A Stable and Consistent Finite Difference Scheme for a Time-Dependent Schrodinger Wave Equation in a Finitely Low Potential Well.

Adeleke O. J.
Department of Computer and Information Science/Mathematics
Covenat University, Ota. Nigeria.
e-mail:wale.adeleke@covenantuniversity.edu.ng

Oke M. O.
Department of Mathematical Sciences, Ekiti State University, Ado-Ekiti.
e-mail: femioke91@gmail.com

Adewumi O. A.
School of Mathematics, Statistics and Computer Science, University of KwaZulu-Natal, Westville Campus. South Africa.
e-mail: Adewumia@ukzn.ac.za

Abstract

In this paper, we present a stable and consistent criterion to an explicit finite difference scheme for a time-dependent Schrodinger wave equation. This paper is a departure from the well-established time independent Schrodinger Wave Equation (SWE). We do this for a particular case of a finitely low potential well.

Keywords: Time-Dependent Schrodinger Wave Equation, Stability, Consistency, Finite Potential Well, Finite Difference.

1. Introduction

Two forms of the Schrodinger wave equation (SWE) exist. In the first, the time factor is explicitly expressed, for which reason it is widely referred to as the time-dependent SWE. In the second, known as the time-independent SWE, the time factor is removed. In practice though these two equations are separate, the latter, which is the time-independent SWE can be derived from the former. The only exception to this order is if the potential is time dependent.

The Schrodinger equation, which was developed by Erwin Schrodinger, is very central to the study of quantum mechanics as it defines the permissibility of a stationary state of a quantum mechanics [7]. Accordingly, it tells how the quantum state of a physical system changes with time [7].

2. Time-Dependent SWE

According to Shanker [5], the form of Schrodinger equation depends on the physical situation. The most general form is the time-dependent Schrodinger wave equation (TDSWE), which gives a description of a system evolving with time.

This time-dependent SWE is given as

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x) + v(x)\psi = i\hbar\frac{\partial\psi}{\partial t} \tag{1}$$

where $\hbar = \frac{h}{2\pi}$, h being the Planck's constant, m is the mass of particle, $\psi(x,t)$, is the wave function, x is the position of any particular particle in time t, $v(x)$ is the time-dependent potential, and t is the time.

When this equation is set up for analysis, it forms the bedrock for wave mechanics which is a branch of quantum mechanics. This equation, when solved, is capable of generating solutions that depict a wave propagating through space. This explains the rationale behind being termed a wave equation even though it does not represent properly the more familiar classical wave equation.

Koch [2] developed a numerical scheme that is workable with the TDSWE in an Ultrafast Laser e. The scheme so developed by Koch approximates the original wave equation on a linear manifold.

With basis on a discretizing space and time on a grid, Kosloff and Kosloff [3] developed a new method through the Fourier method to produce a spatial derivatives and the second-order differencing for time derivatives.

We follow a similar numerical approach in this paper. But instead of solving the TDSWE, we only develop a numerical scheme that is both stable and consistent, thereby establishing it convergence property.

3. Stability and Consistency Criteria for a Finite Difference Scheme

To investigate the stability property of the finite difference scheme to be shortly developed, the Fourier series method has been adopted. This method, developed by von Neumann, which was first discussed by O'Brian, Hyman and Kaplan [4], "expressed an initial line of errors in terms of a finite Fourier series, and considers the growth of a function that reduces to this series for $t = 0$ by a separation of variable method commonly used for solving analytically a partial differential equation [6].

The procedure for doing this is as follows.

Suppose we denote the error at the pivotal point [6] by

$$E(ph) = E_P, p = 0(1)N \qquad (2)$$

$$\equiv E_{P,O}$$

Then the $(N + 1)$ equations

$$E_p = \sum_{n=0}^{N} A_n e^{i\beta_n ph}, \; p = 0(1)N \qquad (3)$$

(where A_n is constant and $\beta_n = \frac{n\pi}{Nh}, Nh = 1$)

are sufficient to determine the unknown $A_k, \; k = 0(1)n$, uniquely. For a linear finite difference scheme ours with separate additive solutions, we need only consider the proportion of the error due to a single term, such as $e^{i\beta ph}$. $A_n$being constant may be neglected.

For an increasing t, investigating this error, we need only to find a solution which reduces to $e^{i\beta ph}$ when $t = qk = 0$.

If we assume

$$E_{p,q} = e^{i\beta x}e^{\alpha t} = e^{i\beta ph}e^{\alpha qk} = e^{i\beta ph}\xi^{q} \quad (4)$$

Where $\xi = e^{\alpha k}$ with $\alpha,$ in general, a complex constant.

When $q = 0$, $E_{p,q} = e^{i\beta ph}$.

The only way to keep the error stable as t increases is to make a provision such that

$$|\xi| \leq \quad (5)$$

Equation (5) is known as the stability criterion. It is both necessary and sufficient for two time-level difference scheme but not always for three time-level schemes [6].

For a more concise approach, suppose we take $e = U - u$, where e is the discretization error, U is the exact solution of the partial differential equation (pde) and u, the exact solution of the finite difference scheme. Then, if $u_{m,n}$ is bounded as n increases, the difference equation is said to be stable. In a nutshell, if $e_{m,n} = U_{m,n} - u_{m,n}$ remains bounded as $n \to \infty$, then the difference equation to the pde is stable.

In a similar fashion, suppose $F_{m,n}(u) = 0$ is a difference equation at $(m,n)th$ mesh point, then a finite difference is said to be consistent with the pde if $F_{m,n}(u) \to 0$as $\delta x, \delta t \to 0$.

4. Main Results

In what follows in this paper, we present the results for both stability and consistency of the explicit finite difference equation for TDSWE. We begin by giving the difference equation.

The TDSWE is

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x) + v(x)\psi = i\hbar\frac{\partial\psi}{\partial t} \tag{6}$$

We can write this as

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \mathrm{u}}{\partial u^2} + v(x)\mathrm{u} = i\hbar\frac{\partial \mathrm{u}}{\partial t}, 0 < x < a, t > 0 \tag{7}$$

Let$\frac{\hbar^2}{2m} = -c^2 and\ ih = d$

$\frac{\partial \mathrm{u}}{\partial t} = \frac{u_{m,n+1} - u_{m,n}}{k}$ and $\frac{\partial^2 \mathrm{u}}{\partial x^2} = \frac{u_{m+1,n} - 2u_{m,n+u_{m-1,n}}}{k}$

Here,

$$u = u_{m,n}$$

For a simple case where v is unity i.e $v(x) = 1$

$$\frac{1}{k}\{u_{m,n+1} - u_{m,n}\} - \frac{e}{h^2}\left(u_{m+1,n} - 2u_{m,n+u_{m-1,n}}\right) - fu_{m,n} = 0 \tag{8}$$

Where

$$e = \frac{c^2}{d} and\ f = \frac{1}{d}$$

$$u_{m,n+1} - u_{m,n} - \frac{ke}{h^2}\left(u_{m+1,n} - 2u_{m,n+u_{m-1,n}}\right) - kfu_{m,n} = 0 \tag{9}$$

$$u_{m,n+1} - u_{m,n} - reu_{m,n+1} - 2reu_{m,n\,+\,u_{m-1,n}} - kfu_{m,n} = 0 \tag{10}$$

$$u_{m,n+1} + (2re - kf - 1)u_{m,n} - re(u_{m,n+1} - u_{m-1,n)} = 0 \quad (11)$$

$$u_{m,n+1} = re(u_{m+1,n} - u_{m-1,n)+}(1 + kf - 2re)u_{m,n} \quad (12)$$

We thus come to the difference scheme given by

$$u_{m,n+1} = \frac{i\hbar k}{2mh^2}(u_{m+1,n} - u_{m-1,n)+}(1 - \frac{ik}{h} - \frac{i\hbar k}{mh^2})u_{m,n} \quad (13)$$

This equation is the finite difference scheme of the TDSWE in a finite potential well, where *v(x) = 1.*

4.1 Stability

In developing a stability criterion for (13), we employ both Courant, Friedrichs andLewy Criteria [CFL criteria] [1] and the Von Neumann method [4]. From the difference scheme for the classical wave equation, the former found that if $c\frac{\partial t}{\partial x} = c\frac{k}{h} > 1$, then the scheme is unstable. The CFL criteria has its origin in the fact that if $c\Delta t > \Delta x$, then the rate at which signals in the numerical scheme travel will be faster than their real world counterparts and this unrealistic expectation leads to instability.

We proceed from the Von Neumann-Fourier method

Let

$$u_{m,n} = e^{-im\theta}e^{in\lambda} \quad (14)$$

whereθ is an arbitrary real number andλ is a complex number yet to be determined.

This choice is motivated by the fact that the initial condition $u_{m,0}$ can be represented by a Fourier series where a typical term behaves as$e^{-im\theta}$.

By substituting (14) into(14) we obtain,

$$e^{im\theta}e^{i(n+1)\lambda} = \frac{i\hbar k}{2mh^2}\left(e^{i(m+1)\theta}e^{in\lambda} + e^{i(m-1)\theta}e^{in\lambda}\right) + (1 - \frac{ik}{h} - \frac{i\hbar k}{mh^2})e^{im\theta}e^{in\lambda} \tag{15}$$

$$e^{i\lambda} = \frac{i\hbar k}{2mh^2}sin^2\left(\frac{\theta}{2}\right) + (1 - \frac{ik}{h} - \frac{i\hbar k}{mh^2}) \tag{16}$$

The quantity $e^{i\lambda}$ will grow exponentially unless

$$-1 \leq e^{i\lambda} = \frac{i\hbar k}{2mh^2}sin^2\left(\frac{\theta}{2}\right) + \left(1 - \frac{ik}{h} - \frac{i\hbar k}{mh^2}\right) < 1 \tag{17}$$

i.e.,

$$-1 \leq 1 - \frac{ik}{h} - \frac{i\hbar k}{mh^2}(1 - \frac{1}{2}sin^2\left(\frac{\theta}{2}\right)) < 1 \tag{18}$$

$$0 \leq -1 - \frac{\hbar}{mh^2}(1 - \frac{1}{2}sin^2\left(\frac{\theta}{2}\right)) < \frac{2}{ik} \tag{19}$$

$$1 \leq -\frac{\hbar}{mh^2}(1 - \frac{1}{2}sin^2\left(\frac{\theta}{2}\right)) < \frac{2}{ik} + 1 \tag{20}$$

$$\{\frac{mh^2}{\hbar} \leq -(1 - \frac{1}{2}sin^2\left(\frac{\theta}{2}\right)) < \frac{mh^2}{\hbar}(1 + \frac{2}{ik})\} \tag{21}$$

$$1 \leq \frac{\hbar}{2mh^2}sin^2\left(\frac{\theta}{2}\right) - \frac{\hbar}{mh^2} < 1 + \frac{2}{ik} \tag{22}$$

Taking the right hand side of (22), i.e.,

$$1 - \frac{ik}{h} - \frac{i\hbar k}{mh^2}(1 - \frac{1}{2}sin^2\left(\frac{\theta}{2}\right)) < 1 \tag{23}$$

$$\frac{\hbar^2 k}{mh^2} > \frac{k}{\frac{1}{2}sin^2\left(\frac{\theta}{2}\right) - 1} \tag{24}$$

$$\frac{\hbar^2 k}{2mh^2}(sin^2\left(\frac{\theta}{2}\right) - 2) > k \tag{25}$$

$$\frac{\hbar^2 k}{2mh^2} > \frac{k}{sin^2\left(\frac{\theta}{2}\right) - 2} \tag{26}$$

For the left hand side inequality of (22) we have

$$1 \leq \frac{\hbar}{2mh^2} sin^2\left(\frac{\theta}{2}\right)) + 1 - \frac{ik}{\hbar} - \frac{ik\hbar}{mh^2} \tag{27}$$

$$\frac{k}{(sin^2\left(\frac{\theta}{2}\right))-2)} < \frac{\hbar^2 k}{2mh^2} \leq \frac{k+2i\hbar}{(sin^2\left(\frac{\theta}{2}\right))-2)} \tag{28}$$

i.e.,

$$\frac{k}{(sin^2\left(\frac{\theta}{2}\right))-2)} < \frac{\hbar^2 k}{2mh^2} \leq \frac{k}{(sin^2\left(\frac{\theta}{2}\right))-2)} + \frac{2i\hbar}{(sin^2\left(\frac{\theta}{2}\right))-2)} \tag{29}$$

$$\Rightarrow \frac{k}{(sin^2\left(\frac{\theta}{2}\right))-2)} \leq \frac{|k|}{|(sin^2\left(\frac{\theta}{2}\right))+(-2)|} + \frac{k}{|(sin^2\left(\frac{\theta}{2}\right))+(-2)|} = \frac{k}{3} \tag{30}$$

Combining inequalities (26) and (30), we get

$$\frac{k}{3} < \frac{\hbar^2 k}{2mh^2} \leq \frac{k+2i\hbar}{3} \tag{31}$$

The result in (31) gives our proposed stability criterion for an explicit finite difference scheme of the TDSWE.

4.2 Consistency

We know that

$$u_{m,n+1} = u_{m,n} + k\frac{\partial \mathrm{u}}{\partial t}|_n^m + \frac{1}{2}k^2\frac{\partial^2 \mathrm{u}}{\partial t^2}|_n^m + \frac{1}{6}k^3\frac{\partial^3 \mathrm{u}}{\partial t^3}|_n^m + \cdots\cdots$$

$$= u_{m,n} + k\frac{\partial \mathrm{u}}{\partial t}(m,n) + \frac{1}{2}k^2\frac{\partial^2 \mathrm{u}}{\partial t^2}(m,n) + \frac{1}{6}k^3\frac{\partial^3 \mathrm{u}}{\partial t^3}(m,n) + \cdots \tag{32}$$

$$u_{m+1,n} = u_{m,n} + h\frac{\partial \mathrm{u}}{\partial x}(m,n) + \frac{1}{2}h^2\frac{\partial^2 \mathrm{u}}{\partial x^2}(m,n) + \frac{1}{6}h^3\frac{\partial^3 \mathrm{u}}{\partial x^3}(m,n) + .. \tag{33}$$

$$u_{m-1,n} = u_{m,n+1} - h\frac{\partial \mathrm{u}}{\partial x}(m,n) + \frac{1}{2}h^2\frac{\partial^2 \mathrm{u}}{\partial x^2}(m,n) - \frac{1}{6}h^3\frac{\partial^3 \mathrm{u}}{\partial x^3}(m,n) + .. \tag{34}$$

By substituting (32) to (34) into (13), we obtain

$$u_{m,n} + k\frac{\partial \mathrm{u}}{\partial t}(m,n) + \frac{1}{2}k^2\frac{\partial^2 \mathrm{u}}{\partial t^2}(m,n) + \frac{1}{6}k^3\frac{\partial^3 \mathrm{u}}{\partial t^3}(m,n) + \cdots\cdots \quad (35)$$

$$= \frac{i\hbar k}{2mh^2}\left(2u_{m,n} + h^2\frac{\partial^2 \mathrm{u}}{\partial x^2}(m,n) + \cdots\right) + (1 - \frac{ik}{h} - \frac{i\hbar k}{mh^2})u_{m,n} \quad (36)$$

$$= \frac{i\hbar k}{mh^2}u_{m,n} + \frac{i\hbar k}{2m}\frac{\partial^2 \mathrm{u}}{\partial x^2}(u_{m,n}) + \cdots + (1 - \frac{ik}{h} - \frac{i\hbar k}{mh^2})u_{m,n} \quad (37)$$

$$= \frac{i\hbar k}{2m}\frac{\partial^2 \mathrm{u}}{\partial x^2}|_n^m + \cdots + (1 - \frac{ik}{h})u_{m,n} \quad (38)$$

$$u_{m,n} + k\frac{\partial \mathrm{u}}{\partial t}|_n^m + \frac{1}{2}k^2\frac{\partial^2 \mathrm{u}}{\partial t^2}|_n^m + \frac{1}{6}k^3\frac{\partial^3 \mathrm{u}}{\partial t^3}|_n^m + \cdots = \frac{i\hbar k}{2m}\frac{\partial^2 \mathrm{u}}{\partial x^2}|_n^m + u_{m,n} - \frac{ik}{h}u_{m,n} \quad (39)$$

$$k\left(\frac{\partial \mathrm{u}}{\partial t} - \frac{i\hbar}{2m}\frac{\partial^2 \mathrm{u}}{\partial x^2}\right)|_n^m = -\frac{ik}{h}u_{m,n} - \frac{1}{2}k^2\frac{\partial^2 \mathrm{u}}{\partial t^2}|_n^m - \frac{1}{6}k^3\frac{\partial^3 \mathrm{u}}{\partial t^3}|_n^m - \cdots \quad (40)$$

The term on the LHS vanishes because u(x,t) satisfies the wave equation. Likewise, as $k = \Delta t \longrightarrow 0$, the terms on the RHS tend to zero(0) and so (13) is a consistent finite difference approximation to the Schrodinger wave equation.

5. Conclusion

In the course of this paper, we have been able to develop criteria for both the stability and consistency for the difference equation of a TDSWE. The consequential effect of these results is that the scheme is convergent as it approaches a continuous solution as $\Delta x, \Delta t \rightarrow 0$.

6. Future Work

Future research will be aimed at numerical test of the criteria developed this paper. Anotjher interesting work to be further carried out is the analytic and computational comparison with existing solution of the TDSWE.

7. References

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