Spline Solution for the Nonlinear Schrödinger Equation

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Abstract

We develop an exponential spline interpolation method to solve the nonlinear Schrödinger equation. The truncation error and stability analysis of the method are investigated and the method is shown to be unconditionally stable. The conservation quantities are computed to determine the conservation properties of the problem. We will describe the method and present numerical tests by two problems. The numerical simulations results demonstrate the well performance of the proposed method.

Keywords

Nonlinear Schrödinger Equation, Exponential Spline Interpolation, Gross-Pitaevskii Equation, Mass and Energy Conservation

1. Introduction

Consider the following nonlinear Schrödinger equation

\[ mu_t + \lambda_1 u_{xx} + \lambda_2 |u|^2 u + \varepsilon(x,t)u = 0, \]  
\[ u(x,0) = u^0(x), x \in \mathbb{R}, \]  
where \( m = \sqrt{-1} \), \( u(x,t) \) is the complex-valued wave function. \( \lambda_1 \) and \( \lambda_2 \) are constant, \( \varepsilon(x,t) \) is a
bounded real function. This equation plays important roles in nonlinear physics. It can describe many nonlinear phenomena including plasma physics [1], hydrodynamics [1] [2], self-focusing in laser pulses [3], propagation of heat pulses in crystals, models of protein dynamics [4], quantum mechanics [5], models of energy transfer in molecular systems [6] and quantum mechanics and optical communication [7]-[9] and so on.

In the past few years a great deal of efforts has been expended to solve NLS equations. It is more difficult to find the analytical solutions of the NLS equation, so the study of the numerical solution of NLS equation in the theory and application is important. Its numerical solutions have been researched by many authors. For example, finite difference method [10] [11], quasi-interpolation scheme [12], quadratic B-spline finite element scheme [13], compact split-step finite difference method and pseudo-spectral collocation method [14] [15], exponential spline method [16], spline methods [17] [18], split-step orthogonal spline collocation method [19], a high-order and accurate method [20], linearly implicit conservative scheme [21].

The aim of this paper is to give an exponential spline interpolation method for the NLS equation. The paper is organized as follows. In Section 2, construction of the method is presented. The stability analysis of the scheme is investigated in Section 3. In Section 4, the computation of conserved quantities and error norms are given. In Section 5, two numerical examples are presented to demonstrate our theoretical results. The last section is a brief conclusion.

2. Construction of Exponential Spline Interpolation Method

We set up a grid in the \( x, t \) plane with grid points \( (x_i, t_j) \) and uniform grid spacing \( h \) and \( k \), where \( x_i = a + ih, h_{x_i} = x_{i+1} - x_i, i = 0, 1, 2, \ldots, N \) and \( t_j = jk, j = 0, 1, 2, \ldots \).

In the interval \( [x_i, x_{i+1}] \), a exponential spline function \( S_i(x, t_j) \) is given by

\[
S_i(x, t_j) = c_{ij}^0 + c_{ij}^1 (x - x_i) + c_{ij}^2 \psi_i (x - x_i) + c_{ij}^3 \phi_i (x - x_i),
\]

where \( c_{ij}^0, c_{ij}^1, c_{ij}^2, c_{ij}^3 \) are coefficients to be determined, \( \psi_i \) and \( \phi_i \) are the auxiliary functions which contain a stiffness parameter \( p_{i+1} \) which will be used to raise the accuracy of the method, on the support \( [x_i, x_{i+1}] \) and are given by

\[
\psi_i (x) = 2 \left[ \cosh \left( p_{i+1} (x - x_i) \right) - 1 \right] / p_{i+1}^2,
\]

\[
\phi_i (x) = 6 \left[ \sinh \left( p_{i+1} (x - x_i) \right) - p_{i+1} (x - x_i) \right] / p_{i+1}^2.
\]

Since the Taylor series expansions of the hyperbolic functions are

\[
\sinh (px) = px + \frac{(px)^3}{3!} + \frac{(px)^5}{5!} + \cdots,
\]

\[
\cosh (px) = 1 + \frac{(px)^2}{2!} + \frac{(px)^4}{4!} + \cdots.
\]

We note that \( \psi_i \) and \( \phi_i \) tend to \( (x - x_i)^2 \) and \( (x - x_i)^3 \) in the limit of \( p \) tending to zero, and in the opposite limit of \( p \) tending to infinity the nonlinear terms in \( \psi_i \) and \( \phi_i \) vanish as \( 1/p \).

So the exponential spline defined above share a number of interesting properties:

1. When \( p \to 0 \), \( S_i(x, t_j) \) reduces to cubic spline; when \( p \to \infty \), \( S_i(x, t_j) \) reduces to linear spline.

2. A change of character of the exponential spline function is from linear to third order polynomial on adjacent support intervals.

3. In the general case the stiffness parameters \( p \) are different on every interval which provides the extremely high flexibility of the exponential spline function.

We wish to find \( c_{ij}^0 \) in Equation (4), \( n = 1, 2, 3, 4 \), Letting \( M_{ij}^j = S_i^{(2)} (x, t_j) \) be the unknown second derivative of the exponential spline of interpolation at the grid points, we can obtain the following representation for \( S_i^j (x, t_j) \) on \( [x_i, x_{i+1}] \) in terms of the known interpolation data \( u_i', u_{i+1}' \) and the unknown spline second derivatives \( M_{ij}', M_{ij+1}' \).
The terms involving the values \( u_i^j \) and \( u_{i+1}^j \) represent the linear interpolation part of \( S_\lambda(x, t_j) \). The terms involving the second derivatives \( M_i^j \) and \( M_{i+1}^j \) introduce the curvature. The function \( S_\lambda(x, t_j) \) on the interval \( [x_{i-1}, x_i] \) is obtained with \( i-1 \) replacing \( i \) in Equation (9).

The continuity requirement for the first derivative \( (S_\lambda)_{x_i} \) at the point \( x_i \) yields the following equation:

\[
A_i M_{i+1}^j + (B_i + B_{i+1}) M_i^j + A_{i+1} M_{i+1}^j = \frac{u_{i+1}^j - u_i^j}{h_{i+1}} - \frac{u_i^j - u_{i-1}^j}{h_i},
\]

where \( A_i = \frac{h}{p_i^2} \sinh (p_i h_i) - \frac{p_i h_i}{p_i^2} \sinh (p_i h_i) \), \( B_i = \frac{p_i h_i}{p_i^2} \cosh (p_i h_i) - \sinh (p_i h_i) \).

**Remark 1.**

1. By expanding Equation (10) in Taylor series, the truncation error for Equation (10) is of the form

\[
T_i^j = \frac{u_{i+1}^j - u_i^j}{h_{i+1}} - \frac{u_i^j - u_{i-1}^j}{h_i} - A_i D^2 u_i^j - \frac{B_i + B_{i+1}}{2} D^2 u_i^j - A_{i+1} D^2 u_{i+1}^j
\]

\[
= \left[ \frac{h}{2} \left( \sigma_i + 1 \right) - A_i - A_{i+1} - B_i - B_{i+1} \right] (u_{2i})'_j + \left[ \frac{h}{6} \left( \sigma_i^2 - 1 \right) + A_i - A_{i+1} \right] h_i (u_{3i})'_j
\]

\[
+ \left[ \frac{h}{12} \left( \sigma_i^2 + 1 \right) - A_i - A_{i+1} \sigma_i \right] h_i^2 (u_{4i})'_j + \left[ \frac{h}{20} \left( \sigma_i^4 - 1 \right) + A_i - A_{i+1} \sigma_i^2 \right] h_i^4 (u_{5i})'_j
\]

\[
+ \left[ \frac{h}{30} \left( \sigma_i^4 + 1 \right) - A_i - A_{i+1} \sigma_i^2 \right] h_i^4 (u_{6i})'_j + O(h^5),
\]

where \( \sigma_i = h_{i+1}/h_i, \) \( h_{i+1} = x_{i+1} - x_i \).

For \( A_i = \frac{h}{12} (-\sigma_i^2 + \sigma_i + 1), A_{i+1} = \frac{h}{12} \sigma_i (\sigma_i^2 + \sigma_i - 1), B_i + B_{i+1} = \frac{h}{12} \sigma_i (\sigma_i^4 + 4 \sigma_i^2 + 4 \sigma_i + 1), \) the truncation error in space of the relation (10) is of \( O(h^6) \).

From Equation (10), we can obtain

\[
A_i M_{i+1}^j + (B_i + B_{i+1}) M_i^j + A_{i+1} M_{i+1}^j = \frac{\sigma_i u_{i+1}^j - (\sigma_i + 1) u_i^j + u_{i-1}^j}{\sigma_i h_i},
\]

or

\[
A_i M_{i+1}^{j+1} + (B_i + B_{i+1}) M_i^{j+1} + A_{i+1} M_{i+1}^{j+1} = \frac{\sigma_i^{j+1} u_{i+1}^{j+1} - (\sigma_i + 1) u_i^{j+1} + u_{i-1}^{j+1}}{\sigma_i h_i},
\]

Further, when \( \sigma_i = 1, \) then \( h = h_i = h_{i+1}, \) \( A_i = A_{i+1} = \frac{h}{12} \), \( B_i + B_{i+1} = \frac{10h}{12} \), the truncation error in space of the relation (10) is of \( O(h^5) \). Equation (2.7) can be rewritten as

\[
M_{i+1}^j + 10 M_i^j + M_{i-1}^j = \frac{12}{h^2} (u_{i+1}^j - 2u_i^j + u_{i-1}^j),
\]

\[
M_{i+1}^{j+1} + 10 M_i^{j+1} + M_{i-1}^{j+1} = \frac{12}{h^2} (u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}),
\]

In order to get the error estimates of Equation (10), we put \( E = e^{hD} \) in Equation (12), where \( E \) and \( D \) are the
shift and differential operators respectively, and expand them in powers of $hD$, we have

$$M'_j = \frac{12}{h^2} E - 2I + E^{-1} u'_j = u'_n(x_i, t_j) + O(h^4), i = 1, 2, \cdots, N. \quad (16)$$

Or

$$(u'_n)' = M'_j + O(h^4), i = 1, 2, \cdots, N. \quad (17)$$

At the grid point $(x_i, t_j)$, Equation (1) can be discretized by

$$m \frac{u_{i+1}^{j+1} - u_{i-1}^{j+1}}{2k} + \lambda_1 (u_{i+1}^{j+1} + u_{i-1}^{j+1}) + \lambda_2 \left[ |u_{i+1}^{j+1}|^2 + |u_{i-1}^{j+1}|^2 \right] + O(k^2) = 0, \quad (18)$$

From Equation (18), we have

$$M_{i+1}^{j+1} = -m \frac{u_{i+1}^{j+1} - u_{i-1}^{j+1}}{k\lambda_1} - \frac{1}{\lambda_1} \left( \lambda_1 \frac{|u_{i+1}^{j+1}|^2 + |u_{i-1}^{j+1}|^2}{2} \right) u_{i+1}^{j+1} + O(k^2), \quad (19)$$

$$M_{i}^{j+1} = -m \frac{u_{i}^{j+1} - u_{i}^{j}}{k\lambda_2} - \frac{1}{\lambda_2} \left( \lambda_2 \frac{|u_{i}^{j+1}|^2 + |u_{i}^{j}|^2}{2} \right) u_{i}^{j+1} + O(k^2), \quad (20)$$

$$M_{i-1}^{j+1} = -m \frac{u_{i-1}^{j+1} - u_{i-1}^{j}}{k\lambda_1} - \frac{1}{\lambda_1} \left( \lambda_1 \frac{|u_{i-1}^{j+1}|^2 + |u_{i-1}^{j}|^2}{2} \right) u_{i-1}^{j+1} + O(k^2), \quad (21)$$

Substituting Equation (19), Equation (20) and Equation (21) into Equation (15) and after some simplifications, we obtain

$$F_i u_{i+1}^{j+1} + F_{i+1} u_{i+1}^{j+1} + F_j u_{i}^{j+1} = F_i u_{i}^{j} + F_{i+1} u_{i+1}^{j} + F_{i+2} u_{i+2}^{j} \quad (22)$$

where $i = 1, 2, \cdots, N, j = 1, 2, \cdots, \delta_{i} e_1^{j+1} = e_1^{j+1} + \lambda_2 \left[ \frac{|u_{i+1}^{j+1}|^2 + |u_{i-1}^{j+1}|^2}{2} \right].$

The boundary conditions (2) and the system given in the Equation (22) consists of $N + 2$ equations in $N + 2$ unknowns. We can write this system in a matrix form as follows:

$$FU^{j+1} = F^* U^j, \quad (23)$$

where $U^j = (u_{i}^{j}, u_{i}^{j}, \cdots, u_{i-1}^{j})^T.$

Once the vectors $U^j$ are computed, $U^{n+1}, n = 1, 2, 3, \cdots$, unknown vectors can be found repeatedly by solving the recurrence relation (23).

### 3. Stability Analysis

Following the von Neumann technique, we first linearize the nonlinear term in Equation (18) by making the quantity $\delta_{i} \delta_{j}$ as locally constant $\delta$ and assume that the numerical solution can be expressed by means of a
Fourier series

\[ u_j^i = \eta_j \exp(m \varphi h) \]  

(24)

where \( m = \sqrt{-1} \), \( \eta_j \) is the amplitude at time level \( j \), \( \varphi \) is the wave number and \( h \) is the element size. Substituting Equation (24) into Equation (22), the amplification factor can be written as

\[ \eta = \frac{F_{1j} \exp(-m \varphi h) + F_{3j} \exp(m \varphi h)}{F_{1j} \exp(-m \varphi h) + F_{2j} \exp(m \varphi h)} \]  

(25)

Using Euler's formula, we have

\[ \eta = \frac{X_j + mY_j}{X_j + mY_j}, \]

where \( X_j = X_2 = 12 \left( \frac{\delta}{\lambda_j} + 1 \right) \cos(\varphi h) + \frac{10\delta}{\lambda_j} - \frac{24}{h^2} \), \( Y_2 = Y_1 = 4 \left( \frac{\lambda_j}{k} \right) \cos(\varphi h) + \frac{40}{k\lambda_j} \).

Since

\[ |\eta| = \sqrt{X_j^2 + Y_j^2} = 1, \]

Thus this method is unconditionally stable.

### 4. Computation of Conserved Quantities and Error Norms

The nonlinear Schrödinger equation possesses two conservation quantities:

1. **Mass conservation:**

\[ C_1^{\text{exact}} = \int_a^b |u(x,t)|^2 \, dx, \]  

Calculated by

\[ C_1 = h \sum_{j=0}^N |u_j^*|^2, \]  

(27)

2. **Energy conservation:** If \( \lambda_1(t) \) and \( \lambda_2(t) \) are independent of \( t \), then

\[ C_2^{\text{exact}} = \int_a^b \left( \lambda_1 \|u_j^*\| - \varepsilon \|u_j^*\|^2 - \frac{\lambda_2}{2} |u_j^*|^2 \right) \, dx, \]  

Calculated by

\[ C_2 = h \sum_{j=0}^N \lambda_j \|u_j^*\|^2 - \varepsilon \|u_j^*\|^2 - \frac{\lambda_2}{2} |u_j^*|^2, \]  

(29)

where \( u_j^* \) and \( u \) are the approximate solution at \( n \)-th time step at \( j \)-th node and exact solution, respectively.

The maximum error norm \( L_{\infty} \) and discrete root mean square error norm \( L_2 \) will be calculated

\[ L_{\infty} (h,k) = \|u - u^*\|_{\infty} = \max_{0 \leq x \leq L} |u(x) - u_j^*| \]  

(30)

\[ L_2 (h,k) = \|u - u^*\|_2 = \left( \sum_{j=0}^N \|u(x_j) - u_j^*\|^2 \right)^{1/2} \]  

(31)

The relative error of numerical solution is defined as

\[ E^r = \sqrt{\frac{\sum_{j=0}^N |u(x_j) - u_j^*|^2}{\sum_{j=0}^N |u_j^*|^2}} \]  

(32)
5. Numerical Results

In the section, we present the results of our numerical experiments for the proposed scheme described in the previous section.

Example 1. Consider the one dimensional Gross-Pitaevskii equation

\[ \mu u_t + \frac{1}{2} u_{xx} - \cos^2(x) u - |u|^2 u = 0, x \in [0, 2\pi], t \geq 0 \]  

(33)

With the analytical solution

\[ u(x,t) = e^{-\frac{2i}{\pi}} \sin(x), \]  

(34)

Conserved quantities and error norms at various times are recorded in Table 1. The real and imaginary parts of the numerical and exact solutions are tabulated in Table 2, the numerical results reveal the accuracy of the proposed method.

The absolute error at different space step sizes \( h \) at time \( t = 1 \) are shown in Figure 1, it can be seen that the absolute errors becomes smaller as decreasing \( h \).

Example 2. Consider the equation (1) with \( \lambda_1 = -1, \lambda_2 = 1 \),

\[ e(x,t) = 4(x - 2t)^2 - e^{-3(x-2t)^2}, \]  

(35)

The exact solution of this problem is

\[ u(x,t) = e^{(x-2t)^2 + i(x-3t)}, \]  

(36)

Table 1. Conserved quantities and error norms at various times for example 1 with \( k = 0.01, h = \frac{2\pi}{64}, a = 0, b = 2\pi \).

<table>
<thead>
<tr>
<th>( t )</th>
<th>( C_L )</th>
<th>( C_{Lr} )</th>
<th>( L_r )</th>
<th>( L_{rE} )</th>
<th>( E' )</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.0</td>
<td>3.14159265358952</td>
<td>5.00720563249462</td>
<td>1.4158e-004</td>
<td>2.5096e-004</td>
<td>1.4158e-004</td>
</tr>
<tr>
<td>10</td>
<td>3.14159265358946</td>
<td>5.00720563249418</td>
<td>2.8317e-004</td>
<td>5.0191e-004</td>
<td>2.8317e-004</td>
</tr>
<tr>
<td>20</td>
<td>3.14159265358965</td>
<td>5.00720563249524</td>
<td>5.6635e-004</td>
<td>1.0038e-003</td>
<td>5.6635e-004</td>
</tr>
<tr>
<td>30</td>
<td>3.14159265358984</td>
<td>5.00720563234957</td>
<td>8.4953e-004</td>
<td>1.5057e-003</td>
<td>8.4953e-004</td>
</tr>
</tbody>
</table>

\( C_{Lr}^{\text{exact}} = C_{Lr} = 3.14159265358979 \)

Table 2. The real and imaginary parts of the numerical and exact solutions for Example 1 with \( k = 0.001, h = \frac{2\pi}{64}, a = 0, b = 2\pi, t = 1 \).

<table>
<thead>
<tr>
<th>( x )</th>
<th>Real parts</th>
<th>Imaginary parts</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Exact solution</td>
<td>Approximation</td>
</tr>
<tr>
<td>( \frac{\pi}{4} )</td>
<td>0.05001875498139</td>
<td>0.05001908991577</td>
</tr>
<tr>
<td>( \frac{\pi}{2} )</td>
<td>0.07073720166770</td>
<td>0.07073767533643</td>
</tr>
<tr>
<td>( \frac{3\pi}{4} )</td>
<td>0.05001875498139</td>
<td>0.05001908991578</td>
</tr>
<tr>
<td>( \frac{5\pi}{4} )</td>
<td>-0.05001875498139</td>
<td>-0.05001908991578</td>
</tr>
<tr>
<td>( \frac{7\pi}{4} )</td>
<td>-0.07073720166770</td>
<td>-0.07073767533646</td>
</tr>
<tr>
<td>( \frac{9\pi}{4} )</td>
<td>-0.05001875498139</td>
<td>-0.05001908991577</td>
</tr>
</tbody>
</table>
Figure 1. The absolute error at different h for example 1 with $k=0.001, t=1$.

Table 3. Conserved quantities and error norms at various times for example 2 with $k=0.01, h=0.1, a=-10, b=20$.

<table>
<thead>
<tr>
<th>$t$</th>
<th>$C_1$</th>
<th>$C_2$</th>
<th>$L_\infty$</th>
<th>$L_2$</th>
<th>$E^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.25331413731550</td>
<td>-3.31870453365852</td>
<td>2.1940e-003</td>
<td>2.8448e-003</td>
<td>2.5411e-003</td>
</tr>
<tr>
<td>2</td>
<td>1.25331413731550</td>
<td>-3.33237042327679</td>
<td>2.3980e-004</td>
<td>3.2407e-003</td>
<td>2.8948e-003</td>
</tr>
<tr>
<td>3</td>
<td>1.25331413731550</td>
<td>-3.32685242595849</td>
<td>7.7694e-004</td>
<td>9.4702e-004</td>
<td>8.4592e-004</td>
</tr>
<tr>
<td>4</td>
<td>1.25331435202165</td>
<td>-3.31733074605112</td>
<td>2.2382e-003</td>
<td>2.5906e-003</td>
<td>2.3140e-003</td>
</tr>
</tbody>
</table>

$C_1^{\text{exact}} = C_1^* = 1.25331413731550, C_2^{\text{exact}} = C_2^* = -3.32358067657703$

Figure 2. The numerical solution at various times $t=1, 2, 3, 4$ with $k=0.01, h=0.1$. 

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Conserved quantities and error norms at various times are presented in Table 3. The numerical results reveal that the values of $C_1$ is almost constant while the values of $C_2$ differ slightly and the errors are very small.

The numerical solutions at various times are given in Figure 2. The numerical solutions and analytical solutions at time $t = 3$ and $t = 4$ are shown in Figure 3 and Figure 4, respectively. The absolute error at time $t = 3$ and $t = 4$ are plotted in Figure 5 and Figure 6, respectively. It observed that (1) the propagation of solitary wave is rightward while preserving unchanged shape; (2) our method gives a good approximation compared with the exact solutions.

6. Conclusion

A numerical method based on exponential spline interpolation function is applied to study a class of nonlinear Schrödinger equation. We use exponential spline collocation method, which results in tri-diagonal systems of
equations that can be solved efficiently by the Thomas algorithm. The numerical simulations confirm and demonstrate the reliability and efficiency of the schemes and tell us that the method is applicable technique, relatively simple and approximates the exact solution very well.

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**References**


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