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HIGH-ORDER B-SPLINE FINITE DIFFERENCE APPROACH FOR SCHRODINGER EQUATION IN QUANTUM MECHANICS

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This paper presents a new numerical method for solving the quantum mechanical complex-valued Schrodinger equation (CSE). The technique combines a second-order Crank-Nicolson scheme based on the finite element method (FEM) for temporal discretisation with nonic B-spline functions for spatial discretisation. This method is unconditionally stable with the help of Von-Neumann stability analysis. To verify our methodology, we examined an experiment utilising a range of error norms to compare experimental outcomes with analytical solutions. Our investigation verifies that the suggested approach works better than current methods, providing better accuracy and efficiency in quantum mechanical error analysis.
Keywords: *Crank-Nicolson Method; Finite element scream; Von-Neumann stability assessment; Nonic B-spline*
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1. INTRODUCTION

Differential equations (DEs) are fundamental tools for analysing dynamic phenomena across various fields and are indispensable in mathematically representing physical systems. They find extensive application in simulating diverse physical problems such as fluid dynamics, signal processing, and electrical engineering. Dynamic systems with measurement errors often necessitate numerical treatment due to the complexity of obtaining analytical solutions.

The Schrodinger equation (SE), formulated by Austrian physicist Erwin Schrodinger in 1926, stands as a cornerstone in quantum theory and mechanics, governing sub-microscopic events. And the probabilistic nature of wave functions. Its significance permeates through atomic, nuclear, and solid-state physics. Schrodinger's experimental validation of SE, particularly with the hydrogen atom, underscored its efficacy in describing quantum phenomena.

SE exists in two primary forms: the time-dependent Schrodinger wave equation, portraying wave function evolution over time, and the time-independent Schrödinger equation, elucidating stationary states. While the former characterises progressive waves pertinent to free particle motion, the latter describes standing waves, especially when the particle's potential energy is independent of time and solely dependent on position.

The solutions to the time-dependent Schrodinger equation mirror the dynamic properties of particles, analogous to Newton's force definition (F= ma) in classical physics. Furthermore, nonlinear Schrodinger equations find applications in various fields, such as plasma physics[2], nonlinear optics [19], and water waves [26].

Recent research delves into specialised solutions and applications of SE variants, including Haar wavelet and finite difference method [1], quantic Hermite collocation method [3], differential quadrature method (DQM) [4], quadratic B-Spline FEM [6], reverse-time SE [9], cubic spline technique [17]. Additionally, studies explore specific solutions and phenomena like breather-type solutions and rogue waves in generalised nonlinear SE formulations [5], highlighting the versatility and ongoing research interest in SE and its extensions.

Many approaches have been used with finite differences [18], and the finite element method [21] is designed specifically for fractional Schrodinger equations with trigonometric B-splines [8]. It has also been investigated to analyse the superconvergence of linearised MFEM for nonlinear Schrödinger equations [24]. Additionally, specialised methods have addressed time-dependent singly perturbed convection-diffusion equations, such as the Crank-Nicolson finite difference approach with a midpoint upwind scheme on non-uniform meshes [12].

Numerous numerical methods have been studied to solve the coupled nonlinear Schrödinger equation using cubic B-spline Galerkin methods [10]. Furthermore, to approximate solutions to Equation (1), multistep and hybrid approaches [25] and two-step hybrid methods [15] have been proposed. Other techniques include B-Spline collocation technique [11], [7] improvised cubic B-spline collocation [13], Crank-Nicolson scheme [14], homotopy analysis method [20], BFRK scheme [22], septic B-Spline collocation [23] and numerical quadrature schemes, which have also been applied. Despite exploring several ways, difficulties in delivering comprehensive computations for these techniques continue to arise. For example, Lehtovaara *et al.*, by the time propagation method [16], presents viable approaches to solve equation (1), but the computation details are still elusive.

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Adopting the nonic B-spline collocation methodology is a significant step forward in tackling complicated problems like the Schrödinger equation by surpassing the drawbacks of the previous numerical methods. Using this technology, researchers can reduce problems associated with excessive computing complexity, poor precision, and programming difficulties.

Researchers can effectively handle the complex computations needed to approximate solutions using MATLAB and MATHEMATICA for computing. Compared to more conventional approaches, this one simplifies computation, improves accuracy, and simplifies implementation.

Furthermore, this effort offers scholars essential insights into the effectiveness of complex analysis as a physics tool by integrating these techniques within the quantum mechanics curriculum. Comprehending complex analysis broadens researchers' understanding and gives them an advantage when addressing other physics problems requiring advanced mathematical techniques. Using the finite element method in conjunction with the B-spline collocation method promotes a catalytic approach to quantum mechanics research advancement. This work opens the door for revolutionary developments in the discipline by proposing novel approaches and encouraging multidisciplinary collaboration.

The primary goal of the scheme that we suggest in this study is to improve the accuracy of approximate solutions for quantum-mechanical energy, similar to Schrödinger's original answer. Our goal is to show that the nonic B-spline collocation approach, in combination with the finite element method (FEM) and Crank-Nicolson scheme, can be a valuable tool for the efficient implementation of intermediate-level complex analysis of the Schrödinger equation.

The Schrödinger equation is converted into an algebraic system of equations at each step of the procedure, making a numerical solution easier, more dependable, and more effective than other approaches. Optical soliton solutions require managing the complex function's real and imaginary parts.

The Crank-Nicolson method, initially proposed by Crank and Phyllis Nicolson in 1947 for the numerical solution of partial differential equations, emerges as an elegant solution for our purposes. This method is known for its convergence and stability properties across finite values of the Courant number ω, defined as $(\frac{\Delta t}{h^2}) = \omega$. Implementing the Crank-Nicolson method offers an efficient solution to the time-dependent Schrödinger equation, a fundamental tool with extensive utility in various fields of physics such as acoustics and optics. By employing this comprehensive approach, we aim to provide researchers with a robust framework for tackling complex quantum-mechanical problems while shedding light on the practical applications of the Schrödinger equation in diverse physical phenomena.

The non-dimensionalized form of the equation can be written as

$$iv_t + \gamma v_{xx} + p|v|^2 v = 0, \tag{1}$$

with the initial conditions

$$v(x,0) = \mathrm{f}(x),\ a \le x \le b, \tag{2}$$

and the boundary conditions

$$v(a,t) = v(b,t) = 0$$

$$v_{5x}(a,t) = v_{5x}(b,t) = v_{6x}(a,t) = v_{6x}(b,t) = 0$$

$$v_{7x}(a,t) = v_{7x}(b,t) = v_{8x}(a,t) = v_{8x}(b,t) = 0, t \in [0,T]. \tag{3}$$

Here, $\gamma \neq 0$ *and* $i^2 = -1$ is an imaginary unit, and $f(x)$ is a smooth function.
If $\gamma = -1$ and $p = 0$, then equation (1) becomes

$$iv_t - v_{xx} = 0 \tag{4}$$

The current work is organised as follows: Section 2 suggests and constructs the nonic B-spline. The nonic B-spline is implemented in Section 3. The Section 4 is reported with linear stability analysis. Section 5 discusses numerical examples, and corresponding results are reported in the table and surfed in figures. Section 6 contains a portion of the conclusions.

2. B-SPLINE OF ORDER NINE

Let's find the step length $h = x_{m+1} - x_m, m = 0,1,..N$, where m=0,1,..., N, and divide the interval [a,b] into N equally spaced points x_n such that $a = x_0 < x_1 <\ldots< x_N = b$. Next, at the knots x_m, the nonic B-splines $B_m(x),\ m = -4(1)N + 4$ are provided by:

$$B_m(x) = \frac{1}{h^9}\begin{cases} d_1^9 & x \in I_1 \\ d_1^9 - \binom{10}{1} d_2^9 & x \in I_2 \\ d_1^9 - \binom{10}{1} d_2^9 + \binom{10}{2} d_3^9 & x \in I_3 \\ d_1^9 - \binom{10}{1} d_2^9 + \binom{10}{2} d_3^9 - \binom{10}{3} d_4^9 & x \in I_4 \\ d_1^9 - \binom{10}{1} d_2^9 + \binom{10}{2} d_3^9 - \binom{10}{3} d_4^9 + \binom{10}{4} d_5^9 & x \in I_5 \\ d_6^9 - \binom{10}{1} d_7^9 + \binom{10}{2} d_8^9 - \binom{10}{3} d_9^9 + \binom{10}{4} d_{10}^9 & x \in I_6 \\ d_6^9 - \binom{10}{1} d_7^9 + \binom{10}{2} d_8^9 - \binom{10}{3} d_9^9 & x \in I_7 \\ d_6^9 - \binom{10}{1} d_7^9 + \binom{10}{2} d_8^9 & x \in I_8 \\ d_6^9 - \binom{10}{1} d_7^9 & x \in I_9 \\ d_{10}^9 & x \in I_{10} \\ 0 & otherwise \end{cases} \quad (5)$$

where

$d_1 = (x - x_{m-5}),\ d_2 = (x - x_{m-4}),\ d_3 = (x - x_{m-3}),\ d_4 = (x - x_{m-2}),\ d_5 = (x - x_{m-1}),\ d_6 = (x_{m+5} - x),$
$d_7 = (x_{m+4} - x),\ d_8 = (x_{m+3} - x),\ d_9 = (x_{m+2} - x),\ d_{10} = (x_{m+1} - x),$

$$I_1 = [x_{m-5}, x_{m-4}),\ I_2 = [x_{m-4}, x_{m-3}), I_3 = [x_{m-3}, x_{m-2}),\ I_4 = [x_{m-2}, x_{m-1}), I_5 = [x_{m-1}, x_m), I_6 = [x_m, x_{m+1}),$$
$$I_7 = [x_{m+1}, x_{m+2}), I_8 = [x_{m+2}, x_{m+3}), I_9 = [x_{m+3}, x_{m+4}), I_{10} = [x_{m+4}, x_{m+5})$$

The nonic B-splines $B_{-4}, B_{-3}, \dots, B_{N+4}$ constitute a basis over the area of space $[a, b]$.The solution $u(x,t)$, approximating the exact solution $v(x,t)$ of equation (1), is expressed as:

$$u(x,t) = \sum_{m=-4}^{N+4} c_m(t) B_m(x) \quad (6)$$

At each time level, the parameters c_m and $B_m(x)$ are the temporal quantities to be found.
At the mesh points x_m, the nodal values of u_m and its higher-order derivatives were acquired using equations (5) and (6), which are as follows:

$$\begin{aligned}
u_m &= c_{m-4} + 502c_{m-3} + 14608c_{m-2} + 88234c_{m-1} + 156190c_m + 88234c_{m+1} + 4608c_{m+2} + 502c_{m+3} + c_{m+4} \\
u'_m &= \frac{9}{h}(-c_{m-4} - 246c_{m-3} - 4046c_{m-2} - 11326c_{m-1} + 11326c_{m+1} + 4046c_{m+2} + 246c_{m+3} + c_{m+4}) \\
u''_m &= \frac{72}{h^2}(c_{m-4} + 118c_{m-3} + 952c_{m-2} + 154c_{m-1} - 2450c_m + 154c_{m+1} + 952c_{m+2} + 118c_{m+3} + c_{m+4}) \\
u'''_m &= \frac{504}{h^3}(-c_{m-4} - 54c_{m-3} - 134c_{m-2} + 434c_{m-1} - 434c_{m+1} + 134c_{m+2} + 54c_{m+3} + c_{m+4}) \\
u_m^{iv} &= \frac{3024}{h^4}(c_{m-4} + 22c_{m-3} - 32c_{m-2} - 86c_{m-1} + 190c_m - 86c_{m+1} - 32c_{m+2} + 22c_{m+3} + c_{m+4}) \\
u_m^{v} &= \frac{15120}{h^5}(-c_{m-4} - 6c_{m-3} + 34c_{m-2} - 46c_{m-1} + 46c_{m+1} - 34c_{m+2} + 6c_{m+3} + c_{m+4}) \\
u_m^{vi} &= \frac{60480}{h^6}(c_{m-4} - 2c_{m-3} - 8c_{m-2} + 34c_{m-1} - 50c_m + 34c_{m+1} - 8c_{m+2} - 2c_{m+3} + c_{m+4}) \\
u_m^{vii} &= \frac{181440}{h^7}(-c_{m-4} + 6c_{m-3} - 14c_{m-2} + 14c_{m-1} - 14c_{m+1} + 14c_{m+2} - 6c_{m+3} + c_{m+4}) \\
u_m^{viii} &= \frac{362880}{h^8}(c_{m-4} - 8c_{m-3} + 28c_{m-2} - 56c_{m-1} + 70c_m - 56c_{m+1} + 28c_{m+2} - 8c_{m+3} + c_{m+4}).
\end{aligned} \quad (7)$$

The continuity of nonic B-splines and their first eight derivatives is ensured.

3. EXECUTION

The current implementation strategy revolves around leveraging a hybrid numerical approach to approximate the equation's solution. The temporal derivatives within the equation are discretised using the forward finite difference method. This method, known for its simplicity and ease of implementation, involves approximating the derivatives by the difference between neighbouring points in time. Discretizing the time derivatives transforms the continuous-time problem into a discrete-time one, enabling numerical computation using iterative techniques.

$$i\,\frac{(v^{n+1}) - (v^n)}{\Delta t} = \frac{(v_{xx}^{n+1}) + (v_{xx}^n)}{2} \quad (8)$$

With equation (8) established, we derive the recurrence relation (9) through a systematic analysis of the simplified system's behaviour. This involves identifying recurring patterns or dependencies among the system's variables across consecutive time steps, which can be expressed using a recursive formula.

$$\delta_{m,1}c_{m-4}^{n+1}+\delta_{m,2}c_{m-3}^{n+1}+\delta_{m,3}c_{m-2}^{n+1}+\delta_{m,4}c_{m-1}^{n+1}+\delta_{m,5}c_{m}^{n+1}+\delta_{m,4}c_{m+1}^{n+1}+\delta_{m,3}c_{m+2}^{n+1}+\delta_{m,2}c_{m+3}^{n+1}+\delta_{m,1}c_{m+4}^{n+1}$$
$$=\delta_{m,6}c_{m-4}^{n}+\delta_{m,7}c_{m-3}^{n}+\delta_{m,8}c_{m-2}^{n}+\delta_{m,9}c_{m-1}^{n}+\delta_{m,10}c_{m}^{n}+\delta_{m,9}c_{m+1}^{n}+\delta_{m,8}c_{m+2}^{n}+\delta_{m,7}c_{m+3}^{n}+\delta_{m,6}c_{m+4}^{n}, \quad (9)$$

where $m=0,1,\dots,N$ and i is an imaginary unit.

$\delta_{m,1}=2ih^2-72\Delta t$ $\delta_{m,2}=1004ih^2-8496\Delta t$

$\delta_{m,3}=29216ih^2-68544\Delta t$ $\delta_{m,4}=176468ih^2-11088\Delta t$

$\delta_{m,5}=312380ih^2+176400\Delta t$ $\delta_{m,6}=2ih^2+72\Delta t$

$\delta_{m,7}=1004ih^2+8496\Delta t$ $\delta_{m,8}=29216ih^2+68544\Delta t$

$\delta_{m,9}=176468ih^2+11088\Delta t$ $\delta_{m,10}=312380ih^2-176400\Delta t$

Consequently, with the aid of MATLAB, the augmented system (9) is efficiently formulated, incorporating the additional equations derived from the boundary conditions(3). This expanded system now consists of (N+9) equations, precisely matching the number of unknowns, thereby enabling a comprehensive solution. MATLAB's robust numerical solvers facilitate the exploration of the solution space, allowing for accurate and reliable results to be obtained with minimal effort.

$$A_1\bar{\alpha}^{n+1}=A_2(\alpha^n) \quad (10)$$

where, $\bar{\alpha}^{n+1}=[c_{-4}^{n+1}\ c_{-3}^{n+1}\dots c_{N+4}^{n+1}]^T$, A_1, A_2 are $(N+9)\times(N+9)$ and $(N+9)\times 1$ matrix respectively.

$$A_1=\begin{pmatrix}
1 & 502 & 14608 & 88234 & 156190 & 88234 & 14608 & 502 & 1 & & & & & \\
-1 & -54 & -134 & 434 & 0 & -434 & 134 & 54 & 1 & & & & & \\
-1 & -6 & 34 & -46 & 0 & 46 & -34 & 6 & 1 & & & & & \\
-1 & 6 & -14 & 14 & 0 & -14 & 14 & -6 & 1 & & & & & \\
\delta_{0,1} & \delta_{0,2} & \delta_{0,3} & \delta_{0,4} & \delta_{0,5} & \delta_{0,4} & \delta_{0,3} & \delta_{0,2} & \delta_{0,1} & & & & & \\
 & \delta_{1,1} & \delta_{1,2} & \delta_{1,3} & \delta_{1,4} & \delta_{1,5} & \delta_{1,4} & \delta_{1,3} & \delta_{1,2} & \delta_{1,1} & & & & \\
 & & - & - & - & - & - & - & - & - & & & & \\
 & & & - & - & - & - & - & - & - & - & - & & \\
 & & & \delta_{N-1,1} & \delta_{N-1,2} & \delta_{N-1,3} & \delta_{N-1,4} & \delta_{N-1,5} & \delta_{N-1,4} & \delta_{N-1,3} & \delta_{N-1,2} & \delta_{N-1,1} & & \\
 & & & & \delta_{N,1} & \delta_{N,2} & \delta_{N,3} & \delta_{N,4} & \delta_{N,5} & \delta_{N,4} & \delta_{N,3} & \delta_{N,2} & \delta_{N,1} & \\
 & & & & & 1 & 502 & 14608 & 88234 & 156190 & 88234 & 14608 & 502 & 1 \\
 & & & & & -1 & -54 & -134 & 434 & 0 & -434 & 134 & 54 & 1 \\
 & & & & & -1 & -6 & 34 & -46 & 0 & 46 & -34 & 6 & 1 \\
 & & & & & -1 & 6 & -14 & 14 & 0 & -14 & 14 & -6 & 1
\end{pmatrix}$$

Initial state

To evaluate the initial vector $\alpha^0$and the solution space $u(x,t)$ is decomposed into complex form as follows:

$$u(x,t)=X(x,t)+iY(x,t). \quad (11)$$

Here, X and Y are real coefficients. We derive the associated coupled pair of real differential equations by substituting equation (11) into equation (4).

$$X_t-Y_{xx}=0 \quad \text{and} \quad X_t+Y_{xx}=0 \quad (12)$$

In the collocation method implementation, loops are recognised as collocation sites for systems. (11) and (12). The nonic B-splines $B_m(x)$ provide solutions for global approximation
by expressing $X(x,t)$ and $Y(x,t)$ as expansions:

$$X_N(x,t)=\sum_{m=-4}^{N+4}\alpha_m(t)B_m(x), \quad \text{and} \quad Y_N(x,t)=\sum_{m=-4}^{N+4}\beta_m(t)B_m(x) \quad (13)$$

In this case, the parameters η_i and ζ_i must be found gradually. equation (12) and the B-splines found in equation (5) are used to estimate the solution of equation (4) by obtaining the initial parameters, α_m^0 and β_m^0. This leads to a system of (2N+18) equations containing 2N unknowns. equation (3) yields the subsequent equations derived from boundary conditions.

$$X_N^v(a,0) = (-\alpha_{-4}^0 - 6\alpha_{-3}^0 + 34\alpha_{-2}^0 - 46\alpha_{-1}^0 + 46\alpha_1^0 - 34\alpha_2^0 + 6\alpha_3^0 + \alpha_4^0) = 0$$
$$X_N^{vi}(a,0) = (\alpha_{-4}^0 - 2\alpha_{-3}^0 - 8\alpha_{-2}^0 + 34\alpha_{-1}^0 - 50\alpha_0^0 + 34\alpha_1^0 - 8\alpha_2^0 - 2\alpha_3^0 + \alpha_4^0) = 0$$
$$X_N^{vii}(a,0) = (-\alpha_{-4}^0 + 6\alpha_{-3}^0 - 14\alpha_{-2}^0 + 14\alpha_{-1}^0 - 14\alpha_1^0 + 14\alpha_2^0 - 6\alpha_3^0 + \alpha_4^0) = 0$$
$$X_N^{viii}(a,0) = (\alpha_{-4}^0 - 8\alpha_{-3}^0 + 28\alpha_{-2}^0 - 56\alpha_{-1}^0 + 70\alpha_0^0 - 56\alpha_1^0 + 28\alpha_2^0 - 8\alpha_3^0 + \alpha_4^0) = 0$$
$$X_N(x,0) = (\alpha_{m-4}^0 + 502\alpha_{m-3}^0 + 14608\alpha_{m-2}^0 + 88234\alpha_{m-1}^0 + 156190\alpha_m^0 + 88234\alpha_{m+1}^0 + 4608\alpha_{m+2}^0 + 502\alpha_{m+3}^0 + \alpha_{m+4}^0) = X(x_m,0)$$
$$X_N^v(b,0) = (-\beta_{N-4}^0 - 6\beta_{N-3}^0 + 34\beta_{N-2}^0 - 46\beta_{N-1}^0 + 46\beta_{N+1}^0 - 34\beta_{N+2}^0 + 6\beta_{N+3}^0 + \beta_{N+4}^0) = 0$$
$$X_N^{vi}(b,0) = (\beta_{N-4}^0 - 2\beta_{N-3}^0 - 8\beta_{N-2}^0 + 34\beta_{N-1}^0 - 50\beta_N^0 + 34\beta_{N+1}^0 - 8\beta_{N+2}^0 - 2\beta_{N+3}^0 + \beta_{N+4}^0) = 0$$
$$X_N^{vii}(b,0) = (-\beta_{N-4}^0 + 6\beta_{N-3}^0 - 14\beta_{N-2}^0 + 14\beta_{N-1}^0 - 14\beta_{N+1}^0 + 14\beta_{N+2}^0 - 6\beta_{N+3}^0 + \beta_{N+4}^0) = 0$$
$$X_N^{viii}(b,0) = (\beta_{N-4}^0 - 8\beta_{N-3}^0 + 28\beta_{N-2}^0 - 56\beta_{N-1}^0 + 70\beta_N^0 - 56\beta_{N+1}^0 + 28\beta_{N+2}^0 - 8\beta_{N+3}^0 + \beta_{N+4}^0) = 0. \quad (14)$$

Analogously, $Y_N(x,t)$ may be derived. The initial vector c_m^0 is computed as $c_m^0 = \alpha_m^0 + i\beta_m^0$, where i denotes the imaginary unit.

4. STUDY OF STABILITY

Examining the robustness of a methodology includes pinpointing the scenarios in which the divergence between theoretical expectations and numerical approximations remains limited with successive temporal iterations. Utilising the Von-Neumann technique aids in validating the stability of the method.

Consider

$$\phi_i^n = E\phi^n e^{i\varphi Kh}, \quad (15)$$

where $i = \sqrt{-1}$ represents an imaginary unit, E represents the amplitude, ϕ is the amplification factor, h represents the spatial step length, and φ is the mode number.

Now, applying equation (15) in the equation (9) and after simplification, we obtained

$$\phi^{n+1}[a_1e^{-4i\varphi h} + a_2e^{-3i\varphi h} + a_3e^{-2i\varphi h} + a_4e^{-i\varphi h} + a_5 + a_6e^{i\varphi h} + a_7e^{2i\varphi h} + a_8e^{3i\varphi h} + a_9e^{4i\varphi h}] = \phi^n[b_1e^{-4i\varphi h} + b_2e^{-3i\varphi h} + b_3e^{-2i\varphi h} + b_4e^{-i\varphi h} + b_5 + b_6e^{i\varphi h} + b_7e^{2i\varphi h} + b_8e^{3i\varphi h} + b_9e^{4i\varphi h}] \quad (16)$$

Applying Euler's formula $e^{\pm i\varphi h} = \cos(\varphi h) \pm i(\sin(\varphi h))$ to equation (16)

$$\frac{\phi^{n+1}}{\phi^n} = \frac{B_1 + iC_1}{B_2 - iC_2}, \quad (17)$$

where

$$B_1 = (b_1 + b_9)\cos(4\varphi h) + (b_2 + b_8)\cos(3\varphi h) + (b_3 + b_7)\cos(2\varphi h) + (b_4 + b_6)\cos(\varphi h) + b_5$$
$$C_1 = (b_1 - b_9)\sin(4\varphi h) + (b_2 - b_8)\sin(3\varphi h) + (b_3 - b_7)\sin(2\varphi h) + (b_4 - b_6)\sin(\varphi h)$$
$$B_2 = (a_1 + a_9)\cos(4\varphi h) + (a_2 + a_8)\cos(3\varphi h) + (a_3 + a_7)\cos(2\varphi h) + (a_4 + a_6)\cos(\varphi h) + a_5$$
$$C_2 = (a_1 - a_9)\sin(4\varphi h) + (a_2 - a_8)\sin(3\varphi h) + (a_3 - a_7)\sin(2\varphi h) + (a_4 - a_6)\sin(\varphi h). \quad (18)$$

Check the stability condition $\left|\frac{\phi^{n+1}}{\phi^n}\right| \le 1$, we get

$$B_1^2 + C_1^2 - B_2^2 - C_2^2 \le 1. \quad (19)$$

Consequently, the proposed scheme exhibits unconditional stability.

5. NUMERICAL ILLUSTRATIONS AND CONVERSATIONS

Three test problems are examined to assess the present study's efficiency and accuracy. The accuracy of the methods is evaluated in this section by computing the error norms L_2 and the maximum absolute error norm L_∞, defined as follows:

By computing both the L_2 and L_∞, error norms for each test problem, the study can effectively evaluate the accuracy of the methods across different scenarios and provide a comprehensive assessment of their performance. These error norms serve as valuable metrics for quantifying the discrepancy between computed and exact solutions, thereby informing decisions regarding the suitability and reliability of the computational methods employed in the study.

$$L_{\infty} = \max_{0 \le m \le N} |u_m - v_m|$$

$$L_2 = \sqrt{h \sum_{m=0}^{N} |(u_m - v_m)^2|}$$

Where u_m and v_m represent the exact and numerical solutions, respectively.
MATLAB R2019 and MATHEMATICA software were utilised for numerical simulations.

Example-1. Solve the equation (4) commencing with the exact solution within the domain

$$v(x,t) = e^{\frac{-it+x}{2}} \ , \ x \in [0,\pi]$$

followed by the initial condition $v(x,0) = e^{\frac{x}{2}}$ and boundary conditions

$$v(-\pi,t) = v(\pi,t) = v_{5x}(-\pi,t) = v_{5x}(\pi,t) = v_{6x}(-\pi,t) = v_{6x}(\pi,t) = v_{7x}(-\pi,t) = v_{7x}(\pi,t) = v_{8x}(-\pi,t) = v_{8x}(\pi,t) = 0, t \in [0,T].$$

Solution.

The numerical solution, along with error norms L_2 and L_{∞}, incorporating absolute error at parameters $\Delta t = 0.01$, $h = 0.05$, $x \in [0,\pi]$, and $x \in [0,\pi]$ fo or various time steps t is as follows:

Observations from Table 1.

- As time progresses, the absolute errors in the numerical solution tend to increase. This indicates that the accuracy of the numerical solution decreases over time.
- Conversely, the error norms L_2 *and* L_{∞} decrease as time advances from $t = 2$ to $t = 4$. This implies that, although the absolute errors increase, the overall discrepancy between the numerical and exact solutions decreases.

Table 1. Numerical solution with error norms at the parameters $\Delta t = 0.01, h = 0.05, x \in [0,\pi]$ for Example-1.

x	$t = 1$			$t = 4$		
	Numerical	Exact	Absolute Error	Numerical	Exact	Absolute Error
0.20	$0.329963 - 0.513877i$	$0.329963 - 0.513887i$	$9.712170e-06$	$-0.399172 + 0.462174i$	$-0.399181 + 0.462180i$	$9.841173e-06$
0.30	$0.364670 - 0.567915i$	$0.364665 - 0.567933i$	$1.843042e-05$	$-0.441153 + 0.51078i$	$-0.441163 + 0.510788i$	$1.172312e-05$
0.50	$0.445413 - 0.693649i$	$0.445403 - 0.693675i$	$2.800452e-05$	$-0.538829 + 0.623867i$	$-0.538838 + 0.623878i$	$1.364284e-05$
0.60	$0.492253 - 0.766603i$	$0.492247 - 0.766630i$	$2.672546e-05$	$-0.595497 + 0.689477i$	$-0.595508 + 0.689492i$	$1.795372e-05$
1.20	$0.896940 - 1.396860i$	$0.896933 - 1.396891i$	$3.129149e-05$	$-1.085095 + 1.256315i$	$-1.085086 + 1.256336i$	$2.239132e-05$
1.50	$1.210741 - 1.885569i$	$1.210733 - 1.885605i$	$3.741733e-05$	$-1.464716 + 1.695852i$	$-1.464713 + 1.695876i$	$2.402096e-05$
1.60	$1.338075 - 2.083884i$	$1.338067 - 2.083916i$	$3.310374e-05$	$-1.618761 + 1.874208i$	$-1.618759 + 1.874233i$	$2.529512e-05$
1.70	$1.478800 - 2.303052i$	$1.478793 - 2.303083i$	$3.227069e-05$	$-1.789007 + 2.071320i$	$-1.789005 + 2.071348i$	2.837233e-05
2.50	$3.291092 - 5.125581i$	$3.291114 - 5.125607i$	$3.435566e-05$	$-3.981497 + 4.609828i$	$-3.981504 + 4.609870i$	$4.318684e-05$
3.10	$5.996802 - 9.339465i$	$5.996802 - 9.339465i$	$8.881784e-16$	$-7.254774 + 8.399732i$	$-7.254774 + 8.399732i$	$1.776356e-15$
L_2	5.0676e – 05			4.8695e – 05		
L_{∞}	2.7220e – 05			2.6560e – 05		

Plotting Numerical Solution vs. Exact Solutions.

Figure 1 illustrates the natural part, and Figure 2 depicts the imaginary part of the numerical solutions compared to the exact solutions. The curves in these plots overlap closely, indicating that the numerical solutions are approximately equal to the analytical solution.

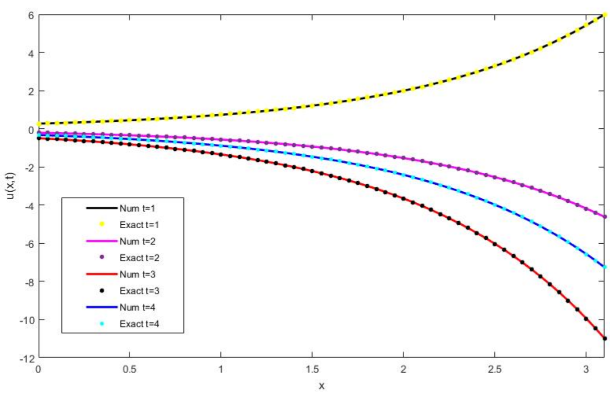

Figure 1. Comparison of numerical solution with exact solution (Real) of Example-1

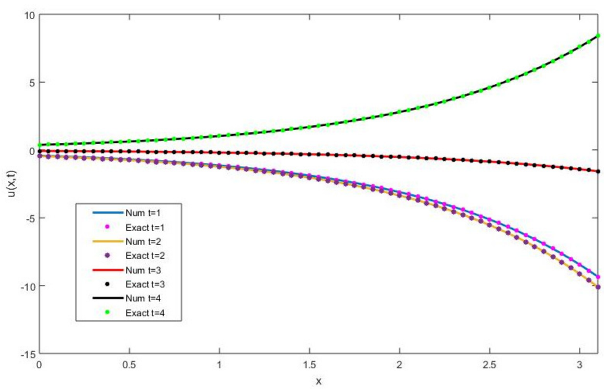

Figure 2. Comparison of numerical solution with analytical solution (Imaginary) of Example 1

3D Comparison of Numerical Solutions and Analytical Solutions:

Figures 3 and 4 present 3D plots comparing the numerical and analytical solutions. These plots, at parameters $h = \Delta t = 0.1, t = 4, x \in [0, \pi]$, demonstrate the approximate nature of the numerical solutions. The close alignment between the surfaces suggests that the numerical solutions closely resemble the analytical solutions.

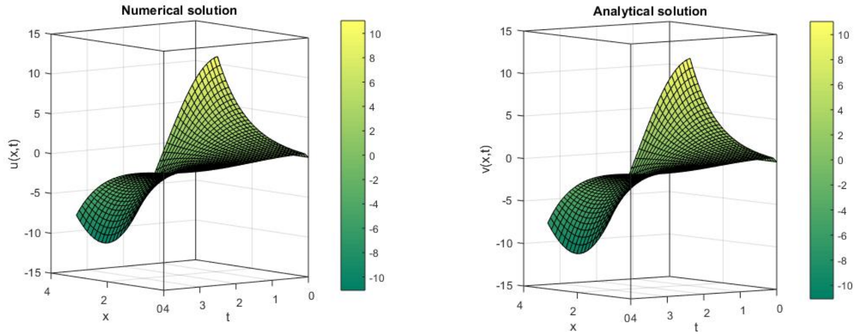

Figure 3. 3D plot of comparison of numerical with analytical solution (Real) of Example 1

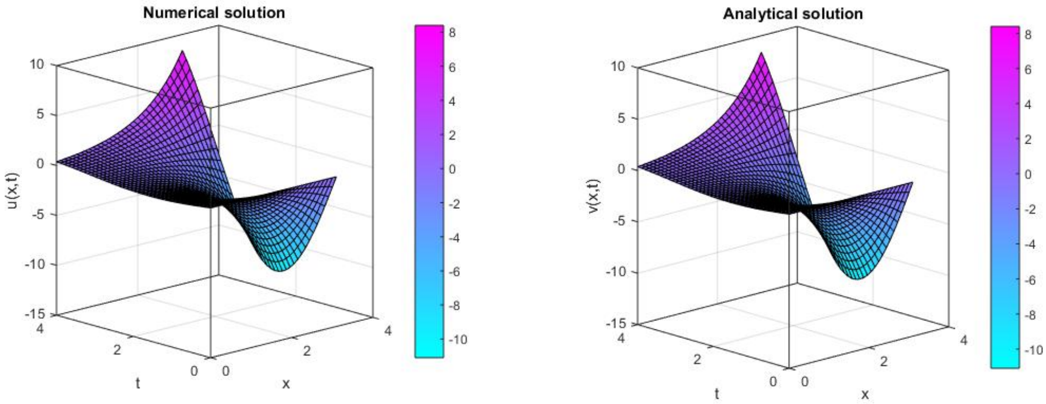

Figure 4. 3D plot of comparison of numerical with analytical solution (Imaginary) of Example 1
The 3D plot of the numerical solution of (a) real and (b) imaginary at $h = \Delta t = 0.1,\ t = 4, x \in [0, \pi]$.

6. CONCLUSION

This study provides a comprehensive approach to approximate solutions to the Schrödinger equation in quantum mechanics using the nonic B-spline technique. An intermediate level of knowledge in complex analysis is necessary for this strategy, especially when defining and applying B-spline collocation techniques. We stress that the B-spline collocation method can solve a broad range of analytically solvable quantum mechanical problems, not just the Schrödinger equation. We provide a reliable framework for solving the Schrödinger equation quickly by fusing the finite element method (FEM) with the nonic B-spline collocation method. We have thoroughly evaluated inaccuracy, stability, and convergence to verify the suggested plan's efficacy. We look into the three conservation constants' approximations and assess them.

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СКІНЧЕННО-РІЗНИЦЕВИЙ ПІДХІД ВИЩОГО ПОРЯДКУ В-СПЛАЙНА ДЛЯ РІВНЯННЯ ШРЕДІНГЕРА У КВАНТОВІЙ МЕХАНІЦІ

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У цій статті представлено новий чисельний метод розв'язування квантово-механічного комплексного рівняння Шредінгера (CSE). Методика поєднує схему Кренка-Ніколсона другого порядку, засновану на методі скінченних елементів (FEM) для часової дискретизації з ненічними В-сплайновими функціями для просторової дискретизації. Цей метод є безумовно стійким за допомогою аналізу стабільності фон-Неймана. Щоб перевірити нашу методологію, ми перевірили експеримент, використовуючи низку норм помилок, щоб порівняти експериментальні результати з аналітичними рішеннями. Наше дослідження підтверджує, що запропонований підхід працює краще, ніж поточні методи, забезпечуючи кращу точність і ефективність квантово-механічного аналізу помилок.

Ключові слова: *метод Кранка-Ніколсона; finite element scream; оцінка стійкості за фон-Нейманом; В-сплайн*