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Stability of Finite Difference Solution of Time-Dependent Schrodinger Equations

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Author's contribution

The sole author designed, analyzed, interpreted and prepared the manuscript.

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Abstract

In this paper, the stability of finite difference methods for time-dependent Schrodinger equation with Dirichlet boundary conditions on a staggered mesh was considered with explicit and implicit discretization. Using the matrix representation for the numerical algorithm, it is shown that for the explicit finite difference method, the solution is conditionally stable while it becomes unconditionally stable for implicit finite difference methods. A 1D Harmonic Oscillator problem shall be used to illustrate this behaviour.

Keywords: Schrodinger equation; finite difference; discretization; dirichlet boundary conditions; crank-nicolson.

1 Introduction

The stability of a differential equation refers to the behaviour of its solutions under small perturbations or changes in the initial conditions. In other words, it describes how sensitive the solution of a differential equation is to changes in the initial conditions or parameters. A differential equation is said to be stable if small perturbations in the initial conditions or parameters lead to correspondingly small changes in the solution over

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time. On the other hand, if small perturbations in the initial conditions or parameters lead to large changes in the solution over time, the differential equation is said to be unstable. The stability of a differential equation is important because it determines the long-term behaviour of its solutions. In particular, a stable differential equation will have solutions that approach a steady-state or equilibrium solution over time, while an unstable differential equation will have solutions that diverge or oscillate indefinitely [1].

The study of stability in differential equations is a fundamental and ongoing area of research in mathematics and applied sciences, with numerous applications and it provides a framework for analyzing the behaviour of dynamical systems and predicting their long-term behaviour. There are many different concepts and techniques that have been developed to analyze the stability of differential equations, depending on the specific properties of the equations and the types of solutions of interest.

1.1 The schrodinger equation

The Schrodinger equation, often called the Schrodinger wave equation is a fundamental equation in quantum mechanics that describes the time evolution of a quantum state [2], which is represented by a wave function. It was developed by the Austrian Physicist Erwin Schrodinger [3] and it is the fundamental equation of Physics for describing quantum mechanical behaviour. In pure mathematics, the Schrodinger equation and its variants are one of the fundamental equations studied in the field of partial differential equations, and has many important applications in geometry, spectral and scattering theory, and integral systems [4]; and quantum mechanics, including the calculation of energy levels and transition probabilities of atoms and molecules, the description of quantum tunnelling and scattering, and the study of the behaviour of condensed matter systems.

The Schrödinger equation is a probabilistic equation, meaning that it gives the probability distribution of the location of a particle in space at any given time. The wave function itself is a complex-valued function that encodes the amplitude and phase of the particle's probability wave. The absolute square of the wave function gives the probability density of finding the particle at a given location.

There are basically two variants of Schrodinger's equation – time-dependent Schrodinger equation (TDSE) and time-independent Schrodinger equation respectively:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V(x)\Psi=i\hbar\frac{\partial\Psi}{\partial t},\ \ 0\le x\le L,\ \ t\ge 0 \tag{1}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x),\ \ 0\le x\le L \tag{2}$$

Where $\hbar = 6.6260693\times10^{-34}\ m^2$ kg / s (reduced Planck constant), $m =$ mass of particle and $V(x) =$ potential energy of particle.

1.2 Finite difference method

The finite difference method is a numerical technique for solving differential equations by approximating their derivatives using finite differences. It involves discretizing the domain of the differential equation into a grid of points and approximating the derivatives of the solution at each point using the values of the solution at neighbouring points [5]. The basic idea of the finite difference method is to approximate the derivatives of the solution using finite difference quotients, which involve differences of the solution values at nearby points. It is based on subdividing the domain of the problem by introducing a mesh of discrete points for each of the independent variables. The resulting system of algebraic equations is then solved by appropriate method.

Finite difference is powerful and one of the most widespread numerical techniques for solving PDE particularly in situations where analytical solutions are difficult or impossible to obtain. It is however important to emphasize that high-order finite difference methods have good properties for solving wave problems efficiently. Nevertheless, for time-dependent wave dominated problems that include boundary conditions, it has historically been challenging to construct stable discretizations with these types of methods [6].

Finite difference method has applications in many fields, including physics, engineering, finance, and biology.

1.3 Discretization of finite differences

We shall assume a hypothetical case of finite domain with a time coordinate $\boldsymbol{t}$, and a spatial coordinate $\boldsymbol{x}$. Thus, a function is only defined for the values of $\boldsymbol{x}$ and t that corresponds to points in the mesh such that for a given continuous function ψ, there are available values of it at (t_i, x_j), denoted by $\psi_{i,j}$. So, for uniformly discretised domain, we have:

$$\Delta x = x_{j+1} - x_j \quad \& \quad \Delta t = t_{i+1} - t_i \tag{3}$$

Constructing the difference operators for the derivatives $\psi_{i,j}$, we have:

- Forward and backward difference respectively as:

$$\psi'(x_j) = \frac{u(x_{j+1}) - u(x_j)}{\Delta x} + 0(\Delta x) \;\; \& \;\; \psi'(x_j) = \frac{u(x_j) - u(x_{j-1})}{\Delta x} + 0(\Delta x) \tag{4}$$

- Centre finite difference approximation:

$$\psi'(x_j) = \frac{u(x_{j+1}) - u(x_{j-1})}{2\Delta x} + 0(\Delta x) \tag{5}$$

2 The Quantum Harmonic Oscillator Problem

The quantum harmonic oscillator problem is a fundamental problem in quantum mechanics that describes the behaviour of a particle in a harmonic oscillator potential. It is a model system that is used to understand the quantum mechanical properties of a wide range of physical systems, including atoms, molecules, and solids. The quantum harmonic oscillator problem is of great importance in quantum mechanics, as it provides a simple model for understanding the behaviour of many physical systems. The problem has many applications in chemistry, physics, and engineering, including the study of molecular vibrations, the behaviour of electrons in solids, and the properties of lasers and other optical devices.

The quantum harmonic oscillator is one of the foundational problems in quantum mechanics and can be applied in the understanding of complex modes of vibration in larger molecules, the theory of heat capacity, the motion of atoms in a solid lattice, etc. [7].

In this example, the time-dependent Schrodinger equation gives us the understanding on how the initial information about the particle in the quantum harmonic system behaves and changes over time. The one-dimensional (ID) Schrodinger wave equation for the Harmonic Oscillator can be put in the following form:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}; \;\; t > 0, \;\; 0 < x < L \tag{6}$$

Subject to the following conditions:

$$\psi(0,t) = \psi(L,t) = 0 \;\; \text{and} \;\; \psi(x,0) = \sqrt{2}\, sin(\pi x)$$

- The equation (6) describes the particle x, in a quantum harmonic oscillator motion with mass, m in the interval $0 < x < L$ and $t > 0$ under the influence of the potential,

$$V(x) = \frac{1}{2}m\omega^2x^2 = \frac{1}{2}kx^2$$

- Discretizing equation (6), by replacing the space derivative by the difference technique at j^{th} time step and the time derivative by a forward difference, gives a linear system of equations for the time given as:
-

$$\frac{i\hbar}{k}\left(\psi_{i,j+1} - \psi_{i,j}\right) = -\frac{\hbar^2}{2m}\frac{1}{h^2}\left(\psi_{i+1,j} - 2\psi_{i,j} + \psi_{i-1,j}\right) + \frac{1}{2}K{x_i}^2\psi_{i,j} \tag{7}$$

Where $V(x) = \frac{1}{2}Kx^2$ (K is a constant - the wave number) and we shall assume $\hbar = m = K = 1$, so that we have equation (8) as follows:

$$\frac{i}{k}\left(\psi_{i,j+1} - \psi_{i,j}\right) = -\frac{1}{2h^2}\left(\psi_{i+1,j} - 2\psi_{i,j} + \psi_{i-1,j}\right) + \frac{1}{2}x_i{}^2\psi_{i,j} \tag{8}$$

i.e.,

$$\left(\psi_{i,j+1} - \psi_{i,j}\right) = \frac{ik}{2h^2}\left(\psi_{i+1,j} - 2\psi_{i,j} + \psi_{i-1,j}\right) - \frac{i}{2}kx_i{}^2\psi_{i,j} \tag{9}$$

Where $0 < k < T$, and $\Delta t = k = t_j - t_{j-1}$ corresponding to the mesh points of T. While the mesh points of x is given as, $\Delta x = h = x_i - x_{i-1}$.

Thus, equation (9) can be re-written as:

$$\psi_{i,j+1} - \psi_{i,j} = \frac{ik}{2h^2}\left(\psi_{i+1,j} - 2\psi_{i,j} + \psi_{i-1,j}\right) - \frac{ik}{2}x_i{}^2\psi_{i,j}$$

Let $\boldsymbol{r = \frac{ik}{2h^2}}$, so that:

$$\begin{aligned}\psi_{i,j+1} &= r\psi_{i-1,j} - 2r\psi_{i,j} + r\psi_{i+1,j} - \frac{ik}{2}x_i{}^2\psi_{i,j} + \psi_{i,j}\\ &= r\psi_{i-1,j} + \left(1 - 2r - \frac{ik}{2}x_i{}^2\right)\psi_{i,j} + r\psi_{i+1,j}\\ &= r\psi_{i-1,j} + s\psi_{i,j} + r\psi_{i+1,j}\end{aligned} \tag{10}$$

where $s = 1 - 2r - \frac{ik}{2}x_i{}^2$.

The graphs below display the stability of the solution at various mesh intervals:

2.1 Crank-nicolson FD approximation for the ID harmonic oscillator

The Crank-Nicolson method provides an implicit scheme that is second-order accurate in both space and time [8]. Again, we consider the same time-dependent equation of equation (6), given below:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t};\quad 0 < x < L, t > 0$$

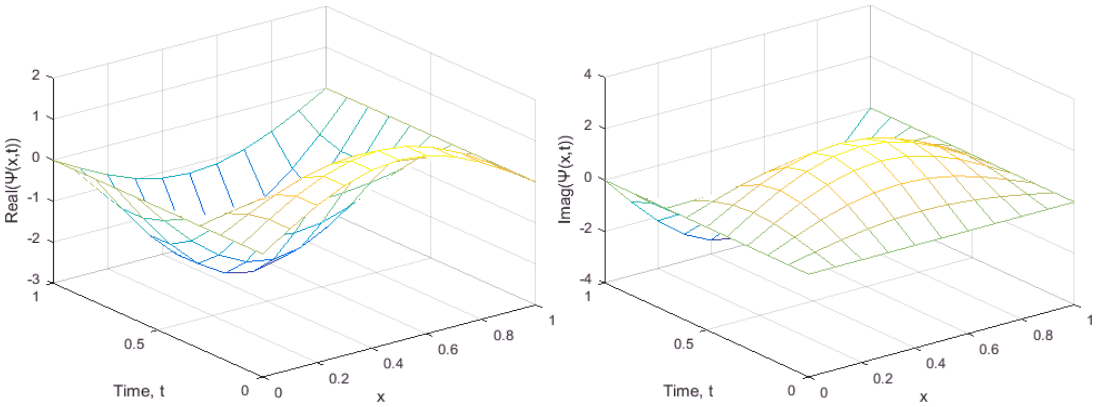

Fig. 1. Real and imaginary part of the central difference numerical solution to equation (6) with $x_0 = 0$, $x_n = 1.0$, $h = 0.1$ at $t_0 = 0$, $t_m = 1.0$, $k = 0.1$, where $m = n = 10$ & $r = 5.0$

Again, we assume, $m = \hbar = 1$, then we have:

$$-\frac{1}{2}\frac{\partial^2\psi(x,t)}{\partial x^2} + \frac{1}{2}kx^2\psi(x,t) = i\frac{\partial\psi(x,t)}{\partial t} \tag{11}$$

Where $V(x) = \frac{1}{2}Kx^2$. Also, taking $K = 1$, yields:

$$-\frac{1}{2}\frac{\partial^2\psi(x,t)}{\partial x^2} + \frac{1}{2}x^2\psi(x,t) = i\frac{\partial\psi(x,t)}{\partial t} \tag{12}$$

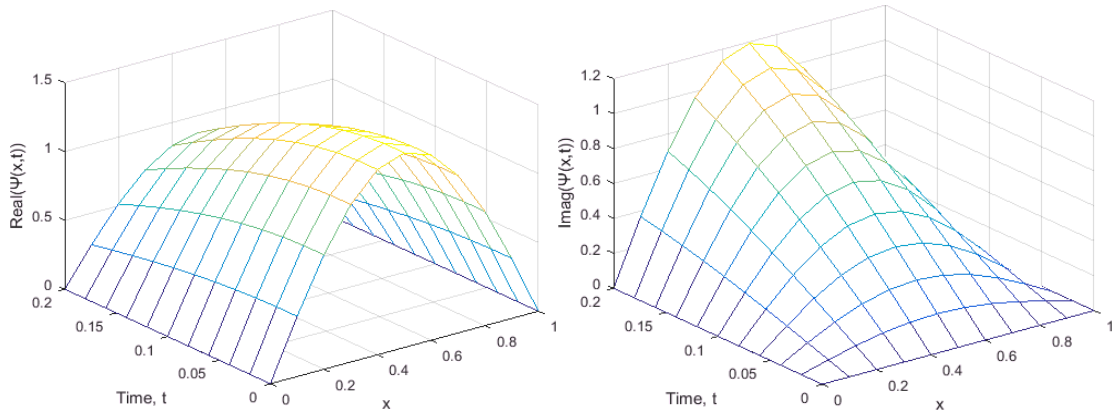

Fig. 2. Real and imaginary part of the central difference numerical solution to equation (3.55) with $x_0 = 0,\ x_n = 1.0,\ h = 0.1$ at $t_0 = 0,\ t_m = \frac{1.0}{5} = 0.2,\ k = 0.02$, where $m = n = 10$ & $r = 1.0$

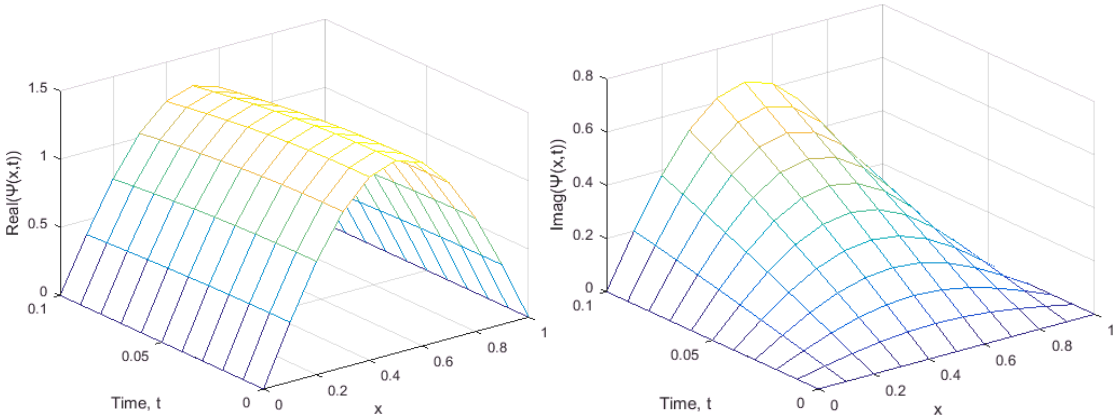

Fig. 3. Real and imaginary part of the central difference numerical solution to equation (6) with $x_0 = 0,\ x_n = 1.0,\ h = 0.1$ at $t_0 = 0,\ t_m = \frac{1.0}{10} = 0.1,\ k = 0.01$, where $m = n = 10$ & $r = 0.5$

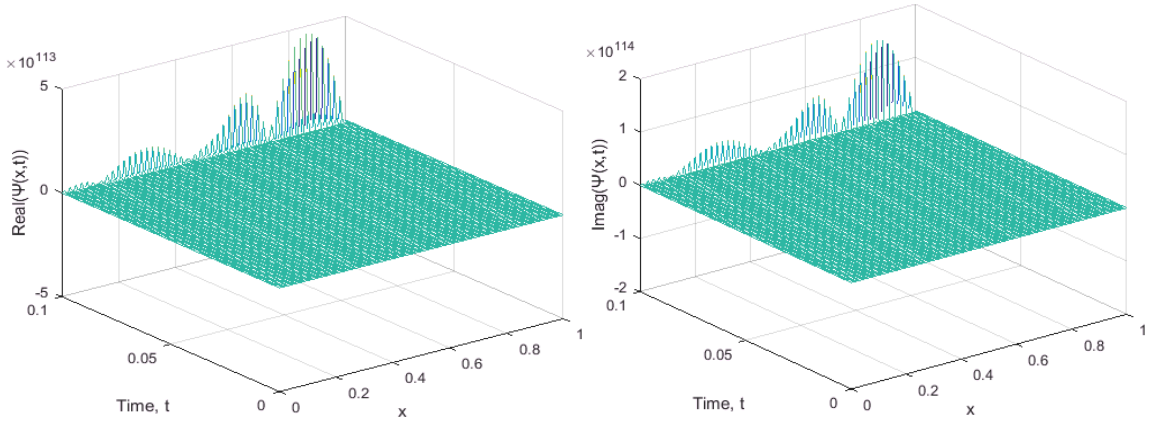

Fig. 4. Real and imaginary part of the central difference numerical solution to equation (6) with $x_0 = 0,\ x_n = 1.0,\ h = 0.01$ at $t_0 = 0,\ t_m = \frac{1.0}{10} = 0.1,\ k = 0.001$, where $m = n = 100$ & $r = 5.0$

From equation (12), using the average centred difference at the forward time step $j+1$, and the current time step j, with $\Delta t = k$, and $\Delta x = h$, gives:

$$\frac{i}{k}\left(\psi_{i,j+1} - \psi_{i,j}\right) = -\frac{1}{2}\left[\frac{1}{2h^2}\left(\left(\psi_{i+1,j} - 2\psi_{i,j} + \psi_{i-1,j}\right) + \left(\psi_{i+1,j+1} - 2\psi_{i,j+1} + \psi_{i-1,j+1}\right)\right) + {x_i}^2\psi_{i,j}\right] \quad (13)$$

i.e.,

$$i\left(\psi_{i,j+1} - \psi_{i,j}\right) = -\frac{k}{2*2h^2}\left(\psi_{i+1,j} - 2\psi_{i,j} + \psi_{i-1,j} + \psi_{i+1,j+1} - 2\psi_{i,j+1} + \psi_{i-1,j+1}\right) + \frac{k}{2}{x_i}^2\psi_{i,j} \quad (14)$$

Let $r = \frac{ik}{2h^2}$, so that:

$$\left(\psi_{i,j+1} - \psi_{i,j}\right) = \frac{r}{2}\left(\psi_{i+1,j} - 2\psi_{i,j} + \psi_{i-1,j} + \psi_{i+1,j+1} - 2\psi_{i,j+1} + \psi_{i-1,j+1}\right) - \frac{ik}{2}{x_i}^2\psi_{i,j} \quad (15)$$

i.e.,

$$-\frac{r}{2}\psi_{i-1,j+1} + (1+r)\psi_{i,j+1} - \frac{r}{2}\psi_{i+1,j+1} = \frac{r}{2}\psi_{i-1,j} + (1-r)\psi_{i,j} + \frac{r}{2}\psi_{i+1,j} - \frac{ik}{2}x_i \quad (16)$$

3 Order, Accuracy and Stability Analysis of Finite Difference Method

The truncation error and stability issues affect the choice of mesh staggering for most numerical methods and the finite difference method is not an exception.

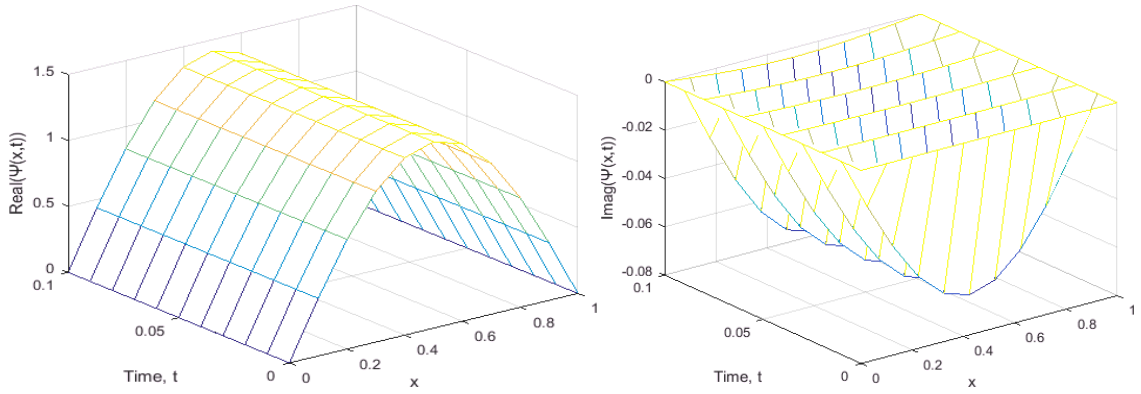

Fig. 5. Real and imaginary part of the Crank-Nicolson finite difference numerical solution of equation (16) with $\Delta x = h = 0.1$ at $t_0 = 0$, $t_m = 0.1$, $k = 0.01$ and $m = n = 10$; $r = 0.5$

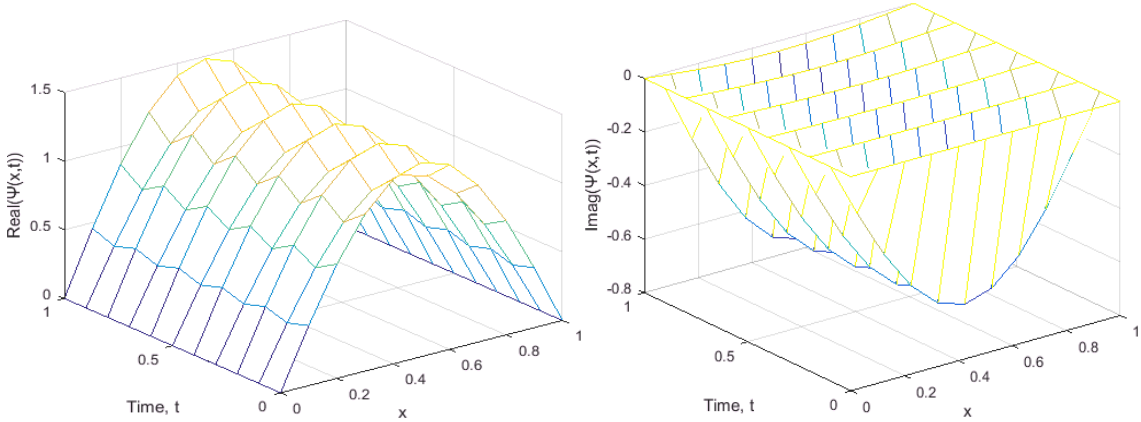

Fig. 6. Real and imaginary part of the Crank-Nicolson finite difference numerical solution of equation (16) with $\Delta x = h = 0.1$ at $t_0 = 0$, $t_m = 1.0$, $k = 0.1$ and $m = n = 10$; $r = 5.0$

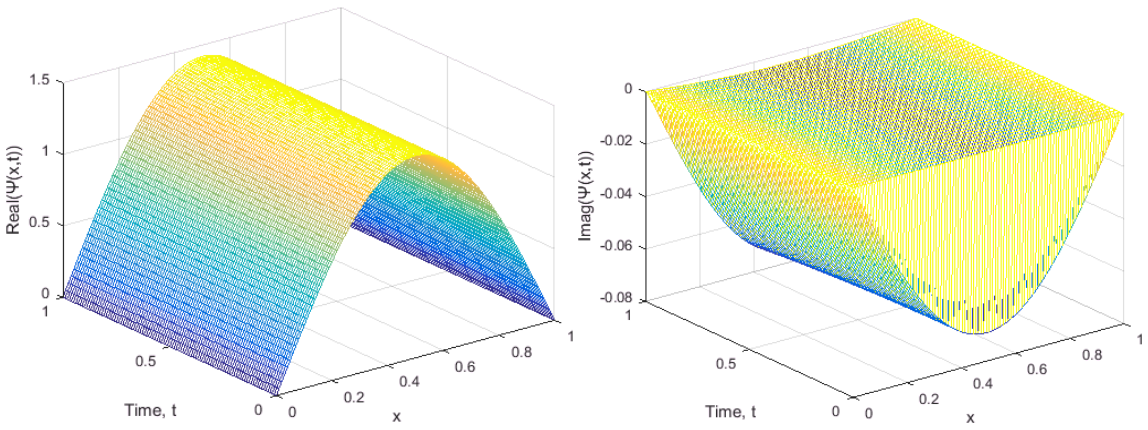

Fig. 7. Real and imaginary part of the Crank-Nicolson finite difference numerical solution of equation (16) with $\Delta x = h = 0.01$ at $t_0 = 0,\ t_m = 1.0,\ k = 0.01$ and $m = n = 100; r = 50$

3.1 Explicit method

Consider the finite difference solution for the one-dimensional Schrodinger equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}; \quad 0 < x < L,\ t > 0$$

Assuming, $m = \hbar = 1$, then we have:

$$-\frac{1}{2}\frac{\partial^2\psi(x,t)}{\partial x^2} + \frac{1}{2}x^2\psi(x,t) = i\frac{\partial\psi(x,t)}{\partial t}$$

or

$$-\frac{1}{2}\psi_{xx} + \frac{1}{2}x^2\psi = i\psi_t \tag{17}$$

Subject to the conditions:

$$\psi(x,0) = f(x), \text{ for } \quad 0 < x < L$$

$$\psi(0,t) = g_0(x),\ \psi(L,t) = g_1(x) \text{ for } \quad 0 < t < T$$

Discretizing, we have:

$$\psi_t = \frac{i}{k}\left(\psi_{i,j+1} - \psi_{i,j}\right) \tag{18}$$

and

$$-\frac{1}{2}\psi_{xx} = -\frac{1}{2h^2}\left(\psi_{i-1,j} - 2\psi_{i,j} + \psi_{i+1,j}\right) \tag{19}$$

where $k = \Delta t$, and $h = \Delta x$.

Combining, we have:

$$\frac{i}{k}\left(\psi_{i,j+1} - \psi_{i,j}\right) = -\frac{1}{2h^2}\left(\psi_{i-1,j} - 2\psi_{i,j} + \psi_{i+1,j}\right) + v_i\psi_{i,j+1} - \psi_{i,j} \tag{20}$$

or

$$\psi_{i,j+1} - \psi_{i,j} = \frac{ik}{2h^2}\left(\psi_{i-1,j} - 2\psi_{i,j} + \psi_{i+1,j}\right) - ikv_i \tag{21}$$

Equation (21) can be simplified by introducing the parameter, $r = \frac{ik}{2h^2}$ and solving for $\psi_{i,j+1}$, we have:

$$\psi_{i,j+1} = r\psi_{i+1,j} + (1-2r)\psi_{i,j} + r\psi_{i-1,j} - ikv_i \tag{22}$$

Note that the x and t meshes must be chosen so that $0 < \Re(r) \leq 0.5$ in order to ensure stability.

Thus, a numerical method is stable if errors that may be present at one stage of the computation do not grow as the process proceeds. In other words, the errors made at one stage of the computation do not cause increasingly large errors as the computations are continued, but rather will eventually damp out [8].

3.2 Implicit method

Consider again, the Schrodinger equation of equation (17):

$$-\tfrac{1}{2}\psi_{xx} + v(x)\psi = i\psi_t; \quad 0 < x < L,\ t > 0$$

Discretizing, we have:

$$\tfrac{i}{k}\left(\psi_{i,j+1} - \psi_{i,j}\right) = -\tfrac{1}{2h^2}\left(\psi_{i-1,j+1} - 2\psi_{i,j+1} + \psi_{i+1,j+1}\right) + v_i$$

which gives:

$$\begin{aligned}\psi_{i,j} &= -\tfrac{ik}{2h^2}\left(\psi_{i-1,j+1} - 2\psi_{i,j+1} + \psi_{i+1,j+1}\right) + \psi_{i,j+1} + ikv_i \\ &= -\tfrac{ik}{2h^2}\left(\psi_{i-1,j+1} - 2\psi_{i,j+1} + \psi_{i+1,j+1}\right) + \psi_{i,j+1} + ikv_i \\ &= -r\psi_{i-1,j+1} + (1+2r)\psi_{i,j+1} - r\psi_{i+1,j+1} + ikv_i\end{aligned} \tag{23}$$

3.3 Truncation error

These are measures of the error by which the analytical solution of a differential equation does not satisfy the difference equation at the grid points and are obtained by substituting the analytical solution of the continuous problem into the numerical scheme. A necessary condition for the convergence of the numerical solutions to the continuous solution is that the local truncation error tends to zero as the mesh size goes to zero. In this case the method is said to be consistent.

The explicit and implicit finite difference representation of the partial derivatives in the Schrodinger equation have the same order except that the second derivative for the implicit method is at step $j+1$ rather than at step j for the explicit method. Thus, we have:

$$\psi_t(x_i, t_j) = \tfrac{i}{k}\left(\psi_{i,j+1} - \psi_{i,j}\right) + 0(k) \tag{24}$$

and

$$\tfrac{1}{2}\psi_{xx}(x_i, t_j) = \tfrac{1}{2h^2}\left(\psi_{i-1,j} - 2\psi_{i,j} + \psi_{i+1,j}\right) + 0(h^2) \tag{25}$$

Substituting into the Schrodinger equation and simplifying, we have the truncation error, $E_{i,j}$ for the explicit method to be:

$$E_{i,j} = \alpha\psi_{xx}(x_i, t_j) - \beta\psi_t(x_i, t_j) = +0(k) + 0(h^2) \tag{26}$$

While, for the implicit scheme/method, the truncation error is given by:

$$E_{i,j+1} = \alpha\psi_{xx}(x_i, t_{j+1}) - \beta\psi_t(x_i, t_j) = +0(k) + 0(h^2) \tag{27}$$

It follows that the truncation error for the explicit method is the same as for the implicit method and it is given as $0(h^2 + k)$. However, for Crank-Nicolson method, the truncation error, $E_{i,j}$ is slightly less and is given by:

$$\frac{\psi_{i,j+1}-\psi_{i,j}}{2.\frac{k}{2}} = \frac{ck}{2(2h^2)}\left[\left(\psi_{i-1,j} - 2\psi_{i,j} + \psi_{i+1,j}\right) + \left(\psi_{i-1,j+1} - 2\psi_{i,j+1} + \psi_{i+1,j+1}\right)\right] + 0(k^2) + 0(h^2) \tag{28}$$

i.e.,

$$E_{i,j+1} = \alpha\psi_{xx}\left(x_i, t_{j+1}\right) - \beta\psi_t\left(x_i, t_j\right) = +0(k^2) + 0(h^2) \tag{29}$$

4 Stability Analysis

There are two primary considerations in choosing the mesh sizes, h and k, for a finite difference solution of a PDE. One issue is the effect of the mesh sizes on the order of the truncation error for the method, the other important issue is the stability of the method.

The primary difficulty with the explicit method is the stability condition, which requires that:

$$r = \frac{ck}{2h^2} \leq \frac{1}{2}$$

A numerical method is said to be stable if errors that may be present at one stage of the computation do not grow as the process proceeds. We consider the explicit form as given in equation (22):

$$\psi_{i,j+1} = r\psi_{i+1,j} + (1-2r)\psi_{i,j} + r\psi_{i-1,j} - ikv_i$$

Hence, expressing in matrix form, we have:

$$\begin{bmatrix} 1-2r & r & & & & \\ r & 1-2r & r & & & \\ & \ddots & \ddots & & & \\ & & \ddots & \ddots & & \\ & & & r & 1-2r & r \\ & & & & r & 1-2r \end{bmatrix} \begin{bmatrix} \psi(1,j) \\ \psi(2,j) \\ \vdots \\ \psi(i,j) \\ \vdots \\ \psi(n-1,j) \\ \psi(n,j) \end{bmatrix} = \begin{bmatrix} \psi(1,j+1) \\ \psi(2,j+1) \\ \vdots \\ \psi(i,j+1) \\ \vdots \\ \psi(n-1,j+1) \\ \psi(n,j+1) \end{bmatrix} \tag{30}$$

Observe that the matrix is tridiagonal and diagonally dominant. We shall use the Fourier method to check if the method is stable [9]. Assume that the numerical method admits a solution of the form:

$$\psi_{i,j} = a^j(\omega)e^{\mathbb{i}i\omega h} \tag{31}$$

where ω is the wave number and $\mathbb{i} = \sqrt{-1}$.

Define:

$$G(\omega) = \frac{a^{j+1}(\omega)}{a^j(\omega)}$$

where $G(\omega)$ is the growth factor [10]. The von Neumann stability condition is given by:

$$|G(\omega)| \leq 1; \quad \text{for} \quad 0 \leq \omega h \leq \pi,$$

where $h = \Delta x$.

It can be shown that the explicit method is stable if $\lambda \leq 1/2$, which implies conditional stability. Thus, substituting equation (31) into equation (22), we get:

$$a^{j+1}(\omega)e^{\mathbb{i}i\omega h} = ra^{j}(\omega)e^{\mathbb{i}(i+1)\omega h} + (1-2r)a^{j}(\omega)e^{\mathbb{i}i\omega h} + ra^{j}(\omega)e^{\mathbb{i}(i-1)\omega h} \tag{32}$$

i.e.,

$$a^{j+1}(\omega)e^{\mathbb{i}i\omega h} = a^{j}(\omega)\left[re^{\mathbb{i}(i+1)\omega h} + (1-2r)e^{\mathbb{i}i\omega h} + re^{\mathbb{i}(i-1)\omega h}\right] \tag{33}$$

or,

$$\frac{a^{j+1}(\omega)}{a^{j}(\omega)} = G(\omega) = re^{\mathbb{i}\omega h} + (1-2r) + re^{-\mathbb{i}\omega h} \tag{34}$$

Thus, the von Neumann stability condition implies that:

$$\begin{aligned} |G(\omega)| \leq 1 \quad &\Leftrightarrow \quad \left|re^{\mathbb{i}\omega h} + (1-2r) + re^{-\mathbb{i}\omega h}\right| \leq 1 \\ &\Leftrightarrow \quad |(1-2r) + 2rcos(\omega h)| \leq 1 \\ &\Leftrightarrow \quad \left|(1-2r) + 2r[1-2sin^2\left(\frac{\omega h}{2}\right)]\right| \leq 1 \\ &\Leftrightarrow \quad \left|1-4rsin^2\left(\frac{\omega h}{2}\right)\right| \leq 1 \\ &\Leftrightarrow \quad 0 \leq r \leq \frac{1}{2sin^2\left(\frac{\omega h}{2}\right)}, \text{ for } \quad 0 \leq \omega h \leq \pi \end{aligned} \tag{35}$$

It follows that $0 \leq r \leq 1/2$.

Thus, the explicit finite difference method is stable if:

$$\frac{ck}{2h^2} \leq \frac{1}{2} \quad \text{or} \quad k \leq h^2, \ \ c = 1$$

So that if h should be reduced by ½, then k must be reduced by $\frac{1}{4}$ in order to achieve stability.

Therefore, for the Schrodinger equation,

$$\frac{1}{2}\psi_{xx} + V(x)\psi = i\psi_t, \ \ (\hbar = 1)$$

the explicit method requires that:

$$\frac{k}{2h^2} \leq 0.5 \ \text{ or } \ k \leq 0.5(2h^2), \ \text{i.e.,} \ \ k \leq h^2$$

4.1 Implicit method

The finite-difference representations of the partial derivatives in the Schrodinger equation is as given for the explicit method, except that the spatial derivative is approximated at step $j+1$, instead of step j. Thus, we have:

$$\psi_t(x_i, t_j) = \ \frac{i}{k}\left[\psi_{i,j+1} - \psi_{i,j}\right] + 0(k)$$

and

$$\psi_{xx}(x_i, t_{j+1}) = \ -\frac{1}{2h^2}\left[\psi_{i-1,j+1} - 2\psi_{i,j+1} + \psi_{i+1,j+1}\right] + 0(h^2)$$

Substituting into the PDE and simplifying, we find that the truncation error for the implicit is the same as for the explicit method, which gives, $0(h^2 + k)$. Now, to show that the implicit method is unconditionally stable, let us consider the implicit solution as contained in equation (23):

$$\psi_{i,j} = -r\psi_{i-1,j+1} + (1+2r)\psi_{i,j+1} - r\psi_{i+1,j+1} + ikv_i$$

The matrix representation of the equation is as given below:

$$\begin{bmatrix} 1+2 & -r & & & & & \\ -r & 1+2 & -r & & & & \\ & \ddots & \ddots & & & & \\ & & \ddots & & \ddots & & \\ & & & -r & 1+2 & -r & \\ & & & & -r & 1+\ 2 \end{bmatrix} \begin{bmatrix} \psi(1,j+1) \\ \psi(2,j+1) \\ \vdots \\ \psi(i,j+1) \\ \vdots \\ \psi(n-1,j+1) \\ \psi(n,j+1) \end{bmatrix} = \begin{bmatrix} \psi(1,j) \\ \psi(2,j) \\ \vdots \\ \psi(i,j) \\ \vdots \\ \psi(n-1,j) \\ \psi(n,j) \end{bmatrix} \tag{36}$$

The matrix is tridiagonal and diagonally dominant. As applicable for the explicit method, w shall also use the Fourier method to check if the method is unconditionally stable. So, assume that the numerical method admits a solution of the form:

$\psi_{i,j} = a^j(\omega)e^{\mathbb{i}i\omega}$, where $\boldsymbol{\omega}$ is the wave number and $\mathbb{i} = \sqrt{-1}$, and define: $G(\omega) = \frac{a^{j+1}(\omega)}{a^j(\omega)}$.

The von Neumann stability condition is given by:

$|G(\omega)| \leq 1, \ \forall k, h;$ where $h = \Delta x$ and $k = \Delta t$

It can be shown that the implicit finite difference method is unconditionally stable if $|G(\omega)| \leq 1$. Thus, substituting equation (31) into equation (23), we get:

$$a^j(\omega)e^{\mathbb{i}i\omega h} = -ra^{j+1}(\omega)e^{\mathbb{i}(i+1)\omega h} + (1+2r)a^{j+1}(\omega)e^{\mathbb{i}i\omega h} - ra^{j+1}(\omega)e^{\mathbb{i}(i-1)\omega h}$$

which yields,

$$a^j(\omega)e^{\mathbb{i}i\omega h} = a^{j+1}(\omega)[-re^{\mathbb{i}(i+1)\omega h} + (1+2r)e^{\mathbb{i}i\omega h} - re^{\mathbb{i}(i-1)\omega h}] \tag{37}$$

i.e.,

$$a^j(\omega)e^{\mathbb{i}i\omega h} = a^{j+1}(\omega)[-re^{\mathbb{i}(i+1)\omega h} + (1+2r)e^{\mathbb{i}i\omega h} - re^{\mathbb{i}(i-1)\omega h}] \tag{38}$$

or,

$$e^{\mathbb{i}i\omega h} = G(\omega)[-re^{\mathbb{i}(i+1)\omega h} + (1+2r)e^{\mathbb{i}i\omega h} - re^{\mathbb{i}(i-1)\omega h}]$$
$$\Rightarrow \qquad 1 = G(\omega)[(1+2r) - r(e^{\mathbb{i}i\omega h} + e^{-\mathbb{i}i\omega h})]$$

or,

$$G(\omega) = \frac{1}{(1+2r)-2rcos\omega h} \leq 1 \ \ and \ \ |G(\omega)| = \left|\frac{1}{1+2r(1-cos\omega h)}\right| \leq 1 \tag{39}$$

i.e.,

$$|G(\omega)| \leq 1$$

Thus, there is no restriction for $\boldsymbol{r}$, hence the implicit finite difference method is unconditionally stable.

5 Crank-Nicolson Method

Crank-Nicolson method is an implicit method. The most important advantage of this method is that it is stable for any values of $\boldsymbol{r}$, however, smaller values usually give better accuracy [11]. It is observed that when the ratio of $\frac{\boldsymbol{ck}}{\boldsymbol{2h^2}}$ is greater than 0.5, the explicit method is found to be unstable. However, the implicit methods, including Crank-Nicolson do not have such a limitation as contained in our analysis above. The truncation error of Crank-Nicolson is slightly less than the general implicit method as contained in equation (29), given as $0(k^2 + h^2)$.

Using the average of the centred difference at the forward time step $j + 1$ and the time step j gives:

$$\psi_{i,j+1} - \psi_{i,j} = \frac{ik}{2(2h^2)}\left[\left(\psi_{i-1,j} - 2\psi_{i,j} + \psi_{i+1,j}\right) + \left(\psi_{i-1,j+1} - 2\psi_{i,j+1} + \psi_{i+1,j+1}\right)\right] - ikv_i \tag{40}$$

Let $\boldsymbol{r} = \frac{\boldsymbol{ik}}{\boldsymbol{2h^2}}$; then we have:

$$\psi_{i,j+1} - \psi_{i,j} = \frac{r}{2}\left[\left(\psi_{i-1,j} - 2\psi_{i,j} + \psi_{i+1,j}\right) + \left(\psi_{i-1,j+1} - 2\psi_{i,j+1} + \psi_{i+1,j+1}\right)\right] - ikv_i \tag{41}$$

So, we have:

$$-\frac{r}{2}\psi_{i-1,j+1} + (1+r)\psi_{i,j+1} - \frac{r}{2}\psi_{i+1,j+1} = \frac{r}{2}\psi_{i-1,j} + (1-r)\psi_{i,j} + \frac{r}{2}\psi_{i+1,j} - ikv_i \tag{42}$$

Now, to show that the implicit method is unconditionally stable, let us consider the matrix-vector representation of the process as given below:

$$\begin{bmatrix} 1-r & \frac{\boldsymbol{r}}{2} & & & & & \\ \frac{\boldsymbol{r}}{2} & 1-r & \frac{\boldsymbol{r}}{2} & & & & \\ \ddots & \ddots & \ddots & & & & \\ & & \frac{\boldsymbol{r}}{2} & 1-r & \frac{\boldsymbol{r}}{2} & & \\ & & & \frac{\boldsymbol{r}}{2} & 1-r & & \end{bmatrix} \begin{bmatrix} \psi(1,j) \\ \psi(2,j) \\ \vdots \\ \psi(i,j) \\ \vdots \\ \psi(n-1,j) \\ \psi(n,j) \end{bmatrix}$$

$$= \begin{bmatrix} 1+r & -\frac{r}{2} & & & & & \\ -\frac{r}{2} & 1+r & -\frac{r}{2} & & & & \\ \ddots & \ddots & \ddots & & & & \\ & & -\frac{r}{2} & 1+r & -\frac{r}{2} & & \\ & & & -\frac{r}{2} & 1+r & & \end{bmatrix} \begin{bmatrix} \psi(1,j+1) \\ \psi(2,j+1) \\ \vdots \\ \psi(i,j+1) \\ \vdots \\ \psi(n-1,j+1) \\ \psi(n,j+1) \end{bmatrix} \tag{43}$$

The matrix is tridiagonal and diagonally dominant. As obtained above when considering the general implicit method, we shall use the Fourier method to check if the method is unconditionally stable.

The von Neumann stability condition is given by:

$$|G(\omega)| \leq 1, \qquad \forall k, h,$$

where $h = \Delta x$ and $k = \Delta t$.

It can be shown that the Crank-Nicolson finite difference method is unconditionally stable if

$$|G(\omega)| \leq 1$$

Substituting, we have:

$$-\frac{r}{2}a^{j+1}(\omega)e^{\mathbb{i}(i-1)\omega h}+(1+r)a^{j+1}(\omega)e^{\mathbb{i}i\omega h}-\frac{r}{2}a^{j+1}(\omega)e^{\mathbb{i}(i+1)\omega h}$$

$$=\frac{r}{2}a^{j}(\omega)e^{\mathbb{i}(i-1)\omega h}+(1-r)a^{j}(\omega)e^{\mathbb{i}i\omega h}+\frac{r}{2}a^{j}(\omega)e^{\mathbb{i}(i+1)\omega h}-ikv_i \tag{44}$$

i.e.,

$$-\frac{r}{2}G(\omega)e^{\mathbb{i}(i-1)\omega h}+(1+r)G(\omega)e^{\mathbb{i}i\omega h}-\frac{r}{2}G(\omega)e^{\mathbb{i}(i+1)\omega h}$$
$$=\frac{r}{2}e^{\mathbb{i}(i-1)\omega h}+(1-r)e^{\mathbb{i}i\omega h}+\frac{r}{2}e^{\mathbb{i}(i+1)\omega h} \tag{45}$$

$\Rightarrow$

$$G(\omega)=\frac{(1-r)+r/2\left(e^{\mathbb{i}\omega h}+e^{-\mathbb{i}\omega h}\right)}{(1+r)-r/2\left(e^{\mathbb{i}\omega h}+e^{-\mathbb{i}\omega h}\right)}=\frac{(1-r)+rcos(\omega h)}{(1+r)-rcos(\omega h)}=\frac{1-r[1-cos(\omega h)]}{1+r[1-cos(\omega h)]} \tag{46}$$

Thus, $|G(\omega)|\leq 1$ for all r, and hence both general implicit and Crank-Nicolson finite difference methods have no restriction for r and are unconditionally stable. However, the truncation error for the Crank-Nicolson method is $0(h^2+k^2)$, while that of the general implicit method is $0(h^2+k)$.

6 Conclusion

It is observed that from equation (33b) that by using von Neumann stability condition , the explicit finite difference method is found to be conditionally stable if only r ≤ *0.5* and thus, if h should be reduced by ½, then k must be reduced by $\frac{1}{4}$ in order to achieve stability. Therefore, for the ID Schrodinger equation for the quantum harmonic equation:

$$\frac{1}{2}\psi_{xx}+V(x)\psi=i\psi_t,\ \ (\mathrm{m}=\hbar=1)$$

Thus, the explicit method requires that:

$$\frac{k}{2h^2}\leq 0.5\quad \text{or}\quad k\leq 0.5(2h^2),\ \ \text{i.e.,}\ k\leq h^2$$

On the other hand, the implicit and Crank-Nicolson finite difference methods for the ID Schrodinger equation are found to be unconditionally Stable using the von Neumann stability condition as $|G(\omega)|\leq 1$ for all r, from equations (39) and (46).

Considering Figs. 1,2 and 4 above, we observe that r = 5.0,1.0 and 5.0 respectively, and thus the effect on the graphs are obvious while, in Fig. 3, $r=0.5$ which satisfies the stability condition of r ≤ *0.5*. On the other hand, we observe that irrespective of the values of r in Figs. 5,6 and 7 which are 0.5, 5.0 and 50.0 respectively, all the graphs appears consistent, which concludes that the implicit and Crank-Nicolson finite difference methods have no restriction for r and are therefore unconditionally stable. However, the Crank-Nicolson has a better truncation error of $0(h^2+k^2)$ while the general implicit method has a truncation error of $0(h^2+k)$.

Competing Interests

Author has declared that no competing interests exist.

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