2008), who explored wave front set analysis of solutions to Schrödinger equations involving long-range perturbed harmonic oscillators. Both studies delve into different aspects of the behaviour and properties of solutions to the Schrödinger equation under various potential perturbations. Mao and Nakamura's study, in turn, connects to the research conducted by Emmanuel and Ogunfiditimi (2018) on the application of the Schrödinger wave equation to develop a quantum finance model for technical analysis in the stock market. While Mao and Nakamura focused on the behaviour of solutions in the presence of perturbations, they utilized the harmonic oscillator model to understand the movement of stocks in a specific market context. Furthermore, the study by Harko and Liang (2016) explores the relationship between the linear harmonic oscillator equation and nonlinear differential equations. This connection extends the understanding of the harmonic oscillator beyond its linear form and has practical implications in various physical systems, as mentioned in the study. Reinhardt *et al*., (2023) conducted research on the Non-Linear Schrödinger Equation (NLSE) and established a comprehensive and unified theory for understanding its solutions. They introduced a classification method based on the cross-ratio and discovered a conformal duality between solutions of different NLSEs. Ikhdair (2012) obtained exact solutions of the Dirac equation for a charged harmonic oscillator in an electric field, enhancing our understanding of the system's

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* Corresponding author. Tel.: +2347031521372
E-mail address: bukar.hassan@naub.edu.ng (Bukar H.).
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behaviour. Das and Arda (2015) derived exact bound state solutions of the N-dimensional radial Schrödinger equation with a pseudo-harmonic potential using the Laplace transform approach. Jaradat *et al*., (2018) approximated analytical solutions for the non-linear Schrödinger equation with a harmonic oscillator, contributing to our understanding of non-linear systems involving harmonic oscillators. Okorie *et al*., (2023) investigated the k-dependent Schrödinger equation using the quantum pseudo-harmonic oscillator, while Kurbonov *et al*., (2023) developed a Crank-Nicolson scheme for solving the first-order diffusion equation. Akaninyeye *et al*., (2019) studied the Schrödinger equation in the cylindrical basis, and Lee and Kim (2022) focused on the stability of numerical solutions for a nonlinear Schrödinger equation. Gao *et al*., (2023) addressed computational challenges in the time-dependent Schrödinger equation with a position-dependent effective mass.

The Crank-Nicolson method is a versatile numerical solution approach that can handle various equations and scenarios, making it a reliable choice in many cases. Braun (2023) introduced a method for solving the Schrödinger equation using sinc functions on a finite interval. Zhao and Sun (2023) focused on numerical methods for the time-dependent Schrödinger equation in molecular dynamics. Bukar and Tahir (2023) developed an approximate solution specifically for the harmonic oscillator. Pathak *et al* (2022) proposed the Kansa method combined with polyharmonic radial basis functions for solving nonlinear Schrödinger equations in two dimensions. Khan *et al* (2022) used the Crank-Nicolson scheme with finite difference approximation for solving the Schrödinger equation, demonstrating convergence and effectiveness for non-homogeneous problems. While the aforementioned literature focused on the Schrödinger equation, which neglected the potential energy and jeopardised the equation's physical meaning, our investigation aims to address this problem. To achieve this, the study utilizes finite difference approximation on the Schrödinger equation and applies a derived technique called the Modified Crank-Nicolson method (MCNM) to obtain numerical solutions.

2. Methodology

2.1 Derivation of the Time-Dependent Schrodinger Equation

Energy conservation can be used to derive the time-dependent Schrodinger equation as

$$Total\ Energy = Kinetic\ energy + Potential\ Energy \tag{1}$$

which is mathematically represented within the context of quantum mechanics as

$$E\Psi = H\Psi \tag{2}$$

now the Left Hand Side (LHS) of equation (2) is

$$E\Psi = \iota\hbar\frac{\partial\Psi}{\partial t}$$

Also, the Right Hand Side (RHS) of equation (2) is

$$H\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi$$

then equation (2) becomes

$$\iota\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi \tag{3}$$

where Ψ is defined as the wave function over time and space as $\Psi(x,t)$, hence we have

$$\iota\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x,t)\Psi(x,t) \tag{4}$$

under Initial Condition,

$$x \in \left[a,b\right], \qquad t \in \left[0,T\right]$$

$$\Psi(x,0) = \beta(x),$$

and the Boundary Conditions,

$$\Psi(a,t) = \alpha_0(a),$$
$$\Psi(b,t) = \alpha_1(b)$$

Equation (4) is the fundamental formula for quantum mechanics, which studies matter in terms of the wave-like characteristics of particles in a field sometimes called the One Dimensional/Time-Dependent Schrodinger Equation.

2.2 Derivation of Modified Crank Nicolson Method for Time - Dependent Schrodinger Equation through Finite Difference Approximation

In the atomic unit ($\hbar = m = e = a_0 = 1$), Hartree, (1928).

Hence equation (4) becomes

$$\iota \frac{\partial}{\partial t}\Psi(x,t) = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x,t)\Psi(x,t) \tag{5}$$

here $x = ih, \quad y = jk$ is denoted by (i,j)

then equation (5) becomes

$$\iota \frac{\partial}{\partial t}\Psi_i^j = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\Psi_i^j + V_i^j\Psi_i^j \tag{6}$$

From the grid point,

Forward Difference	Backward difference
$U_x = \frac{U_{i+1}^j - U_i^j}{\Delta x}$	$U_x = \frac{U_i^j - U_{i-1}^j}{\Delta x}$
$U_y = \frac{U_i^{j+1} - U_i^j}{\Delta y}$	$U_y = \frac{U_i^j - U_i^{j-1}}{\Delta y}$

$$U_{xx} = \frac{U_{i-1}^j - 2U_i^j + U_{i+1}^j}{\Delta x^2}$$

$$U_{yy} = \frac{U_i^{j+1} - 2U_i^j + U_i^{j-1}}{\Delta y^2}$$

From equation (6), let $\frac{\partial}{\partial t}\Psi_i^j = \frac{\partial^2}{\partial x^2}\Psi_i^j$

By the explicit method

$$\frac{\Psi_i^{j+\frac{1}{2}} - \Psi_i^j}{\frac{\Delta t}{2}} = \frac{\Psi_{i-1}^j - 2\Psi_i^j + \Psi_{i+1}^j}{\Delta x^2}$$

Also using the implicit method

$$\frac{\Psi_i^{j+1} - \Psi_i^{j+\frac{1}{2}}}{\frac{\Delta t}{2}} = \frac{\Psi_{i-1}^j - 2\Psi_i^j + \Psi_{i+1}^j}{\Delta x^2}$$

adding the implicit and explicit, we obtain

$$\frac{\Psi_i^{j+1} - \Psi_i^j}{\Delta t} = \frac{1}{2}\left[\frac{\Psi_{i-1}^j - 2\Psi_i^j + \Psi_{i+1}^j}{\Delta x^2} + \frac{\Psi_{i-1}^{j+1} - 2\Psi_i^{j+1} + \Psi_{i+1}^{j+1}}{\Delta x^2}\right] \tag{7}$$

substituting (7) into (6) after simplification, we obtained

$$\iota\left[4\Psi_i^{j+1} - 4\Psi_i^j\right] = -\frac{\Delta t}{\Delta x^2}\left[\Psi_{i-1}^j - 2\Psi_i^j + \Psi_{i+1}^j + \Psi_{i-1}^{j+1} - 2\Psi_i^{j+1} + \Psi_{i+1}^{j+1}\right] + V_i^j\Psi_i^j \tag{8}$$

Let $\frac{\Delta t}{\Delta x^2} = \lambda$, hence the RHS of (8) becomes

$$\iota\left[4\Psi_i^{j+1} - 4\Psi_i^j\right] = -\lambda\Psi_{i-1}^j + 2\lambda\Psi_i^j - \lambda\Psi_{i+1}^j - \lambda\Psi_{i-1}^{j+1} + 2\lambda\Psi_i^{j+1} - \lambda\Psi_{i+1}^{j+1} + V_i^j\Psi_i^j \tag{9}$$

By simplification and collecting like terms gives

$$\lambda\Psi_{i-1}^{j+1}+(4\iota-2\lambda)\Psi_{i}^{j+1}+\lambda\Psi_{i+1}^{j+1}=-\lambda\Psi_{i-1}^{j}+(4\iota+2\lambda)\Psi_{i}^{j}-\lambda\Psi_{i+1}^{j}+V_{i}^{j}\Psi_{i}^{j} \quad (10)$$

This equation (10) is called the Modified Crank-Nicolson method (MCNM) for the solution of the Schrödinger equation.

We are require to compute the values of Ψ_i^{j+1}, which represents the wave function at spatial grid point i and time step $j+1$ in Equation (10) containing initial and boundary conditions attached depending on the specific problem to be solved, which helps to give information about wave function at the boundaries of the system at the initial time step. Specifically, equation (10) becomes

$$\Psi_{i}^{j+1}=\frac{1}{(4\iota-2\lambda)}\Big[(4\iota+2\lambda)\Psi_{i}^{j}-\lambda\ \ \Psi_{i-1}^{j+1}+\Psi_{i+1}^{j+1}+\Psi_{i-1}^{j}+\Psi_{i+1}^{j}\ \Big]+V_{i}^{j}\Psi_{i}^{j} \quad (11)$$

under the following initial and boundary conditions:

initial condition:

$$\Psi_1^0=\beta(x_i), \qquad i=1,2,3,4,5,6\ldots,N$$

boundary conditions:

$$\Psi_1^j=T_1(t_j)$$
$$\Psi_N^j=T_2(t_j), \qquad j=0,1,2,3,4,5,6\ldots,M$$

From equation (10) above it can be seen that the potential energy in the Schrödinger equation has been accounted for. Now let look at the case when there is no potential energy in the Schrodinger equation's modified Crank-Nicolson difference method which means that the particle involved is not subject to any external forces or interactions within the system.

It is important to note that in practical system, complete absence of potential energy is rare. However, this simplified scenario is often used in theoretical discussions to understand the behaviour of free particles, Choy et.al (2014) Consider a particle moving freely in empty space, far away from any external influences such as gravitational or electromagnetic field. In this scenario the particle is not subject to any potential energy, as there are no forces acting on it. Even though there is no potential energy, the particle can still possess kinetic energy if it has a non-zero velocity. For example, let's consider a free electron moving through space. The electron has mass and a non-zero velocity, which means it will have kinetic energy. From equation (10), we obtain

$$-\lambda\Psi_{i-1}^{j+1}+(4\iota+2\lambda)\Psi_{i}^{j+1}-\lambda\Psi_{i+1}^{j+1}=\lambda\Psi_{i-1}^{j}+(4\iota-2\lambda)\Psi_{i}^{j}+\lambda\Psi_{i+1}^{j} \quad (12)$$

Equation (12) above is called the Modified Crank-Nicolson Difference Method for the Schrodinger equation with zero potential energy.

2.3 Transformation of Modified Crank-Nicolson Method with Zero Potential Energy into Matrix Form

In general, the LHS of (12) contains three unknowns and three known values of Ψ for every value of j are also contained in the RHS of (12).

Given that $j=1,2,3,\ldots,N$ has N mesh points, (12) provides $N-1$ simultaneous equations for the $N-1$ unknown values at each time level.

$N-1$ for each j that is $0,1,\ldots,M,$

$$\begin{array}{ll}
i=1: & -\lambda\Psi_0^1+(4\iota+2\lambda)\Psi_1^1-\lambda\Psi_2^1=\lambda\Psi_0^0+(4\iota-2\lambda)\Psi_1^0+\lambda\Psi_2^0\\
i=2: & -\lambda\Psi_1^1+(4\iota+2\lambda)\Psi_2^1-\lambda\Psi_3^1=\lambda\Psi_1^0+(4\iota-2\lambda)\Psi_2^0+\lambda\Psi_3^0\\
i=3: & -\lambda\Psi_2^1+(4\iota+2\lambda)\Psi_3^1-\lambda\Psi_4^1=\lambda\Psi_2^0+(4\iota-2\lambda)\Psi_3^0+\lambda\Psi_4^0\\
i=4: & -\lambda\Psi_3^1+(4\iota+2\lambda)\Psi_4^1-\lambda\Psi_5^1=\lambda\Psi_3^0+(4\iota-2\lambda)\Psi_4^0+\lambda\Psi_5^0\\
i=5: & -\lambda\Psi_4^1+(4\iota+2\lambda)\Psi_5^1-\lambda\Psi_6^1=\lambda\Psi_4^0+(4\iota-2\lambda)\Psi_5^0+\lambda\Psi_6^0\\
\vdots & \qquad\qquad\vdots\qquad\qquad\qquad\qquad\vdots\\
i=N-1: & -\lambda\Psi_{N-2}^1+(4\iota+2\lambda)\Psi_{N-1}^1-\lambda\Psi_N^1=\lambda\Psi_{N-2}^0+(4\iota-2\lambda)\Psi_{N-1}^0+\lambda\Psi_N^0
\end{array} \tag{13}$$

The above system of equation in (13) can be written in matrix form

$$\begin{pmatrix}
(4\iota+2\lambda) & -\lambda & 0 & 0 & \dots & 0\\
\lambda & (4\iota+2\lambda) & -\lambda & 0 & \dots & 0\\
0 & \lambda & (4\iota+2\lambda) & -\lambda & \dots & 0\\
0 & 0 & \lambda & (4\iota+2\lambda) & -\lambda & 0\\
\vdots & \vdots & \vdots & \ddots & \ddots & \ddots\\
0 & 0 & 0 & 0 & -\lambda & (4\iota+2\lambda)
\end{pmatrix}
\begin{pmatrix}
\Psi_1^{j+1}\\ \Psi_2^{j+1}\\ \vdots\\ \vdots\\ \Psi_{N-2}^{j+1}\\ \Psi_{N-1}^{j+1}
\end{pmatrix}=$$

$$\begin{pmatrix}
(4\iota-2\lambda) & \lambda & 0 & 0 & \dots & 0\\
\lambda & (4\iota-2\lambda) & \lambda & 0 & \dots & 0\\
0 & \lambda & (4\iota-2\lambda) & \lambda & \dots & 0\\
0 & 0 & \lambda & (4\iota-2\lambda) & \lambda & 0\\
\vdots & \vdots & \vdots & \ddots & \ddots & \ddots\\
0 & 0 & 0 & 0 & \lambda & (4\iota-2\lambda)
\end{pmatrix}
\begin{pmatrix}
\Psi_1^{j}\\ \Psi_2^{j}\\ \vdots\\ \vdots\\ \Psi_{N-2}^{j}\\ \Psi_{N-1}^{j}
\end{pmatrix}+
\begin{pmatrix}
\lambda\Psi_0^j+\lambda\Psi_0^{j+1}\\ 0\\ \vdots\\ \vdots\\ 0\\ \lambda\Psi_N^j+\lambda\Psi_N^{j+1}
\end{pmatrix}. \tag{14}$$

Equation (14) can be written as

$$A\Psi_{j+1}=B\Psi_j+C_j, \tag{15}$$

where,

$$A=\begin{pmatrix}
(4\iota+2\lambda) & -\lambda & 0 & 0 & \dots & 0\\
-\lambda & (4\iota+2\lambda) & -\lambda & 0 & \dots & 0\\
0 & \lambda & (4\iota+2\lambda) & -\lambda & \dots & 0\\
0 & 0 & -\lambda & (4\iota+2\lambda) & -\lambda & 0\\
\vdots & \vdots & \vdots & \ddots & \ddots & \ddots\\
0 & 0 & 0 & 0 & -\lambda & (4\iota+2\lambda)
\end{pmatrix},$$

$$B=\begin{pmatrix}
(4\iota-2\lambda) & \lambda & 0 & 0 & \dots & 0\\
\lambda & (4\iota-2\lambda) & \lambda & 0 & \dots & 0\\
0 & \lambda & (4\iota-2\lambda) & \lambda & \dots & 0\\
0 & 0 & \lambda & (4\iota-2\lambda) & \lambda & 0\\
\vdots & \vdots & \vdots & \ddots & \ddots & \ddots\\
0 & 0 & 0 & 0 & \lambda & (4\iota-2\lambda)
\end{pmatrix},$$

$$C_j = \begin{pmatrix} \lambda\Psi_0^j + \lambda\Psi_0^{j+1} \\ 0 \\ \vdots \\ \vdots \\ 0 \\ \lambda\Psi_N^j + \lambda\Psi_N^{j+1} \end{pmatrix}, \quad where \quad \Psi_{j+1} = \begin{pmatrix} \Psi_1^{j+1} \\ \Psi_2^{j+1} \\ \vdots \\ \vdots \\ \Psi_{N-2}^{j+1} \\ \Psi_{N-1}^{j+1} \end{pmatrix}, \qquad \Psi_j = \begin{pmatrix} \Psi_1^j \\ \Psi_2^j \\ \vdots \\ \vdots \\ \Psi_{N-2}^j \\ \Psi_{N-1}^j \end{pmatrix}$$

hence, we can obtain solution for Ψ_{j+1} from equation (15)

$$\Psi_{j+1} = A^{-1}B\Psi_j + A^{-1}C_j \tag{16}$$

To obtain the required solution, where $T = M\Delta t$, evaluation for $j = 1,2,3,\ldots,M$ can also be made.

3. Numerical Results and Discussion

Three different problems were used to ascertain the efficiency of the method. Using a variety of three test problems, the method's accuracy and applicability were evaluated. To assess their accuracy, the derived numerical results were compared with the exact solution. MATLAB R2021 software was employed for the numerical simulations. Consider the Schrödinger equation in:

Problem 1:

$$\iota\frac{\partial}{\partial t}\Psi(x,t) = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x,t)\Psi(x,t)$$

with boundary and initial conditions set as:

$$\Psi(x,0) = 0$$

$$\Psi(0,t) = 0$$

$$\Psi(3,t) = 0$$

$$V(x,t)\Psi(x,t) = \sin(V) + \cos(\Psi(x,t)) + e^{2V}$$

at $\Delta t = 0.01, \quad \Delta x = 0.1118$

substituting the conditions and data given into equation (11),

Given that the initial condition $\Psi(x,0) = 0$, we know that the first row $(j = 0)$ will be all zeros and the first column should also be all zeros based on the given boundary condition $\Psi(0,t) = 0$ and $\lambda = 0.8$, the numerical solution is represented below on a table.

Table 1: Numerical results for Problem 1 at $\Delta t = 0.01, \quad \Delta x = 0.1118$ using Matlab2021

j/*i*	0	1	2	3
Ψ_1^{j+1}	0	0	0	0
Ψ_2^{j+1}	0	$2.0000-0.0000\iota$	$2.0321-1.3793\iota$	$0.5802-0.7345\iota$
Ψ_3^{j+1}	0	$2.1379+0.3448\iota$	$2.7324-0.9213\iota$	$1.5527-1.8263\iota$
Ψ_4^{j+1}	0	$2.0880+0.3924\iota$	$2.6849-0.7058i\iota$	$2.0962-1.4757\iota$
Ψ_5^{j+1}	0	$2.0763+0.3871\iota$	$2.6327-0.6975\iota$	$2.0367-1.2788\iota$
Ψ_6^{j+1}	0	$2.0765+0.3847\iota$	$2.6266-0.7079\iota$	$1.9790-1.2767\iota$

Ψ_7^{j+1}	0	$2.0769+0.3845\imath$	$2.6282-0.7100\imath$	$1.9733-1.2907\imath$
Ψ_8^{j+1}	0	$2.0769+0.3846\imath$	$2.6287-0.7098\imath$	$1.9761-1.2933\imath$
Ψ_9^{j+1}	0	$2.0769+0.3846\imath$	$2.6287-0.7097\imath$	$1.9769-1.2928\imath$
Ψ_{10}^{j+1}	0	$2.0769+0.3846\imath$	$2.6287-0.7097\imath$	$1.9769-1.2926\imath$
Ψ_{11}^{j+1}	0	$2.0769+0.3846\imath$	$2.6287-0.7097\imath$	$1.9769-1.2926\imath$
Ψ_{12}^{j+1}	0	$2.0769+0.3846\imath$	$2.6287-0.7097\imath$	$1.9769-1.2926\imath$
Ψ_{13}^{j+1}	0	0	0	0

Problem 2

$$\imath \frac{\partial}{\partial t}\Psi(x,t) = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x,t)\Psi(x,t)$$

with boundary and initial conditions set as:

$$\Psi(x,0) = 0$$

$$\Psi(0,t) = 0$$

$$\Psi(5,t) = 0$$

$$V(x,t)\Psi(x,t) = \sin(V)$$

at $M = 5, \Delta t = 0.1, \Delta x = \sqrt{0.2}$

substituting the conditions and data given into equation (11), we have the following numerical solution.

Table 2: Numerical results for Problem 2 at $\Delta t = 0.1, \Delta x = \sqrt{0.2}$ using Matlab2021

j/i	0	1	2	3	4	5
Ψ_1^{j+1}	0	0	0	0	0	0
Ψ_2^{j+1}	0	0.0100	$0.0188 - 0.0047\iota$	$0.0244 - 0.0130\iota$	$0.0254 - 0.0230\iota$	$0.0216 - 0.0322\iota$
Ψ_3^{j+1}	0	$0.0103 + 0.0012i$	$0.0210 - 0.0006\iota$	$0.0317 - 0.0058\iota$	$0.0409 - 0.0152\iota$	$0.0468 - 0.0288\iota$
Ψ_4^{j+1}	0	$0.0102 + 0.0012i$	$0.0204 + 0.0000\iota$	$0.0303 - 0.0036\iota$	$0.0397 - 0.0095\iota$	$0.0483 - 0.0180\iota$
Ψ_5^{j+1}	0	$0.0102 + 0.0012i$	$0.0203 - 0.0001\iota$	$0.0298 - 0.0037\iota$	$0.0381 - 0.0095\iota$	$0.0450 - 0.0167\iota$
Ψ_6^{j+1}	0	$0.0102 + 0.0012i$	$0.0203 - 0.0001\iota$	$0.0298 - 0.0038\iota$	$0.0380 - 0.0098\iota$	$0.0445 - 0.0175\iota$
Ψ_7^{j+1}	0	$0.0102 + 0.0012i$	$0.0203 - 0.0001\iota$	$0.0298 - 0.0038\iota$	$0.0381 - 0.0098\iota$	$0.0446 - 0.0177\iota$
Ψ_8^{j+1}	0	$0.0102 + 0.0012i$	$0.0203 - 0.0001\iota$	$0.0298 - 0.0038\iota$	$0.0381 - 0.0098\iota$	$0.0447 - 0.0177\iota$
Ψ_9^{j+1}	0	$0.0102 + 0.0012i$	$0.0203 - 0.0001\iota$	$0.0298 - 0.0038\iota$	$0.0381 - 0.0098\iota$	$0.0447 - 0.0177\iota$
Ψ_{10}^{j+1}	0	$0.0102 + 0.0012i$	$0.0203 - 0.0001\iota$	$0.0298 - 0.0038\iota$	$0.0381 - 0.0098\iota$	$0.0447 - 0.0177\iota$
Ψ_{11}^{j+1}	0	0	0	0	0	0

Remark: The modified Crank-Nicolson method is the numerical technique used to solve problem 1 and 2. It updates the values of Ψ_i^{j+1} iteratively based on the given equation that considers neighbouring values of Ψ , V , and the parameter λ . The method calculates λ using the provided values of Δt and Δx . The equation is applied for a specified number of time steps, progressively updating the values of Ψ_i^{j+1} . As the iterations progress, the computed values of Ψ_i^{j+1} in the table gradually approach a steady state, representing a solution to the problem at hand.

Problem 3

$$\iota \frac{\partial \Psi}{\partial t} = -\frac{1}{2}\frac{\partial^2 \Psi}{\partial x^2}$$

with initial and boundary conditions as:

$$\Psi(0,t) = 0$$

$$\Psi(1,t) = 0$$

$$\Psi(x,0) = \sin \pi x$$

the analytical solution is $\Psi(x,t) = \sin \pi x$

at $\Delta t = 0.01, \Delta x = 0.1$ $: [0-10]$

substituting the conditions and data given into equation (12), gives

$$\lambda \Psi_{i-1}^{j+1} + (4\iota - 2\lambda)\Psi_i^{j+1} + \lambda \Psi_{i+1}^{j+1} = -\lambda \Psi_{i-1}^{j} + (4\iota + 2\lambda)\Psi_i^{j} - \lambda \Psi_{i+1}^{j}$$

$$\text{where } \lambda = \frac{\Delta t}{\Delta x^2}$$

Table 3: Numerical results for Problem 3 at $\Delta x = 0.1, \Delta t = 0.01$ using Matlab2021

		$j = 1$	$j = 2$	
	t	0.01	0.02	*exact solution*
$i = 0$	$x = 0$	$0.0585 - 0.1205\iota$	$0.1742 - 0.1467\iota$	0.0000
$i = 1$	$x = 0.1$	$0.2901 - 0.0073\iota$	$0.2798 - 0.0641\iota$	0.3090
$i = 2$	$x = 0.2$	$0.5810 + 0.0304\iota$	$0.5534 + 0.0531\iota$	0.5878
$i = 3$	$x = 0.3$	$0.8078 + 0.0409\iota$	$0.8002 + 0.0868\iota$	0.8090
$i = 4$	$x = 0.4$	$0.9502 + 0.0467\iota$	$0.9479 + 0.0949\iota$	0.9511
$i = 5$	$x = 0.5$	$0.9989 + 0.0488\iota$	$0.9965 + 0.0975\iota$	1.0000
$i = 6$	$x = 0.6$	$0.9502 + 0.0467\iota$	$0.9479 + 0.0949\iota$	0.9511
$i = 7$	$x = 0.7$	$0.8078 + 0.0409\iota$	$0.8002 + 0.0868\iota$	0.8090
$i = 8$	$x = 0.8$	$0.5810 + 0.0304\iota$	$0.5534 + 0.0531\iota$	0.5878
$i = 9$	$x = 0.9$	$0.2901 - 0.0073\iota$	$0.2798 - 0.0641\iota$	0.3090
$i = 10$	$x = 1$	$0.0585 - 0.1205\iota$	$0.1742 - 0.1467\iota$	0.0000

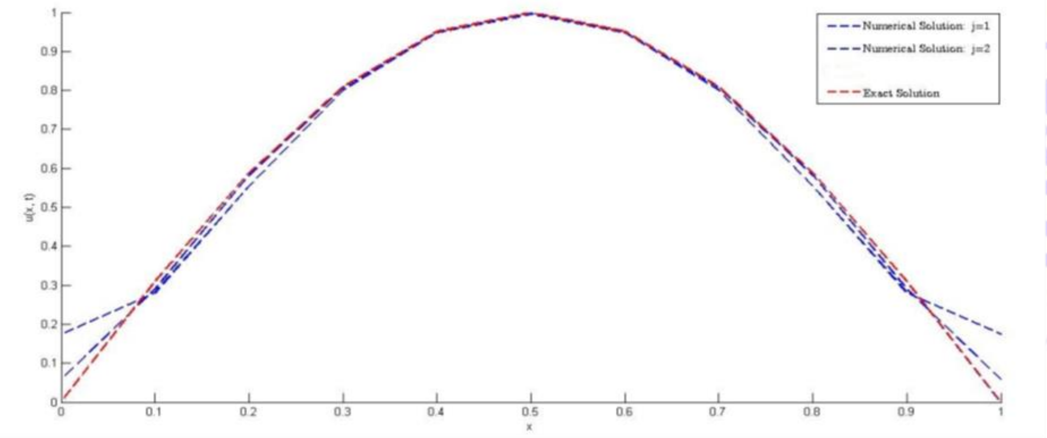

Figure 1: Numerical solution against exact solution

4. Discussion of Results

The numerical solution (blue lines) and the exact solution (red dashed line) represent the estimated and ideal behaviours, respectively, of the partial differential equation in problem 3 above. The comparison of the numerical and exact solutions reveals similarities and differences in their behaviour, indicating the accuracy of the numerical approach. The error value calculated using the max(abs(UN) - Uexact)) which is 1.9058. The provided error calculation assumes the existence of variables UN and Uexact which represent the numerical solution and exact solution, respectively. The performance of the method was assessed by presenting the numerical solutions for different points within the interval, and the results are summarized in Table 3 above. The error analysis quantifies the discrepancies between the two solutions, with lower errors indicating higher accuracy. Overall, numerical methods enable the practical approximation of solutions for challenging PDEs in real-world scenarios.

5. Conclusion

This study examined the accuracy and efficiency of the modified Crank-Nicolson method for solving the time-dependent Schrödinger equation, with and without potential energy. From problem 1 and 2, the modified Crank-Nicolson method is used to solve the given Schrodinger equations. It updates variable values iteratively by considering neighbouring values and a parameter. The method utilizes initial conditions to calculate values and applies the equation for a specified number of time steps until a steady state is achieved. It is known for its accuracy, stability, and applicability in physics, engineering, and computational modelling for solving partial differential equations. Comparing the numerical and exact solutions in problem 3 reveals similarities and differences, showcasing the accuracy of the numerical approach. Error analysis quantifies discrepancies, with lower values indicating higher accuracy. Numerical simulations using MATLAB software were compared to exact solutions. The method demonstrated accuracy, convergence, and computational requirements, addressing computational challenges and preserving the equation's physical meaning of the time-dependent Schrödinger equation unlike the ones in previous literatures. It is recommended to use the modified Crank-Nicolson method for solving the time-dependent Schrödinger equation.

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