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Solving the Generalized Nonlinear Schrödinger Equation via Quartic Spline Approximation[1]

Q. Sheng,*,[2] A. Q. M. Khaliq,† and E. A. Al-Said‡

*Department of Mathematics, University of Louisiana, Lafayette, Louisiana 70504-1010; †Department of Mathematics, Western Illinois University, Macomb, Illinois 61455; and ‡Department of Mathematics, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia
E-mail: SHENG@louisiana.edu

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This paper is concerned with a new conservative finite difference method for solving the generalized nonlinear Schrödinger (GNLS) equation $iu_t + u_{xx} + f(|u|^2)u = 0$. The numerical scheme is constructed through the semidiscretization and an application of the quartic spline approximation. Central difference and extrapolation formulae are used for approximating the Neumann boundary conditions introduced. Both continuous and discrete energy conservation and the stability property are investigated. The numerical method provides an efficient and reliable way for computing long-time solitary solutions given by the GNLS equation. Numerical examples are given to demonstrate our conclusions. © 2001 Academic Press

Key Words: generalized Schrödinger equation; solitary waves; quartic spline approximation; energy conservation; stability; semidiscretization.

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1. INTRODUCTION

There has been a high level of interest in computations of nonlinear waves, pulses, and beams. This is particularly the case for solitary waves, including the study of single solitary waves and collision of several solitary waves. Schrödinger type equations have been fundamental in modeling the physical processes.

In this paper, we study a highly efficient method of computations for the generalized nonlinear Schrödinger equation (GNLS),

$$i\frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} + f(|u|^2)u = 0, \quad -\infty < x < \infty,\ t \ge t_0, \tag{1.1}$$

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together with the initial condition

$$u(x, t_0) = \phi(x) + i\psi(x), \quad -\infty < x < \infty, \tag{1.2}$$

where $i = \sqrt{-1}$, and $f(s)$ is sufficiently smooth with $f(0) = 0$. Functions $\phi(x)$ and $\psi(x)$ are real valued and are sufficiently smooth in the domain considered. The most frequently used functions f include $f(s) = s^r$, $f(s) = 1 - e^{-s}$, $f(s) = s/(1+s)$, and $f(s) = \ln(1+s)$, $r > 0$ [1–3, 6, 7]. Equation (1.1) arises from plasma physics and quantum theory. It reduces to the nonlinear Schrödinger equation (NLS) as $f(s) = s$ [5, 17].

The nonlinear term in (1.1) helps prevent dispersion of the wave. It balances the forces of dispersion and nonlinearity in solutions. These balanced solutions include different kinds of interesting solitary waves including the single solitary wave and collision of two or more solitons [15].

It is observed that, when the nonlinear term in (1.1) is canceled, we obtain the linear version of the Schrödinger equation (LS):

$$i\frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} = 0, \quad -\infty < x < \infty,\ t > t_0. \tag{1.3}$$

The above equation provides a useful governing law for the propagation of dispersive waves. In fact, for given initial profile $\exp(inx)$, the Fourier solutions of (1.2), $u(x,t) = \exp[i(nx - \omega(n)t)]$, $\omega(n) = n^2$, demonstrate clearly the relation with the wave number n. It can be further shown that the solution of (1.3) has an amplitude which decays like $1/\sqrt{t}$ as $t, x \to \infty$ with $x/t = c$ fixed [1, 17].

The x-free version of the GNLS,

$$i\frac{du}{dt} + f(|u|^2)u = 0, \quad t > t_0,$$

is also frequently considered in the investigation. This nonlinear equation possesses a general solution $u(t) = c\exp(i\alpha|c|^2 t)$ when $f(s) = \alpha s$, which is particularly important in the study of instabilities with respect to long-wave perturbations [11, 15].

It has been shown that Eq. (1.1) in general possesses an infinite set of conservation laws [10, 11]. The conservation in time of the energy can be expressed through the $\mathcal{L}_2$-norm,

$$\|u\|_2 = \sqrt{\int_{-\infty}^{\infty} |u(x,t)|^2\, dx} = c, \quad t > t_0, \tag{1.4}$$

or the weighted $\mathcal{L}_2$-norm,

$$\|u\|_{2,\gamma} = \sqrt{\int_{-\infty}^{\infty} \gamma(x)|u(x,t)|^2\, dx} = c, \quad t > t_0, \tag{1.5}$$

where $\gamma(x)$ is positive and c is a constant. Condition (1.4), or (1.5), provides an $\mathcal{L}_2$-boundness of the solution and plays a crucial part in the dynamics of the solitary wave models. The initially unstable Fourier modes of the wave draw energy from the stable modes, but because of conservation, the process must come to an end, and, in fact, it is possible for the energy to return to its initial distribution among the modes. This is referred to as the so-called Fermi–Pasta–Ulam recurrence [1, 10, 17].

Various kinds of numerical methods can be found nowadays for simulating solutions of NLS and GNLS problems (for instance, cf. [5, 8, 10–12, 15] and references therein). Much effort has been devoted to developing algorithms which conserve the energy of the wave exactly when time advances. Among the most popular and efficient finite difference schemes, are five classical algorithms using semidiscretization, moving grid adaptation, and Crank–Nicolson type approximations [4, 5, 10, 16] and those based on pseudospectral considerations [9]. In [5], several important different schemes are tested, analyzed, and compared.

During the recent development in spline collocated computations and higher order approximations, in 1996, quartic spline collocations are introduced and studied for computing solutions of partial differential equations with singularities [14, 18, 19]. In this paper, we will extend the existing concept and propose a special quartic spline approximation to replace conventional finite differences in approximating the spatial derivative. Properties of the discrete conservation law and weak-conservation law of the numerical scheme will be investigated under the ℓ_2-norms, which is consistent with the original $\mathcal{L}_2$-norms used for continuous problems. Numerical examples will be given.

2. SEMIDISCRETIZATIONS VIA QUARTIC SPLINE

Under the assumption that $\lim |x| \to \infty |u| = 0$, $t_0 < t \le T$, for the purpose of computation, we may consider as an approximation to the original GNLS problem (1.1), (1.2) the initial boundary value problem

$$i\frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} + f(|u|^2)u = 0, \quad a \le x \le b, t_0 < t \le T, \tag{2.1}$$

$$u(x, t_0) = \phi(x) + i\psi(x), \quad a \le x \le b, \tag{2.2}$$

$$\frac{\partial u}{\partial x}(a, t) = \frac{\partial u}{\partial x}(b, t) = 0, \quad t_0 < t \le T, \tag{2.3}$$

where $|a|$ and $|b|$ are sufficiently large.

We further express the solution of (2.1)–(2.3) as

$$u(x, t) = p(x, t) + iq(x, t), \quad a \le x \le b, t \ge t_0,$$

where p and q are real functions. Let $v = (p, q)^T$. Under the new notation, the problem (2.1)–(2.3) can be written as

$$\frac{\partial v}{\partial t} + A\frac{\partial^2 v}{\partial x^2} + g(v) = 0, \quad a \le x \le b, t_0 < t \le T, \tag{2.4}$$

$$v(x, t_0) = (\phi(x), \psi(x))^T, \quad a \le x \le b, \tag{2.5}$$

$$\frac{\partial v}{\partial x}(a, t) = \frac{\partial v}{\partial x}(b, t) = 0, \quad t_0 < t \le T, \tag{2.6}$$

where

$$A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \text{and} \quad g(v) = f(|v|^2)Av.$$

Given that $N > 1$ and $h = (b - a)/(N - 1) < 1$, we define the spatial mesh region $\Omega = \{x_j : x_1 = a, x_j = x_{j-1} + h, j = 2, 3, \ldots, N, x_N = b\}$ over the interval $[a, b]$. The spatial derivative in (2.4) can then be approximated via the derivative of a quartic spline function $s = s(x, t)$:

$$\frac{\partial v}{\partial t} + A\frac{\partial^2 s}{\partial x^2} + g(v) = O(h^2), \quad x = x_j,\, j = 1, 2, \ldots, N,\, t_0 < t \le T. \tag{2.7}$$

Removing the local truncation error term, we obtain

$$\frac{dw_j}{dt} + Am_j + g(w_j) = 0, \quad j = 1, 2, \ldots, N,\, t_0 < t \le T, \tag{2.8}$$

where $w_j = w(x_j, t)$ are approximations of $v(x_j, t)$, and $m_j = s_{xx}(x_j, t)$, $x_j \in \Omega$.

For a given function $\nu(x)$, we denote

$$\delta_x^2 \nu_j = \nu_{j-1} - 2\nu_j + \nu_{j+1}, \quad j = 1, 2, \ldots, N.$$

According to the Numerov condition, we have the spline collocation relation

$$m_{j-1} + 10m_j + m_{j+1} = \frac{12}{h^2}\delta_x^2 s_j = \frac{12}{h^2}\delta_x^2 w_j + e_j, \quad j = 1, 2, \ldots, N. \tag{2.9}$$

It can be shown that the local truncation error e_j associated with the above approximation is given by

$$e_j = -\frac{h^4}{240} v_{x^6}(\xi_j, t),$$

where ξ_j is inside a neighborhood of x_j. The above indicates that it is a fourth-order approximation to the second derivative [19]. It follows immediately from (2.8), (2.9) that

$$\left(1 + \frac{1}{12}\delta_x^2\right)\frac{dw_j}{dt} + \frac{1}{h^2}A\delta_x^2 w_j + \left(1 + \frac{1}{12}\delta_x^2\right)g(w_j) = 0, \quad j = 1, 2, \ldots, N,\ t_0 < t \le T. \tag{2.10}$$

Based on different approximation strategies for the Neumann boundary conditions, we introduce the following methods.

Method 1. By means of the central difference approximation to (2.6), we obtain the relations

$$\begin{aligned} w(x_1 - h, t) &= w(x_2, t) + O(h^2), \quad w(x_N + h, t) = w(x_{N-1}, t) + O(h^2), \\ w_t(x_1 - h, t) &= w_t(x_2, t) + O(h^2), \quad w_t(x_N + h, t) = w_t(x_{N-1}, t) + O(h^2), \end{aligned}$$

where $t_0 < t \le T$.

Let $I \in \mathcal{R}^{2\times 2}$ be the identity matrix and $B \in \mathcal{R}^{2N\times 2N}$ be the block-diagonal matrix diag$\{A, A, \ldots, A\}$. By denoting $g_j = (\phi_j, \psi_j)^T$, $w_j = (p_j, q_j)^T$, and $\sigma_j = f(p_j^2 + q_j^2)$, $j = 1, 2, \ldots, N$, where $\phi_j = \phi(x_j)$, $\psi_j = \psi(x_j)$, $p_j = p(x_j)$, and $q_j = q(x_j)$, $x_j \in \Omega$, we may further define dimension-$2N$ vectors $\theta_0 = (g_1, g_2, \ldots, g_N)^T$ and $w = (w_1, w_2, \ldots, w_N)^T$. Adopting Method 1 for approximating the boundary values, from (2.5), (2.10) we obtain the second-order nonlinear scheme for approximating the initial boundary value problem (2.1)–(2.3),

$$P^{(1)}\frac{dw}{dt} + \left(\frac{12}{h^2}BQ^{(1)} + P^{(1)}RB\right)w = 0, \quad t > t_0, \tag{2.11}$$

$$w(t_0) = \theta_0, \tag{2.12}$$

where for the block-tridiagonal matrices $P^{(1)}$, $Q^{(1)}$, and $R(w)$, we have

$$\begin{aligned}
&P^{(1)}_{1,1} = P^{(1)}_{N,N} = 5I, \quad P^{(1)}_{1,2} = P^{(1)}_{N,N-1} = I,\\
&P^{(1)}_{j,j} = 10I, \quad P^{(1)}_{j,j-1} = P^{(1)}_{j,j+1} = I, \quad j = 2, 3, \ldots, N-1,\\
&Q^{(1)}_{1,1} = Q^{(1)}_{N,N} = -Q^{(1)}_{1,2} = -Q^{(1)}_{N,N-1} = -I,\\
&Q^{(1)}_{j,j} = -2I, \quad Q^{(1)}_{j,j-1} = Q^{(1)}_{j,j+1} = I, \quad j = 2, 3, \ldots, N-1,\\
&R_{j,j} = \sigma_j I, \quad j = 1, 2, \ldots, N.
\end{aligned}$$

We note that $P^{(1)}$ is symmetric, positive definite, and nonsingular.

Method 2. By means of Richardson's extrapolation for approximating (2.6), we have

$$\begin{aligned}
w(x_1 - h, t) &= -\frac{4}{11}w(x_1, t) + \frac{2}{11}w(x_2, t) + \frac{2}{11}w(x_3, t) + O(h^4),\\
w(x_N + h, t) &= \frac{2}{11}w(x_{N-2}, t) + \frac{2}{11}w(x_{N-1}, t) - \frac{4}{11}w(x_N, t) + O(h^4),\\
w_t(x_1 - h, t) &= -\frac{4}{11}w_t(x_1, t) + \frac{2}{11}w_t(x_2, t) + \frac{2}{11}w_t(x_3, t) + O(h^4),\\
w_t(x_N + h, t) &= \frac{2}{11}w_t(x_{N-2}, t) + \frac{2}{11}w_t(x_{N-1}, t) - \frac{4}{11}w_t(x_N, t) + O(h^4),
\end{aligned}$$

where $t_0 \le t < T$.

Using the above for eliminating unknowns located at $(x_1 - h, t)$ and $(x_N + h, t)$ in (2.10), we derive from (2.10) the following system:

$$\begin{aligned}
&106w_1' + 13w_2' + 2w_3' + \frac{12}{h^2}A(-26w_1 + 13w_2 + 2w_3)\\
&\quad + (-4\sigma_0 + 110\sigma_1)Aw_1 + (2\sigma_0 + 11\sigma_2)Aw_2 + 2\sigma_0 Aw_3 = 0,\\
&w_{j-1}' + 10w_j' + w_{j+1}' + \frac{12}{h^2}A(w_{j-1} - 2w_j + w_{j+1})\\
&\quad + \sigma_{j-1}Aw_j + 10\sigma_j Aw_j + \sigma_{j+1}Aw_{j+1} = 0, \quad j = 2, 3, \ldots, N-1,\\
&2w_{N-2}' + 13w_{N-1}' + 106w_N' + \frac{12}{h^2}A(2w_{N-2} + 13w_{N-1} - 26w_N)\\
&\quad + 2\sigma_{N+1}Aw_{N-2} + (11\sigma_{N-1} + 2\sigma_{N+1})Aw_{N-1} + (110\sigma_N - 4\sigma_{N+1})Aw_N = 0.
\end{aligned}$$

Note that quantities of σ_j, $x_j \in \Omega$, are extremely small as x_j are close enough to the left or right boundary according to our earlier assumption. We may therefore replace σ_0 in the first equation by $\sigma_1, \sigma_2, \sigma_3$ in turn, and σ_{N+1} in the last equation by $\sigma_{N-2}, \sigma_{N-1}, \sigma_N$ in turn.

It follows immediately that the system can be conveniently written into a matrix form

$$P^{(2)}\frac{dw}{dt}+\left(\frac{12}{h^2}BQ^{(2)}+P^{(2)}RB\right)w=0,\quad t>t_0, \tag{2.13}$$

$$w(t_0)=\theta_0, \tag{2.14}$$

where the block-tridiagonal matrices $P^{(2)}$ and $Q^{(2)}$ are defined through

$$\begin{aligned}
&P_{1,1}^{(2)}=P_{N,N}^{(2)}=106I,\quad P_{1,2}^{(2)}=P_{N,N-1}^{(2)}=13I,\quad P_{1,3}^{(2)}=P_{N,N-2}^{(2)}=2I,\\
&P_{j,j}^{(2)}=10I,\quad P_{j,j-1}^{(2)}=P_{j,j+1}^{(2)}=I,\quad j=2,3,\ldots,N-1,\\
&Q_{1,1}^{(2)}=Q_{N,N}^{(2)}=-26I,\quad Q_{1,2}^{(2)}=Q_{N,N-1}^{(2)}=13I,\quad Q_{1,3}^{(2)}=Q_{N,N-2}^{(2)}=2I,\\
&Q_{j,j}^{(2)}=-2I,\quad Q_{j,j-1}^{(2)}=Q_{j,j+1}^{(2)}=I,\quad j=2,3,\ldots,N-1.
\end{aligned}$$

Therefore $P^{(2)}$ is nonsingular and positive. The scheme (2.13), (2.14) is of fourth order ignoring the trivial replacements near the boundary.

3. CONSERVATION LAWS

An analog of (1.4), (1.5) in the finite domain problem (2.1)–(2.3) can be established as

$$\|u\|_{\bar{2}}=\sqrt{\int_a^b |u(x,t)|^2\,dx}=c,\quad t>t_0, \tag{3.1}$$

$$\|u\|_{\bar{2},\gamma}=\sqrt{\int_a^b \gamma(x)|u(x,t)|^2\,dx}=c,\quad t>t_0. \tag{3.2}$$

In view that strict conservation laws may be difficult to follow in actual computations, for given $0\le\epsilon\ll 1$, we may introduce the following pair of weaker conservation conditions:

$$|\|u\|_{\bar{2}}-c|\le\epsilon(t-t_0),\quad t>t_0, \tag{3.3}$$

$$|\|u\|_{\bar{2},\gamma}-c|\le\epsilon(t-t_0),\quad t>t_0. \tag{3.4}$$

Problems satisfying (3.3) or (3.4) are considered as weakly conservative.

Given that $u, v\in\mathcal{R}^{2N}$, we define the inner product

$$\langle u,v\rangle=u^Tv=\sum_{j=1}^{2N}u_jv_j.$$

It follows that, for $u=u(t)\in\mathcal{R}^{2N}$, $t_0<t\le T$, a discretized version of (3.1), (3.2) and (3.3), (3.4) can be defined as

$$\|u\|_2=\sqrt{\langle u,u\rangle}=c,\quad t_0<t\le T, \tag{3.5}$$

$$\|u\|_{2,\Gamma}=\sqrt{\langle \Gamma u,u\rangle}=c,\quad t_0<t\le T, \tag{3.6}$$

and

$$||\|u\|_2 - c| \le \epsilon(t - t_0), \quad t_0 < t \le T, \tag{3.7}$$

$$||\|u\|_{2,\Gamma} - c| \le \epsilon(t - t_0), \quad t_0 < t \le T, \tag{3.8}$$

respectively, where $\Gamma \in \mathcal{R}^{2N \times 2N}$ is nonsingular and positive.

THEOREM 1. *The semidiscretized problem* (2.11), (2.12) *is conservative.*

Proof. Let w be the solution of (2.11), (2.12). According to the symmetric property of $P^{(1)}$, and the skew symmetric property of A, we have

$$\left\langle \left(P^{(1)}\right)^{-1} B Q^{(1)} w, w \right\rangle = 0.$$

Similarly, we find that

$$\langle R(w)Bw, w\rangle = w^T \begin{pmatrix} \sigma_1 I & 0 & & & \\ 0 & \sigma_2 I & & 0 & \\ & & \ddots & & \\ & 0 & & \sigma_{N-1} I & 0 \\ & & & 0 & \sigma_N I \end{pmatrix} \times \begin{pmatrix} A & & & & \\ & A & & & \\ & & \ddots & & \\ & & & A & \\ & & & & A \end{pmatrix} w$$

$$= \sum_{j=1}^{N} \sigma_j w_j^T A w_j = 0.$$

However, we observe that

$$\frac{1}{2}\frac{d}{dt}\|w\|_2^2 = \left\langle \frac{dw}{dt}, w \right\rangle = \frac{12}{h^2}\left\langle \left(P^{(1)}\right)^{-1} B Q^{(1)} w, w \right\rangle + \langle RBw, w\rangle = 0, \quad t_0 < t \le T.$$

Thus the semidiscretized problem is conservative. ■

We note that discrete conservative laws using different norms can be found frequently in many publications. A well-known example is given in [11], where

$$\|u\| = \sqrt{\frac{1}{2}u_1^T u_1 + \sum_{j=2}^{N-1} u_j^T u_j + \frac{1}{2}u_N^T u_N}, \quad t_0 < t \le T.$$

However, many such norms, including this one, are not consistent with the original $\mathcal{L}_2$-norms used for the continuous problem. Thus the numerical schemes developed may not be conservative under the ℓ_2-norm we used. For instance, the semidiscretized scheme derived in [11] can be written as

$$u' = [S + T(u)]u,$$

where

$$S = -\frac{1}{h^2} \begin{pmatrix} -2A & 2A & & & \\ A & -2A & A & & \\ & & \ddots & & \\ & & A & -2A & A \\ & & & 2A & -2A \end{pmatrix},$$

$$T(u) = \operatorname{diag}(\sigma_1 A, \sigma_2 A, \ldots, \sigma_N A),$$

and $u = (u_1, u_2, \dots, u_N)^T$, $u_j \in \mathcal{R}^2$. By means of the skew symmetric property of A, we arrive at

$$\begin{aligned}\langle Su, u\rangle + \langle Tu, u\rangle &= -\frac{1}{h^2}u_1^T A u_2 - \frac{1}{h^2}u_N^T A u_{N-1}\\ &= -\frac{1}{h^2}(p_1q_2 - q_1p_2) - \frac{1}{h^2}(p_Nq_{N-1} - q_Np_{N-1}) \neq 0\end{aligned}$$

in general. Thus the scheme is not conservative according to (3.5).

THEOREM 2. *Let $|a|$, $|b|$ be sufficiently large. Then the solution of the problem* (2.13), (2.14) *is weakly conservative in the sense of* $\|\cdot\|_{2,P^{(1)}}$.

Proof. It is observed that

$$P^{(2)} = P^{(1)} + \tilde{P}, \quad Q^{(2)} = Q^{(1)} + \tilde{Q}, \tag{3.9}$$

in which for the block perturbation matrices $\tilde{P}$, $\tilde{Q}$,

$$\begin{aligned}&\tilde{P}_{1,1} = \tilde{P}_{N,N} = 101I, \quad \tilde{P}_{1,2} = \tilde{P}_{N,N-1} = 12I, \quad \tilde{P}_{1,3} = \tilde{P}_{N,N-2} = 2I,\\ &\tilde{Q}_{1,1} = \tilde{Q}_{N,N} = -25I, \quad \tilde{Q}_{1,2} = \tilde{Q}_{N,N-1} = 12I, \quad \tilde{Q}_{1,3} = \tilde{Q}_{N,N-2} = 2I,\end{aligned}$$

and the rest of $\tilde{P}_{i,j} = \tilde{Q}_{i,j}$ are null matrices. Let w be the solution of the problem (2.13), (2.14). Since that f is sufficiently smooth and the numerical scheme is at least of first order accuracy, for given ϵ, we have

$$\begin{aligned}\max_k\{|p_k - p_{k+1}|, |q_k - q_{k+1}|\} &\leq c_1 h,\\ \max_k |p_kq_{k+1} - q_kp_{k+1}| &\leq c_2\epsilon,\end{aligned}$$

where $c_1, c_2 > 0$ are constants. The above imply that

$$|\sigma_k - \sigma_{k-1}| \leq \tilde{c}\left|p_k^2 + q_k^2 - p_{k-1}^2 - q_{k-1}^2\right| \leq c_3 h.$$

However, for sufficiently large $|a|$, $|b|$, based on (2.3) we may assume that

$$\|w_j'\|_2 \leq \epsilon, \quad j = 1, 2, 3, N-2, N-1, N. \tag{3.10}$$

$$|p_1q_3 - q_1p_3|, \; |p_Nq_{N-2} - q_Np_{N-2}| \leq \epsilon. \tag{3.11}$$

Note that

$$\left\langle BQ^{(1)}w, w\right\rangle = 0,$$

$$\left\langle P^{(1)}RBw, w\right\rangle = w^T P^{(1)}RBw = \sum_{k=1}^{N-1}(\sigma_k - \sigma_{k+1})(q_kp_{k+1} - p_kq_{k+1})$$

due to the skew symmetric property of A. It follows therefore that

$$\left|\left\langle P^{(1)}RBw, w\right\rangle\right| \leq c_2c_3(N-1)h\epsilon = c_4\epsilon.$$

Substituting (3.9) into (2.13) and multiplying both sides of the equation by w, we readily obtain

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt}\|w\|^2_{2,P^{(1)}} &= \left\langle P^{(1)}\frac{dw}{dt}, w\right\rangle \\
&= \left\langle -\left(\frac{12}{h^2}BQ^{(1)} + P^{(1)}RB\right)w - \tilde{P}w' - \left(\frac{12}{h^2}B\tilde{Q} + \tilde{P}RB\right)w, w\right\rangle \\
&= -\left\langle P^{(1)}RBw, w\right\rangle - \langle \tilde{P}w', w\rangle - \left\langle\left(\frac{12}{h^2}B\tilde{Q} + \tilde{P}RB\right)w, w\right\rangle. \qquad (3.12)
\end{aligned}$$

It can be shown that

$$\begin{aligned}
\langle \tilde{P}w', w\rangle &= (w_1')^T(101w_1 + 12w_2 + 2w_3) + (w_N')^T(2w_{N-2} + 12w_{N-1} + 101w_N), \\
\langle B\tilde{Q}w, w\rangle &= 12\left(w_1^TAw_2 + w_N^TAw_{N-1}\right) + 2\left(w_1^TAw_3 + w_N^TAw_{N-2}\right) \\
&= 12[(p_1q_2 - q_1p_2) + (p_Nq_{N-1} - q_Np_{N-1})] + 2[(p_1q_3 - q_1p_3) \\
&\quad + (p_Nq_{N-2} - q_Np_{N-2})] \\
\left\langle \tilde{P}RBw, w\right\rangle &= 12\sigma_2w_1^TAw_2 + 2\sigma_3w_1^TAw_3 + 2\sigma_{N-2}w_N^TAw_{N-2} + 12\sigma_{N-1}w_N^TAw_{N-1} \\
&= 12\sigma_2(p_1q_2 - q_1p_2) + 2\sigma_3(p_1q_3 - q_1p_3) \\
&\quad + 2\sigma_{N-2}(p_Nq_{N-2} - q_Np_{N-2}) + 12\sigma_{N-1}(p_Nq_{N-1} - q_Np_{N-1}).
\end{aligned}$$

Recall (3.10)–(3.12). From the above we obtain immediately that

$$\left|\frac{d}{dt}\left(\|w\|^2_{2,P^{(1)}}\right)\right| \le c\epsilon,$$

where $c \ge 0$ is a constant. Therefore (2.13), (2.14) is weakly conservative. ■

4. TIME INTEGRATION AND LINEAR STABILITY

The formal solution of (2.11), (2.12), or (2.13), (2.14), can be expressed as

$$\begin{aligned}
w(t) &= E\left(\frac{-12(t-t_0)}{h^2}\left(P^{(\ell)}\right)^{-1}BQ^{(\ell)}\right)\theta_0 \\
&\quad - \int_{t_0}^{t} E\left(\frac{-12(t-\tau)}{h^2}P^{-1}BQ^{(\ell)}\right)R(w(\tau))Bw(\tau)\,d\tau, \quad t_0 < t \le T,\ \ell = 1, 2,
\end{aligned}$$

respectively, where $E(\alpha M) = \exp(\alpha M)$ is the matrix exponential operator involved. A direct calculation via the above, however, can be difficult. Instead, based on Method 1 and Method 2, we consider the two adaptive difference schemes

$$\begin{aligned}
P^{(\ell)}\left(w^{(k+1)} - w^{(k)}\right) + \tau_k\left(\frac{12}{h^2}BQ^{(\ell)} + P^{(\ell)}R\left(\frac{1}{2}\left(w^{(k+1)} + w^{(k)}\right)\right)B\right)& \\
\times\left(\frac{1}{2}\left(w^{(k+1)} + w^{(k)}\right)\right) = 0, \quad k = 0, 1, \ldots,\ \ell = 1, 2,& \qquad (4.1)
\end{aligned}$$

$$w^{(0)} = \theta_0, \qquad (4.2)$$

where $w^{(k)}$ is an approximation to $w(t_k)$, and the adjustable time step size $0 < \tau_k = t_{k+1} - t_k < 1,\ k = 0, 1, 2, \ldots$ [13]. Both algorithms are of second order in time.

THEOREM 3. *The implicit scheme* (4.1), (4.2) *is conservative when* $\ell = 1$ *and weakly conservative in the sense of* $\|\cdot\|_{2,P^{(2)}}$ *when* $\ell = 2$.

Proof. Let $\ell = 1$. Similar to the proof of Theorem 1, we may observe that

$$\left\langle \left(P^{(1)}\right)^{-1} B Q^{(1)}\left(w^{(k+1)} + w^{(k)}\right), \left(w^{(k+1)} + w^{(k)}\right)\right\rangle = 0,$$
$$\left\langle R\left(\frac{1}{2}\left(w^{(k+1)} + w^{(k)}\right)\right) B\left(w^{(k+1)} + w^{(k)}\right), \left(w^{(k+1)} + w^{(k)}\right)\right\rangle = 0.$$

Recall (4.1). We find immediately from the above that

$$\left\langle \left(w^{(k+1)} - w^{(k)}\right), \left(w^{(k+1)} + w^{(k)}\right)\right\rangle = \left\|w^{(k+1)}\right\|_2^2 - \left\|w^{(k)}\right\|_2^2 = 0.$$

Therefore the scheme is conservative. However, for $\ell = 2$, according to properties (3.10), (3.11), we have

$$\left\langle B\tilde{Q}\left(w^{(k+1)} + w^{(k)}\right), \left(w^{(k+1)} + w^{(k)}\right)\right\rangle \le c_1\epsilon,$$
$$\left\langle \tilde{P} R\left(\frac{1}{2}\left(w^{(k+1)} + w^{(k)}\right)\right) B\left(w^{(k+1)} + w^{(k)}\right), \left(w^{(k+1)} + w^{(k)}\right)\right\rangle \le c_2\epsilon.$$

Further,

$$\begin{aligned}\left\langle P^{(2)}\left(w^{(k)} - w^{(k+1)}\right), \left(w^{(k)} + w^{(k+1)}\right)\right\rangle &= \left\|w^{(k)}\right\|_{2,P^{(2)}}^2 - \left\|w^{(k+1)}\right\|_{2,P^{(2)}}^2 \\ + \left\langle \tilde{P} w^{(k)}, w^{(k+1)}\right\rangle - \left\langle \tilde{P} w^{(k+1)}, w^{(k)}\right\rangle &\le \left\|w^{(k)}\right\|_{2,P^{(2)}}^2 - \left\|w^{(k+1)}\right\|_{2,P^{(2)}}^2 + c_3\epsilon,\end{aligned}$$

where c_1, c_2, and c_3 are positive constants. It therefore follows that

$$\left\|w^{(k+1)}\right\|_{2,P^{(2)}}^2 \le \left\|w^{(k)}\right\|_{2,P^{(2)}}^2 + c\epsilon,$$

and this indicates the weak conservation law. ■

THEOREM 4. *The adaptive schemes* (4.1), (4.2) *are unconditionally stable in the von Neumann sense.*

Proof. Noting the fact that $|a|$, $|b|$ can be arbitrarily large, and recalling (2.10), we study the systems derived from (4.1),

$$\begin{aligned}&\left(1 + \frac{1}{12}\delta_x^2\right)\left(w_j^{(k+1)} - w_j^{(k)}\right) + \frac{\tau_k}{2h^2} A\delta_x^2\left(w_j^{(k+1)} + w_j^{(k)}\right) \\ &\quad + \tau_k\left(1 + \frac{1}{12}\delta_x^2\right) g\left(\frac{1}{2}\left(w_j^{(k+1)} + w_j^{(k)}\right)\right) = 0, \quad j = 1, 2, \ldots, N,\ k = 0, 1, \ldots \end{aligned} \tag{4.3}$$

where $g(w) = f(p^2 + q^2)Aw$. Following conventional linearization process, we assume that

$$g(w) \approx f(\xi)Aw.$$

Replacing g by the above in (4.3), we obtain subsequently the following linearized systems of equations:

$$\left(1+\frac{1}{12}\delta_x^2\right)\left(w_j^{(k+1)}-w_j^{(k)}\right)+\frac{\tau_k}{2}\left\{\frac{1}{h^2}A\delta_x^2+f(\xi)A\left(1+\frac{1}{12}\delta_x^2\right)\right\}$$
$$\times\left(w_j^{(k+1)}+w_j^{(k)}\right)=0,\quad j=1,2,\ldots,N,\ k=0,1,\ldots. \tag{4.4}$$

Let $w_j^{(k)} = \exp(i\gamma hj)M^k\phi$ be the test function, where $\gamma \in \mathcal{R}$, $\phi \in \mathcal{R}^2$, and $M \in \mathcal{R}^{2\times 2}$ being the amplifying matrix. Substituting the test function into (4.4), we immediately obtain

$$(\alpha I+\beta A)M-(\alpha I-\beta A)=0,$$

where

$$\alpha=\frac{1}{6}(5+\cos\gamma h),\ \beta=\frac{\tau_k}{h^2}\left(\cos\gamma h-1+\frac{\alpha h^2}{2}f(\xi)\right).$$

Recall the skew symmetric property of A. It is easy to see that the matrix $\alpha I+\beta A$ is nonsingular and shares the same set of eigenvalues, $\{\alpha+\beta i, \alpha-\beta i\}$, with $\alpha I-\beta A$. Thus the maximal module of the eigenvalues of M is one. Hence the linearized scheme is nondissipative and the schemes (4.1), (4.2) are stable. ■

Let

$$F_k^{(\ell)}=\frac{12}{h^2}\left(P^{(\ell)}\right)^{-1}BQ^{(\ell)}+R\left(\frac{1}{2}\left(w^{(k+1)}+w^{(k)}\right)\right)B.$$

Then (4.1), (4.2) can be written in the embedded form

$$\left(I+\frac{\tau_k}{2}F_k^{(\ell)}\right)w^{(k+1)}=\left(I-\frac{\tau_k}{2}F_k^{(\ell)}\right)w^{(k)},\quad k=0,1,2,\ldots,\ \ell=1,2, \tag{4.5}$$
$$w^{(0)}=\theta_0, \tag{4.6}$$

which can be solved through employing a proper iterative method.

5. NUMERICAL TESTS

We consider numerical solutions of two standard NLS/GNLS model problems via the quartic spline associated scheme developed. The solutions give two different solitary waves. For simplicity, we let the step size, $\tau_k=\tau$, $k=0,1,2,\ldots,$ be uniform. Both methods developed work well in the computation and solutions are satisfactory. For the same testing problem, it is also observed that there is no significant difference between the numerical results given by Method 1 and those by Method 2. Therefore, for simplicity in discussions, we only present results obtained using Method 1 in the first numerical experiment, while presenting those given by Method 2 in the second experiment.

TABLE I
The Energy Conservation of Numerical Solution of (5.1), (5.2)

n	t_n	$\|u_n\|_2$	n	t_n	$\|u_n\|_2$	n	t_n	$\|u_n\|_2$
1	0.25	2.82842742	180	45.0	2.82842795	330	82.5	2.82842788
10	2.5	2.82842742	200	50.0	2.82842826	340	85.0	2.82842789
30	7.5	2.82842742	220	55.0	2.82842821	350	87.5	2.82842795
80	20.0	2.82842787	240	60.0	2.82842805	360	90.0	2.82842789
100	25.0	2.82842798	260	65.0	2.82842816	370	92.5	2.82842793
120	30.0	2.82842794	280	70.0	2.82842875	380	95.0	2.82842807
140	35.0	2.82842803	300	75.0	2.82842848	390	97.5	2.82842783
160	37.5	2.82842797	320	80.0	2.82842801	400	100.0	2.82842752

(i) Single soliton case. The cubic Schrödinger equation is also a basic GNLS equation. We consider the initial value problem

$$i\frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} + |u|^2 u = 0, \quad -\infty < x < \infty,\ t \ge 0, \tag{5.1}$$

$$u(x,0) = \sqrt{\frac{2\alpha}{\beta}}\exp\left(\frac{i\gamma x}{2}\right)\operatorname{sech}(\sqrt{\alpha}x), \quad -\infty < x < \infty, \tag{5.2}$$

where $\alpha = \beta = \gamma = 1$.

In our numerical calculation, boundary condition (2.3) is introduced with $a = -30$ and $b = 70$. We choose relatively large step sizes $h = 0.50$, $\tau = 0.25$. According to the exact solution of the problem (5.1), (5.2), we have $\|u\|_2 \approx 2.8284270$, $t \ge 0$. Let n denote the time level index, $t_n = n\tau$ be the corresponding time, and u_n be the numerical solution at the time level t_n. In Table I, we list the energy profile of the numerical solution u_n obtained via Method 1. There is no significant improvement found in the numerical solution for this particular example when Method 2 is used.

It is observed that the total energy of the numerical solution is preserved very well during the computation, though small disturbances start to appear at time level 80. These disturbances are possibly due to the rounding errors in the process and are insignificant compared to the total energy in the l_2-norm. The solution is plotted in Figs. 1–3. Figure 1 shows the real part, p_n, of u_n. Figure 2 shows the imaginary part, q_n, of u_n. In Fig. 3, we plot the modules of u_n at each grid point. In Fig. 4, we show detailed p_n when $0 \le t \le 10$ on the p–t plane as well as on the x–t plane for the solitary wave locations. Iterations are used in solving the nonlinear equations involved. It is found that the numerical error $\|u(t_n) - u_n\|_2$ increases linearly and reaches 10^{-3} at t_{400}. There is no visible change in the computed solitary wave pattern except that the wave shifts slightly to the right when time increases. This may indicate an accumulated round-off error and suggest further improvements of the programming and controls.

(ii) Collision of two solitons case. We consider interacting solitons for the cubic Schrödinger equation (5.1) with the initial condition

$$\begin{aligned} u(x,0) = \sqrt{\frac{2\alpha}{\beta}}\Bigg[&\exp\left(\frac{i\gamma_1 x}{2}\right)\operatorname{sech}(\sqrt{\alpha}x) \\ &+ \exp\left(\frac{i\gamma_2(x-\gamma_3)}{2}\right)\operatorname{sech}(\sqrt{\alpha}(x-\gamma_3))\Bigg], \quad -\infty \le x \le \infty, \end{aligned} \tag{5.3}$$

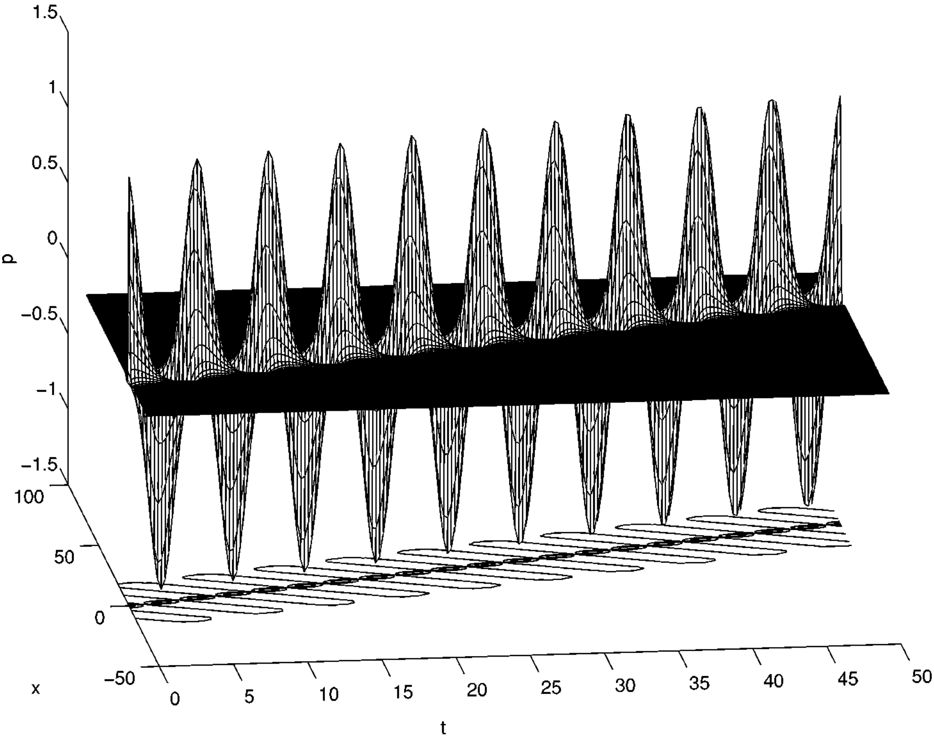

FIG. 1. The computed function $p_n(x, t)$ for problem (5.1), (5.2).

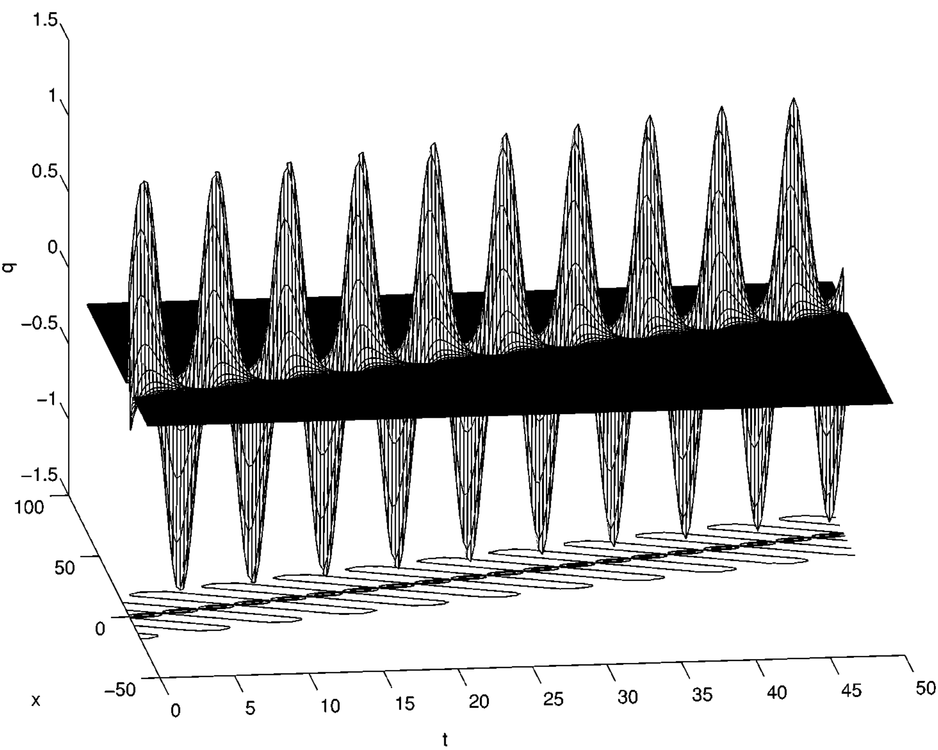

FIG. 2. The computed function $q_n(x, t)$ for problem (5.1), (5.2).

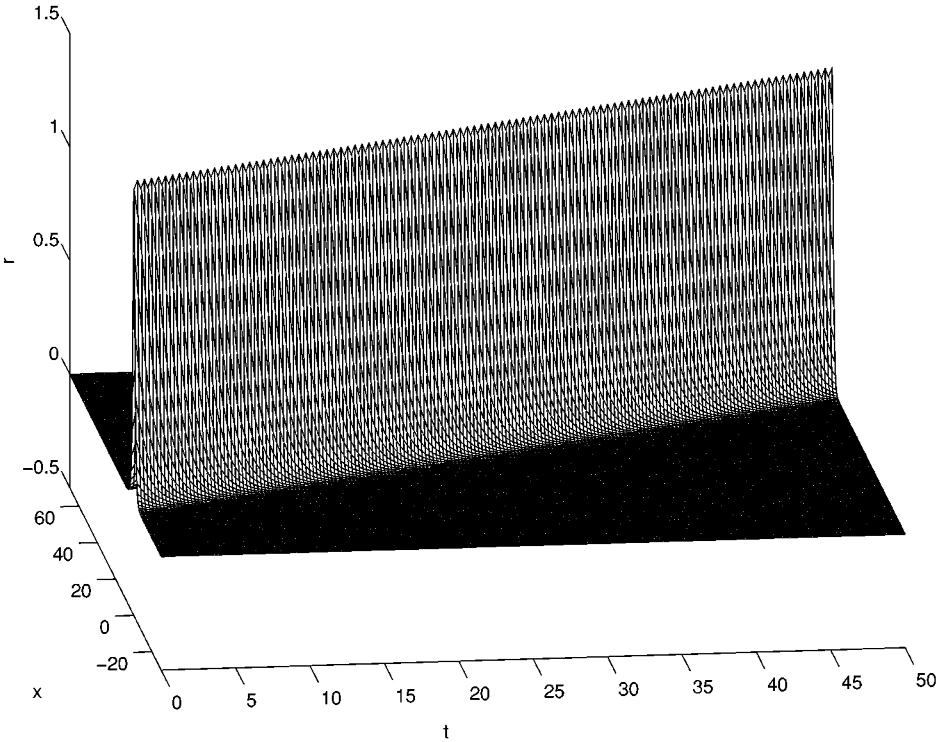

FIG. 3. The computed function $r_n(x,t) = \sqrt{p_n^2(x,t) + q_n^2(x,t)}$ for problem (5.1), (5.2).

where $\alpha = 0.5$, $\beta = \gamma_1 = 1$, $\gamma_2 = 0.1$, and the initial location of the slower solitary wave is $\gamma_3 = 25$. We choose $a = -20$, $b = 80$ and let $h = 0.5$ and $\tau = 0.25$ as in [11]. It is known that the total energy is $\|u(t)\|_2 \approx 4.756828290610$, $t > 0$, where u is the exact solution of (5.1), (5.3). In Table II, we give the energy profile of the numerical solution u_n given by Method 2.

Again, we observe that the approximation of total energy of the numerical solution is acceptable, and the energy conservation is well preserved. Iterations are used in the process for nonlinear equations and the average number of iterations is 2. We also note that, similar to the previous case, the computing error increases almost linearly and reaches about 10^{-3} in 200 time steps in l_2-norm due to the effect that the computed solution slowly shifts

TABLE II
The Energy Conservation of Numerical Solution of (5.1), (5.3)

n	t_n	$\|u_n\|_2$	n	t_n	$\|u_n\|_2$	n	t_n	$\|u_n\|_2$
2	0.5	4.75682827	70	17.5	4.75682833	140	35.0	4.75683406
10	2.5	4.75682829	80	20.0	4.75682836	150	37.5	4.75683670
20	5.0	4.75682827	90	22.5	4.75682832	160	40.0	4.75683754
30	7.5	4.75682839	100	25.0	4.75682950	170	42.5	4.75683587
40	10.0	4.75682838	110	27.5	4.75683008	180	45.0	4.75683338
50	12.5	4.75682831	120	30.0	4.75683320	190	47.5	4.75683333
60	15.0	4.75682833	130	32.5	4.75683252	200	50.0	4.75683469

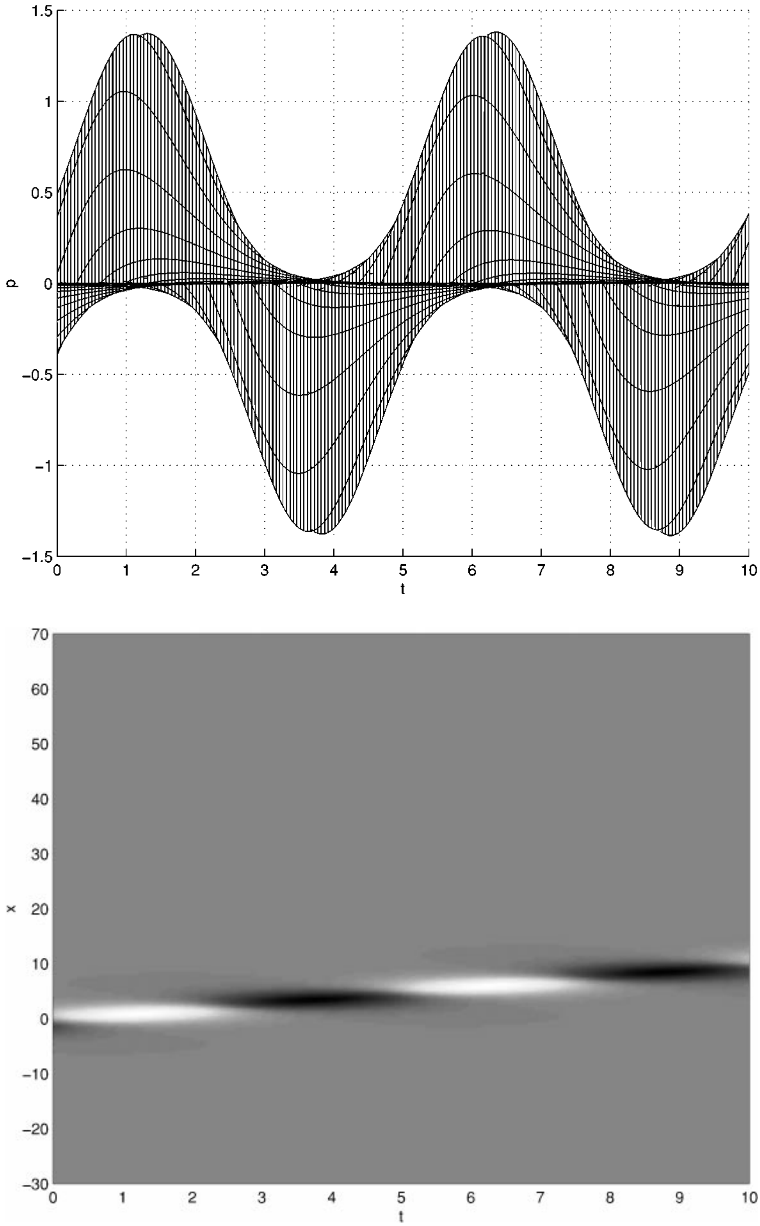

FIG. 4. Projections of the solitary function p_n in the first stage as $0 < t < 10$. (Above) Projection on the u–t plane. (Below) Projection on the x–t plane. The case for q_n is similar. Problem (5.1), (5.2) is considered.

to the right. This is possibly because of the accumulated round-off error or programming controlling error.

In Figs. 5 and 6, we plot the real part and imaginary part of the solution, respectively. The energy function, $\sqrt{p_n^2 + q_n^2}$, is plotted in Fig. 7. Finally, we show contour maps of p_n and q_n in Fig. 8. It is interesting to see that the solitary waves calculated agree well with predictions and studies in earlier investigations [1, 8, 10, 11, 17].

Thus we conclude that the conservative schedules are applicable and the computation procedures developed are reliable and accurate. The numerical methods may possess a

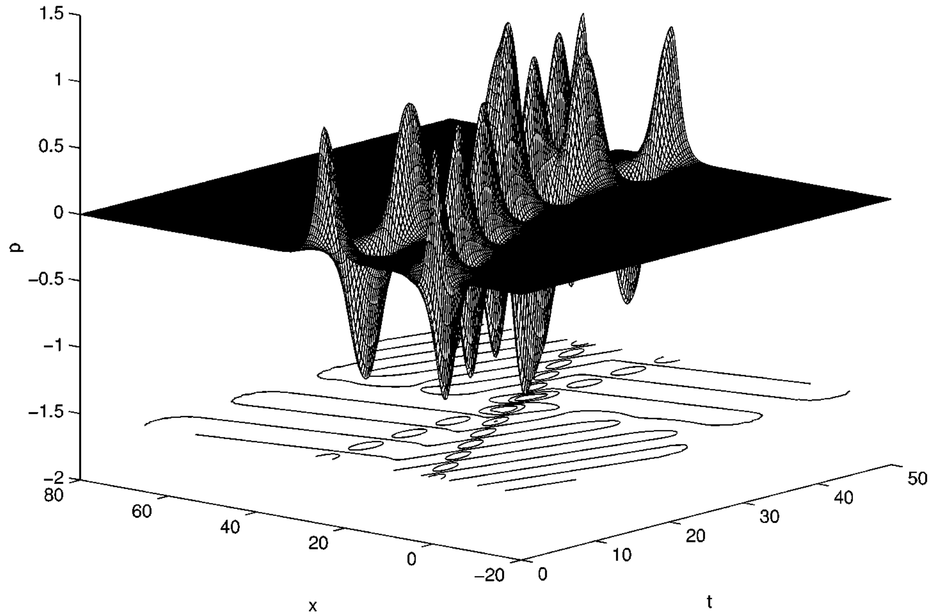

FIG. 5. The computed function $p_n(x, t)$ for problem (5.1), (5.3).

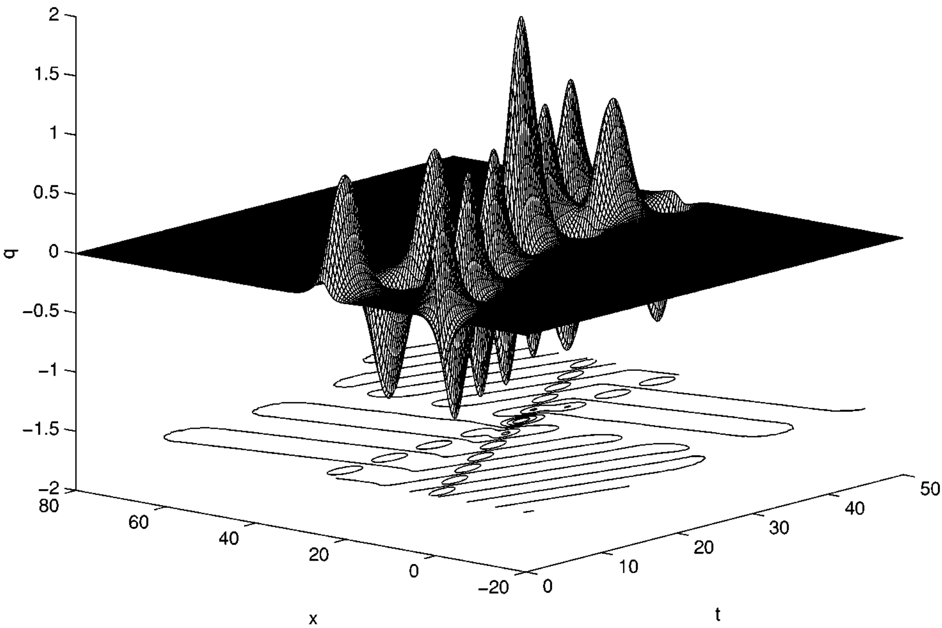

FIG. 6. The computed function $q_n(x, t)$ for problem (5.1), (5.3).

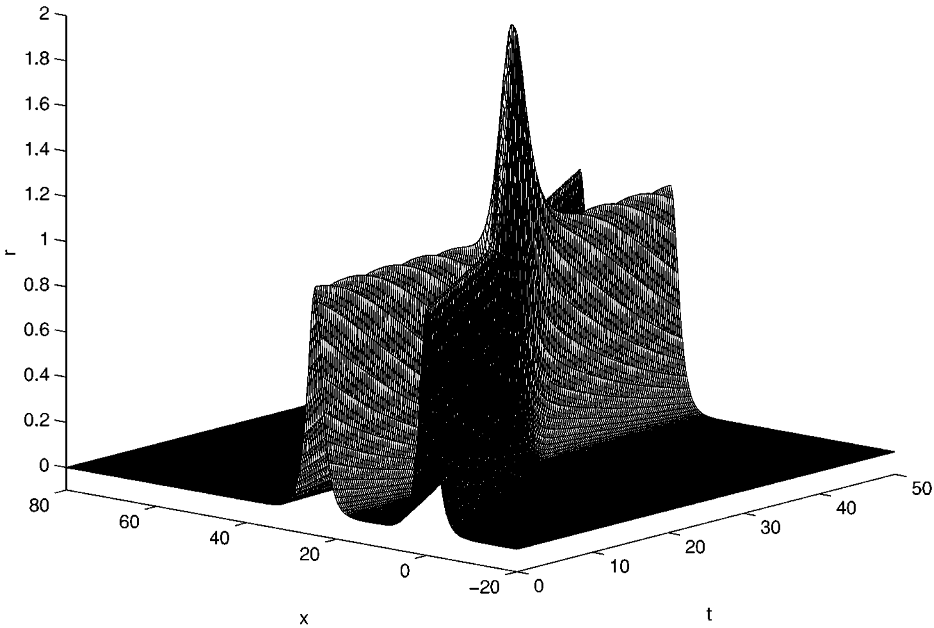

FIG. 7. The computed function $r_n(x,t) = \sqrt{p_n^2(x,t) + q_n^2(x,t)}$ for problem (5.1), (5.3).

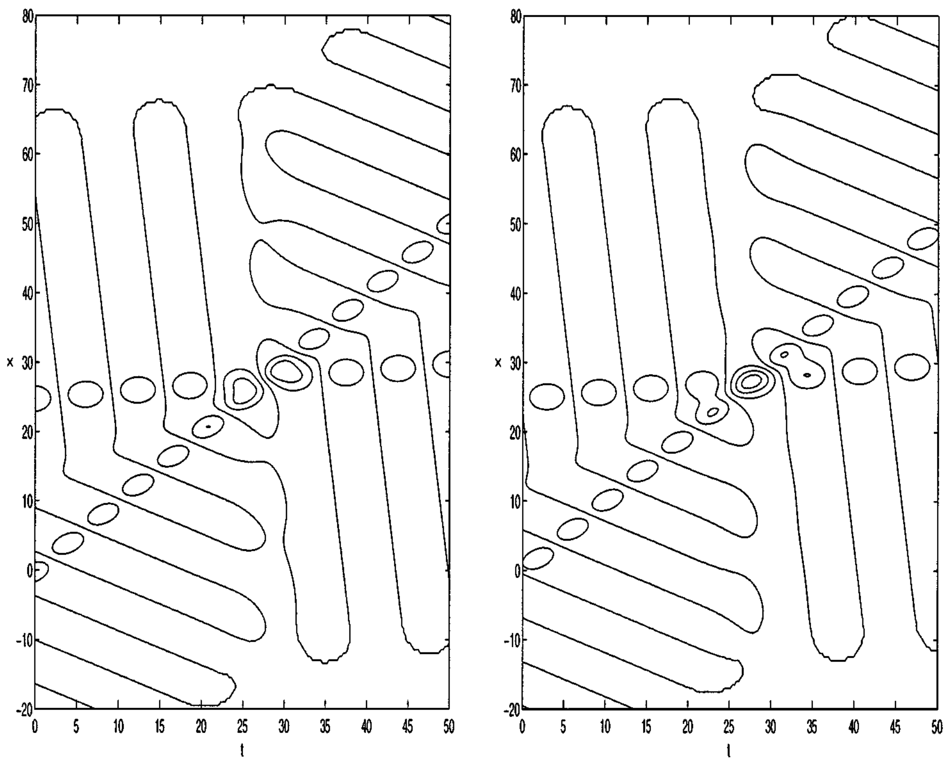

FIG. 8. Projections of the solitary functions $p_n(x,t)$ (left) and q_n (right) on the x–t plane ($0 < t < 50$, $-20 < x < 80$). Problem (5.1), (5.3) is considered.

strong potential for application and extension to solving more general and more difficult problems.

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