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Higher-order split-step Fourier schemes for the generalized nonlinear Schrödinger equation

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Dedicated to Professor E.S. Suhubi on the occasion of his 70th birthday

Abstract

The generalized nonlinear Schrödinger (GNLS) equation is solved numerically by a split-step Fourier method. The first, second and fourth-order versions of the method are presented. A classical problem concerning the motion of a single solitary wave is used to compare the first, second and fourth-order schemes in terms of the accuracy and the computational cost. This numerical experiment shows that the split-step Fourier method provides highly accurate solutions for the GNLS equation and that the fourth-order scheme is computationally more efficient than the first-order and second-order schemes. Furthermore, two test problems concerning the interaction of two solitary waves and an exact solution that blows up in finite time, respectively, are investigated by using the fourth-order split-step scheme and particular attention is paid to the conserved quantities as an indicator of the accuracy. The question how the present numerical results are related to those obtained in the literature is discussed.

Keywords: Split-step method; Fourier method; Generalized nonlinear Schrödinger equation; Solitary waves

1. Introduction

The generalized nonlinear Schrödinger (GNLS) equation is a nonlinear partial differential equation given by

$$iw_t + w_{xx} + q_1|w|^2w + q_2|w|^4w + iq_3(|w|^2)_x w + iq_4|w|^2w_x = 0, \tag{1.1}$$

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where $\mathrm{i} = \sqrt{-1}$, w is a complex-valued function of the spatial coordinate x and the time t, the parameters q_1, q_2, q_3 and q_4 are real constants and the subscripts t and x denote differentiation with respect to time and space, respectively. Compared to the nonlinear Schrödinger (NLS) equation with a cubic nonlinearity, the GNLS equation possesses both cubic and quintic nonlinearities and nonlinear terms that contain derivatives. It has been derived as a model equation governing the modulation of a quasi-monochromatic wave train in a weakly nonlinear, dispersive medium. Certain cases of the GNLS equation have found application in fluid dynamics, nonlinear optics and plasma physics (see [8,9] and references therein).

Some properties of the GNLS equation are summarized here. Assume that w and all its derivatives converge to zero sufficiently rapidly as $x \to \pm\infty$. Solutions of the GNLS equation subjected to these boundary conditions are known to satisfy some conservation laws [8,9]. According to these conservation laws, the conserved quantities

$$I_1 = \int_{-\infty}^{\infty} |w|^2 \, \mathrm{d}x \tag{1.2}$$

$$I_2 = \int_{-\infty}^{\infty} \{|w_x|^2 - \tfrac{1}{2}(2q_3 + q_4)|w|^2 \mathrm{Im}(ww_x^*) - \tfrac{1}{2}q_1|w|^4 + \tfrac{1}{6}[q_3(2q_3 + q_4) - 2q_2]|w|^6\} \, \mathrm{d}x \tag{1.3}$$

$$I_3 = \int_{-\infty}^{\infty} [2\,\mathrm{Im}(ww_x^*) - q_3|w|^4] \, \mathrm{d}x, \tag{1.4}$$

where the symbol $(*)$ denotes complex conjugation, remain constant in time [8,9]. Note that I_1 represents the theoretical L_2 norm of the system. Although the general case of the GNLS equation is known as a nonintegrable equation in the sense of the inverse scattering method, certain cases of the GNLS equation are completely integrable and such equations possess soliton solutions and an infinite number of conservation laws. For certain values of the coefficients and certain initial conditions, solutions of the general equation (1.1) experience finite-time blow up [8]. Only a few analytical solutions corresponding to some special cases of the GNLS equation are available [8,9]. Therefore, numerical studies are essential to develop an understanding of the phenomena related to the GNLS equation.

The difficulties in obtaining the exact solutions of nonlinear dispersive wave equations have stimulated considerable research effort on the development of numerical methods in recent years. One of the numerical methods employed for nonlinear dispersive wave equations is the split-step method proposed by Tappert [16]. The basic idea in the split-step method is to decompose the original problem into subproblems which are simpler than the original problem and then to compose the approximate solution of the original problem by using the exact or approximate solutions of the subproblems in a given sequential order. The choice of operator splitting one should use depends solely on a particular application, and no general method is known. However, for nonlinear dispersive wave equations that are derived by balancing the effects of dispersion and nonlinearity, such as the GNLS equation that we will be solving, an appropriate approach is to split the original problem into linear and nonlinear subproblems that take into account purely dispersive and purely nonlinear effects, respectively. For both a more complete account of split-step methods and a comprehensive list of references the reader is referred to a recent review [5]. While various numerical methods have been employed for the numerical solutions of the cubic NLS equation (see [4,15,17] and references therein) in which the split-step method profits from the existence of a simple analytical solution for the nonlinear subproblem, less attention has been paid to the numerical solution of the GNLS equation for which the cubic NLS equation is a special case. The GNLS equation has been solved numerically using the split step method in [9] by Pathria and Morris. They have compared

four different first-order split-step Fourier schemes, which exhibit different conservation properties, from a computational efficiency point of view [9].

The main purpose of this paper is to introduce higher-order split-step Fourier schemes for the GNLS equation and is to compare these schemes from a computational efficiency viewpoint. To this end, as in [9], the initial and boundary-value problem is decomposed into linear and nonlinear subproblems. A Fourier method is employed for the spatial discretizations of both linear and nonlinear subproblems. While the linear subproblem is treated exactly, a fourth-order Runge–Kutta scheme is used for the time integration of the nonlinear subproblem. Three different numerical schemes that are basically the first-order, second-order and fourth-order versions of the present split-step Fourier method are proposed. The present application of the split-step Fourier method to the GNLS equation is set in a framework which differs in two aspects from that presented in [9]. First, we solve numerically the nonlinear subproblem using a fourth-order Runge–Kutta scheme, whereas Pathria and Morris [9] have used an approximate analytical technique for the solution of the nonlinear subproblem. Another difference between [9] and the present study arises in consideration of the order of splitting formula. Pathria and Morris [9] have pointed out that higher-order splittings are possible but they have restricted their attention to the first-order splitting. Until now, there has been no study of what exactly happens when higher-order splittings are considered. It is not a great surprise that the method becomes more accurate at the cost of increasing computation time as the order of splitting increases. However, the question remains as to whether higher-order extensions of the method are worthwhile to use from a computational efficiency point of view. Therefore, in the present study, in addition to the first-order splitting, we consider higher-order splittings, in particular second- and fourth-order splittings, for solving the GNLS equation and compare the schemes in terms of computational efficiency. Also we discuss how the results obtained in the present study are related to those obtained in [8,9] (and those obtained in [10] by Robinson, where an orthogonal spline collocation semi-discretization has been used for the GNLS equation). For an application of the present split-step Fourier method to the complex modified Korteweg-de Vries equation, we refer the reader to [7].

In some earlier numerical studies of the GNLS equation, the contribution from the nonlinear derivatives have been ignored [2,3,13]. In [3] the cubic-quintic nonlinear Schrödinger equation has been solved using a first-order split-step Fourier scheme to confirm numerically the sufficient conditions derived analytically for bounded solutions. In [2] and [13] finite difference methods have been presented for the numerical solution of the equation $\mathrm{i}w_t + w_{xx} + f(|w|^2)w = 0$ which is a special case of the GNLS equation for $f(s) = s^p,\ p = 1, 2$.

The paper is organized as follows. In Section 2, it is shown how the split-step Fourier method can be reformulated for the GNLS equation. In Section 3, numerical experiments with various initial conditions for the GNLS equation are reported and the first- second- and fourth-order schemes are compared from a computational efficiency viewpoint. Comments and conclusions are contained in Section 4.

2. The numerical method

2.1. Review of the split-step method

We first present a brief summary of the split-step method for a general evolution equation in the form

$$w_t = (\mathcal{L} + \mathcal{N})w, \tag{2.1}$$

where $\mathcal{L}$ and $\mathcal{N}$ are linear and nonlinear operators, respectively, and $\mathcal{L}$ and $\mathcal{N}$ do not commute with each other. For instance, we have

$$\mathcal{L} = \mathrm{i}\frac{\partial^2}{\partial x^2}, \qquad \mathcal{N} = \mathrm{i}q_1|w|^2 + \mathrm{i}q_2|w|^4 - q_3(|w|^2)_x - q_4|w|^2\frac{\partial}{\partial x}$$

for the GNLS equation. The main idea in the split-step method is to approximate the exact solution of Eq. (2.1) by solving the purely linear and purely nonlinear equations in a given sequential order, in which the solution of one subproblem is employed as an initial condition for the next subproblem. This may be realized by using a solution operator $\varphi_n(\Delta t)$ that includes an appropriate combination of products of the exponential operators $\exp(\Delta t\mathcal{L})$ and $\exp(\Delta t\mathcal{N})$. This produces a splitting error due to the noncommutativity of $\mathcal{L}$ and $\mathcal{N}$, and at this stage the celebrated Baker-Campbell-Hausdorf formula [5,12] is very useful to reduce noticeably the splitting error. In what follows, we study the first-, second- and fourth-order versions of the method. To this end, we do not record information about higher-order splittings which will not be used in the present paper. According to the BCH formula, the first-order solution operator is given by

$$\varphi_1(\Delta t) = \exp(\Delta t\,\mathcal{L})\exp(\Delta t\,\mathcal{N}). \tag{2.2}$$

In the second-order version of the method, which has also received much attention in the literature, the solution operator is approximated by

$$\varphi_2(\Delta t) = \exp\left(\tfrac{1}{2}\Delta t\,\mathcal{N}\right)\exp(\Delta t\,\mathcal{L})\exp\left(\tfrac{1}{2}\Delta t\,\mathcal{N}\right) \tag{2.3}$$

which is symmetric, that is, $\varphi_2(\Delta t)\varphi_2(-\Delta t) = 1$. Approximations of higher order, that preserve the symmetry, can be constructed by a proper composition of the second-order symmetric approximation [5,6,14,19]. A fourth-order splitting is given in the form [6]

$$\varphi_4(\Delta t) = \varphi_2(\omega\,\Delta t)\varphi_2[(1-2\omega)\Delta t]\varphi_2(\omega\,\Delta t) \tag{2.4}$$

where $\omega = (2 + 2^{1/3} + 2^{-1/3})/3$. Note that the number of products of exponential operators increases with the order of decay of splitting error. According to Suzuki [14], the above formulae (2.2)–(2.4) have a minimal number of exponential operators for the corresponding order of splitting errors. The relations (2.2)–(2.4) are the basic schemes of the present numerical method. In general, the operators $\mathcal{L}$ and $\mathcal{N}$ in Eqs. (2.2)–(2.4) may be interchanged without affecting the order of the method.

2.2. Spatial discretization

Application of the numerical method requires truncation of the infinite interval to a finite interval $[a, b]$. For the numerical experiments considered, the constants a and b must be chosen sufficiently large so that the boundaries do not affect the propagation of solitary waves. We assume that $w(x, t)$ satisfies the periodic boundary condition $w(a, t) = w(b, t)$ for $t \in [0, T]$. If the spatial period is, for convenience, normalized to $[0, 2\pi]$ using the transformation $X = 2\pi(x - a)/(b - a)$, the GNLS equation becomes

$$\mathrm{i}w_t + \bar{p}w_{XX} + q_1|w|^2w + q_2|w|^4w + \mathrm{i}\bar{q}_3(|w|^2)_Xw + \mathrm{i}\bar{q}_4|w|^2w_X = 0 \tag{2.5}$$

where

$$\bar{p} = \left(\frac{2\pi}{b-a}\right)^2, \quad \bar{q}_3 = \left(\frac{2\pi}{b-a}\right) q_3, \quad \bar{q}_4 = \left(\frac{2\pi}{b-a}\right) q_4. \tag{2.6}$$

The interval $[0, 2\pi]$ is divided into N equal subintervals with grid spacing $\Delta X = 2\pi/N$, where the integer N is even. The spatial grid points are given by $X_j = 2\pi j/N$, $j = 0, 1, 2, ..., N$. The approximate solution to $w(X_j, t)$ is denoted by $W_j(t)$. The discrete Fourier transform of the sequence $\{W_j\}$, i.e.

$$\hat{W}_k = \mathcal{F}_k[W_j] = \frac{1}{N}\sum_{j=0}^{N-1} W_j \exp(-\mathrm{i}kX_j), \qquad -\frac{N}{2} \le k \le \frac{N}{2} - 1. \tag{2.7}$$

gives the corresponding Fourier coefficients. Likewise, $\{W_j\}$ can be recovered from the Fourier coefficients by the inversion formula for the discrete Fourier transform (2.7), as follows:

$$W_j = \mathcal{F}_j^{-1}[\hat{W}_k] = \sum_{k=-N/2}^{N/2-1} \hat{W}_k \exp(\mathrm{i}kX_j), \quad j = 0, 1, 2, \ldots, N-1. \tag{2.8}$$

where $\mathcal{F}$ denotes the discrete Fourier transform and $\mathcal{F}^{-1}$ its inverse. These transforms are efficiently computed using a fast Fourier transform (FFT) algorithm. Spatial derivatives of w, in both linear and nonlinear subproblems, may now be computed by first multiplying the Fourier coefficients, $\hat{W}_k$, by the power of ik corresponding to the order of the spatial derivative, and then applying the inverse Fourier transform. For example, the second-order derivative w_{XX} at (X_j, t) is computed by $\mathcal{F}_j^{-1}[-k^2\mathcal{F}_k[W_j]]$ and so on.

2.3. Time integration

As we have already mentioned in Section 1, we consider a split-step method for the GNLS equation, in which the linear equation

$$w_t - \mathrm{i}\bar{p}w_{XX} = 0 \tag{2.9}$$

and the nonlinear equation

$$w_t - \mathrm{i}q_1|w|^2w - \mathrm{i}q_2|w|^4w + \bar{q}_3(|w|^2)_X w + \bar{q}_4|w|^2 w_X = 0 \tag{2.10}$$

are solved in a given sequential order corresponding to one of the splitting formulas (2.2)–(2.4). The linear equation (2.9) is solved by means of the discrete Fourier transform and the advancements in time are performed according to

$$W_j^{m+1} = \mathcal{F}_j^{-1}[\exp(-\mathrm{i}\bar{p}k^2\,\Delta t)\mathcal{F}_k[W_j^m]] \tag{2.11}$$

where Δt is time step and W_j^m denotes the approximation to $w(X_j, m\,\Delta t)$. The nonlinear term in Eq. (2.10) is evaluated in physical space, while the spatial differentiation takes place in spectral space. Then the spatial discretization of the nonlinear partial differential Eq. (2.10) by a Fourier pseudospectral method can be written as

$$\dot{W}_j = \mathrm{i}(q_1|W_j|^2W_j + q_2|W_j|^4W_j) - \mathcal{F}_j^{-1}[\mathrm{i}k\bar{q}_3\mathcal{F}_k[|W_j|^2]]W_j - \mathcal{F}_j^{-1}[\mathrm{i}k\bar{q}_4\mathcal{F}_k[W_j]]|W_j|^2, \quad j = 0, 1, 2, \ldots, N-1 \tag{2.12}$$

where the superposed dot denotes differentiation with respect to time. For the time integration of this equation, as it has been pointed out in Section 1, instead of using an approximate analytical technique [9] we adopt rather a different approach and employ a fourth-order Runge–Kutta method. The choice of this numerical method is due to the fact that "the fourth-order Runge–Kutta method exhibits superior conservation of energy and other invariants" [11]. Now the total error involved in integrating from time t to time $t + \Delta t$ will be the sum of the temporal splitting error and the temporal discretization error of the ordinary differential equations given by (2.12).

The features of the method can be listed as follows: at each time step, depending on our choice of the splitting formulae (2.2)–(2.4), we advance the solution of the GNLS equation in various stages that involve the solution of linear and nonlinear subproblems. The method is first-order, second-order and fourth-order accurate in time depending on which splitting approximation is used. This will be verified through the numerical experiments in Section 3. Note that we use a Runge–Kutta method which has the same order of accuracy as the highest-order splitting approximation considered in this study. Moreover, alternating the order in the steps corresponding to Eqs. (2.9) and (2.10), that is, an interchange of the operators $\mathcal{L}$ and $\mathcal{N}$ in Eqs. (2.2)–(2.4), does not affect the order of the total error. Although a formal proof of this behavior is not presented here, it has been confirmed through the numerical experiments considered. Now the first-order split-step Fourier method for the GNLS equation can be summarized as follows: the advancement in time is carried out in two steps. Given the data W_j at any time step $t = t_m$, first advance the solution according to the nonlinear part, namely solve Eq. (2.12) using the fourth-order Runge–Kutta method for time integration. This intermediate solution becomes the initial data for the linear problem. Secondly, solve the linear problem using the discrete Fourier transform as indicated by Eq. (2.11). The extension of the first-order split-step scheme based on Eq. (2.2) to the second-order and fourth-order split-step schemes based on Eqs. (2.3) and (2.4), respectively, is straightforward.

3. Numerical experiments

To examine the performance of the suggested split-step schemes we now consider the three different problems described below. The conservation properties of the split-step schemes are examined by calculating discrete analogues of the conserved quantities I_1, I_2 and I_3. The relative errors in discrete approximations to the conservation integrals (1.2), (1.3) and (1.4) are denoted by δ_1, δ_2 and δ_3, respectively, and they are defined by $\delta_1 = |\bar{I}_1 - \bar{I}_{10}|/|\bar{I}_{10}|$, $\delta_2 = |\bar{I}_2 - \bar{I}_{20}|/|\bar{I}_{20}|$ and $\delta_3 = |\bar{I}_3 - \bar{I}_{30}|/|\bar{I}_{30}|$ where $\bar{I}_1$, $\bar{I}_2$, $\bar{I}_3$ and $\bar{I}_{10}$, $\bar{I}_{20}$, $\bar{I}_{30}$ represent the calculated values of the conserved quantities I_1, I_2, I_3 at inital and terminating times, respectively. Trapezoidal rule is used for the numerical quadrature of the integrals.

3.1. Solitary wave solution

The purpose of the present numerical experiment is to verify numerically (i) that the proposed split-step schemes exhibit the expected first-order, second-order and fourth-order convergence in time, (ii) that they give spectral accuracy in space and (iii) that the fourth-order scheme is computationally more efficient than the others. The GNLS equation has a travelling solitary wave solution [8–10], which has the form

$$w(x,t) = \left[\frac{4}{4 + 3\sinh^2(x - 2t - 15)}\right]^{1/2} \exp[\mathrm{i}\phi(x,t)] \tag{3.1}$$

$$\phi(x,t) = 2\tanh^{-1}[\tfrac{1}{2}\tanh(x-2t-15)] + x - 15 \tag{3.2}$$

for the choice of coefficients $q_1 = 1/2, q_2 = -7/4, q_3 = -1, q_4 = -2$. This solution represents a solitary wave initially at $x = 15$ moving to the right with speed 2. It follows from Eqs. (1.2)–(1.4) that the exact values of the conserved quantities I_1, I_2, I_3 for this problem are $I_1 = 2\ln 3$, $I_2 = -3/2 + 3.875\ln 3$, $I_3 = 4 - 9\ln 3$, respectively. As in [8,9], the problem is first solved on the space interval $5 \le x \le 35$ for times up to $t = 3$. We present in Fig. 1(a) the L_∞-errors of the first-order, second-order and fourth-order split-step schemes for the final time $t = 3$ as a function of N on a $\log_{10} - \log_{10}$ scale. We use the relation $\Delta t = \nu(\Delta x)^2$ to determine the value of Δt for a given Δx ($\equiv (b-a)/N$), where the value of ν is fixed at $\nu = 0.1$. We observe that the L_∞-errors decrease with increasing N until the boundaries start exerting

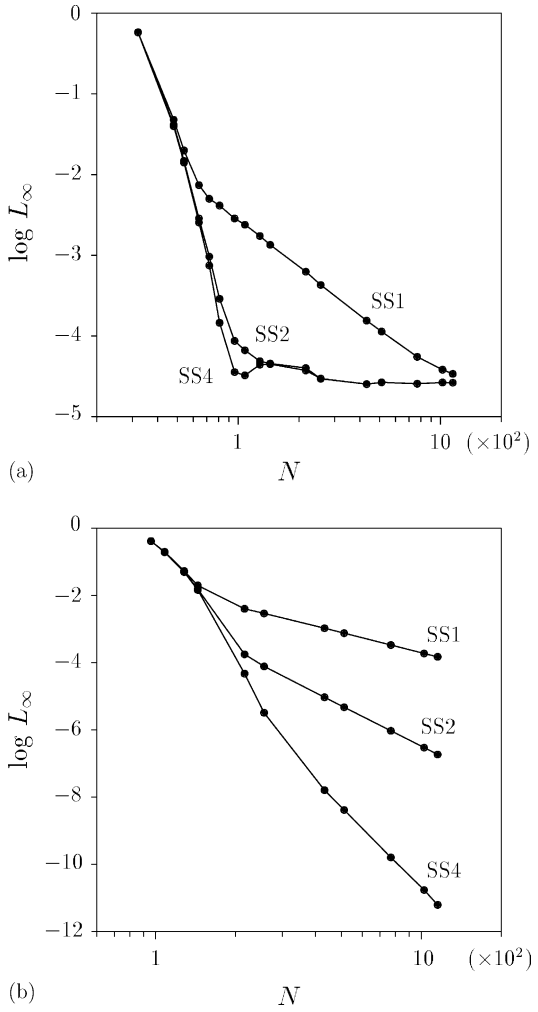

Fig. 1. The L_∞-errors for the terminating time $t = 3$ as a function of the number of spatial grid points for the first-order (SS1), second-order (SS2) and fourth-order (SS4) split-step Fourier schemes: (a) the space interval: $5 \le x \le 35$; (b) the space interval: $-20 \le x \le 60$.

Table 1
Comparison of the convergence rates calculated from the L_∞-errors for the first-order, second-order and fourth-order split-step Fourier schemes in the case of a single solitary wave ($N = 512$, $-20 \le x \le 60$)

Δt	First-order		Second-order		Fourth-order	
	L_∞-error	Order	L_∞-error	Order	L_∞-error	Order
0.0500	1.604E−2	–	2.079E−3	–	4.425E−04	–
0.0100	3.109E−3	1.019	7.975E−5	2.026	1.098E−06	3.727
0.0050	1.552E−3	1.002	1.991E−5	2.002	7.179E−08	3.935
0.0030	9.306E−4	1.001	7.167E−6	2.000	9.436E−09	3.972
0.0010	3.100E−4	1.001	7.962E−7	2.000	1.176E−10	3.991
0.0005	1.549E−4	1.001	1.990E−7	2.000	7.637E−12	3.945

their influence. The nondecreasing error behavior for the second-order and fourth-order schemes after the value of $N = 96$ is due to the limited space interval $5 \le x \le 35$. To show that this behavior can be eliminated by balancing the error due to boundary effects with the error due to internal resolution, we repeat the experiments of Fig. 1(a) but now using the space interval $-20 \le x \le 60$. The results are presented in Fig. 1(b) on a $\log_{10} - \log_{10}$ scale again. But this time the effect of the boundaries disappear and the L_∞-errors continue to decrease with increasing N. Now, for any fixed value of N the fourth-order scheme gives smaller errors than those of the first-order and second-order schemes. The reader is referred to [1,18] for a discussion about the problem of finding the optimal space interval. The relation between the L_2-error and N is also investigated for the split-step schemes. Since the pictures are very similar to those in Fig. 1, we do not reproduce them here.

To test whether the split-step schemes exhibit the expected convergence rates in time we perform some numerical experiments for various values of time step Δt and a fixed value of N. In these experiments we take $N = 512$ to ensure that the spatial error is negligible. The rate of convergence for each scheme is calculated using the formula

$$\text{rate of convergence} \approx \frac{\ln(E(N_2)/E(N_1))}{\ln(N_1/N_2)} \tag{3.3}$$

where $E(N_j)$ is either the L_∞-error or the L_2-error when using N_j subintervals. The L_∞-errors and the L_2-errors for the terminating time $t = 3$ are shown in Tables 1 and 2, respectively. We remark that the L_2-errors are well correlated with the L_∞-errors. The computed convergence rates agree well with the

Table 2
Comparison of the convergence rates calculated from the L_2-errors for the first-order, second-order and fourth-order split-step Fourier schemes in the case of a single solitary wave ($N = 512$, $-20 \le x \le 60$)

Δt	First-order		Second-order		Fourth-order	
	L_2-error	Order	L_2-error	Order	L_2-error	Order
0.0500	9.950E−3	–	7.834E−4	–	1.711E−4	–
0.0100	2.017E−3	0.992	3.047E−5	2.017	2.900E−7	3.964
0.0050	1.010E−3	0.998	7.611E−6	2.001	1.954E−8	3.892
0.0030	6.064E−4	0.999	2.739E−6	2.001	2.607E−9	3.943
0.0010	2.022E−4	1.000	3.043E−7	2.000	3.321E−11	3.971
0.0005	1.011E−4	1.000	7.609E−8	2.000	2.681E−12	3.631

Table 3
The convergence rate in space for the fourth-order split-step Fourier scheme in the case of a single solitary wave ($\Delta t = 0.61038 \times 10^{-3}$, $-20 \le x \le 60$)

N	L_∞-error	Order	L_2-error	Order
96	4.164E−1	–	2.023E−1	–
128	5.004E−2	7.37	2.190E−2	7.73
144	1.477E−2	10.36	8.772E−3	7.77
192	3.495E−4	13.01	4.056E−4	10.69
216	4.740E−5	16.96	7.402E−5	14.44
256	2.510E−6	17.29	4.588E−6	16.37
324	3.071E−8	18.69	5.905E−8	18.48
432	7.139E−11	21.08	1.372E−10	21.08

expected rates for the first-order, second-order and fourth-order split-step schemes. The orders of decay of the L_2-error and the L_∞-error are the ones of the splitting formulae employed for the temporal integration.

To test whether the split-step schemes exhibit the expected convergence rate in space we perform some further numerical experiments for various values of N and a fixed value of time step Δt. In these experiments we take $\Delta t = 0.61038 \times 10^{-3}$ to minimize temporal errors. Furthermore, we make the calculations about the spatial convergence rates under the assumption that the method is an algebraically convergent method in space. In other words, we suppose that $E(N) \sim N^{-p}$ for some $p > 0$, where $E(N)$ is the L_2 (or L_∞) error when using N subintervals. The results corresponding to the fourth-order split-step scheme are shown in Table 3 for an increasing number of subintervals. We present the L_2-errors and the L_∞-errors for the terminating time $t = 3$ together with the observed rates of convergence in each case. These results show that the numerical solution obtained using the fourth-order split-step scheme converges rapidly to the accurate solution in space, which is an indicative of exponential convergence. Since the results corresponding to the first-order and second-order schemes are almost identical to those given in Table 3, we do not reproduce them here.

To compare the proposed split-step Fourier schemes in terms of computational efficiency, we perform two different sets of numerical experiments. In the first set of experiments, we fix Δt and Δx (in particular we take $N = 512$) and measure the computing times, the L_∞-error, the L_2-error and the conservation errors δ_1, δ_2, δ_3 at the terminating time $t = 3$. The results are represented in Table 4. Note that the computing times in Table 4 are normalized so that the computing time of the first-order split-step scheme is one unit. The results show that each of the conserved quantities is extremely well preserved for the split-step schemes. Furthermore, we observe that, for a fixed number of spatial grid points, the computing time increases with the increasing order of the split-step method. For example, as might be expected, the

Table 4
Comparison of the L_∞-error, the L_2-error, the conservation errors δ_1, δ_2, δ_3 and the computing times for the first-order, second-order and fourth-order split-step Fourier schemes in the case of a single solitary wave ($N = 512$, $-20 \le x \le 60$, $\Delta t = 0.61038 \times 10^{-3}$)

Method	L_∞-error	L_2-error	δ_1	δ_2	δ_3	Normalized CPU
First-order	1.892E−04	1.234E−04	1.691E−13	2.243E−07	9.984E−09	1.0
Second-order	2.966E−07	1.134E−07	2.198E−13	1.865E−13	1.381E−13	1.7
Fourth-order	1.716E−11	5.156E−12	5.913E−13	9.309E−14	3.985E−13	4.1

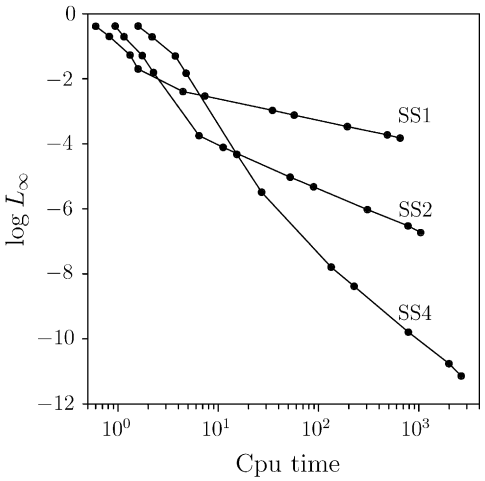

Fig. 2. The L_∞-errors for the terminating time $t = 3$ as a function of the CPU time for the first-order (SS1), second-order (SS2) and fourth-order (SS4) split-step Fourier schemes.

fourth-order scheme is more accurate but more expensive than the others. Note that how a replacement of the second-order scheme by the fourth-order scheme reduces the error by a factor of 10^4, while the computational cost is multiplied only by 2.4. Similar observations are also valid for a replacement between the first-order and second-order schemes with a factor of 10^3. In the second set of our numerical experiments, we consider different values of N and measure both the computing times and the L_∞- and L_2-errors. In Figs. 2 and 3 we plot the L_∞- and L_2-errors, respectively, versus the amount of computing time needed by each scheme to achieve those errors. That is, a horizontal line through a particular value of the error intersects the graphs at the CPU time needed by each scheme. The most efficient scheme is the one that uses the least CPU time to produce a solution of given accuracy. We observe from Fig. 2 that the fourth-order scheme, for the L_∞-error levels less than roughly 10^{-4}, costs less than the cost of the second-order scheme and that the fourth-order scheme is more efficient than the second-order scheme when considering an error of less than 10^{-4}. The difference in computational efficiency becomes more significant as the accuracy level is increased. A similar situation is observed for the L_∞-error levels less than roughly 10^{-2} when comparing the first-order and second-order schemes. It is clear from Fig. 3 that the L_2-errors are well correlated with the L_∞-errors. We conclude that the fourth-order split-step scheme is computationally more efficient than the first-order and second-order schemes, particularly when high accuracy is required.

Pathria and Morris [9] have pointed out that "the behavior of the quantities I_1, I_2 and I_3 provides a valuable check on the numerical results" and that "the computed energy I_2 is the most sensitive of the three in indicating numerical difficulties and, consequently, the application of any numerical scheme should be accompanied by a close watch on its evolution". A similar particular sensitivity of numerical approximations of I_2 in indicating numerical difficulties has been also observed by Robinson in [10] where the present solitary wave problem is solved using an orthogonal spline collocation method which is fourth-order accurate in space. Robinson has pointed out that I_2 experiences a radical change, while I_1 and I_3 are well conserved, and that this radical change is consistent with observations made in [9]. On Table 7 of [10], the calculated values of I_2 at $t = 0$ and $t = 3$ are given as 2.861766 and 3.242514,

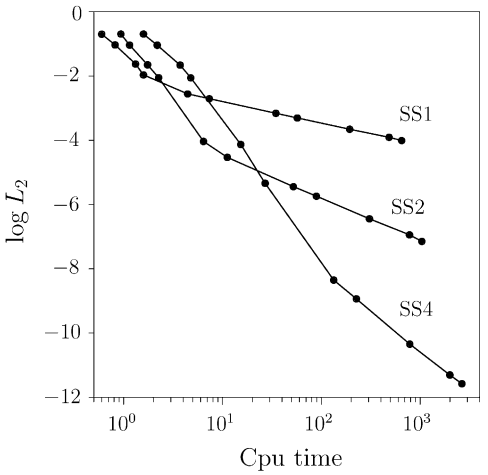

Fig. 3. The L_2-errors for the terminating time $t = 3$ as a function of the CPU time for the first-order (SS1), second-order (SS2) and fourth-order (SS4) split-step Fourier schemes.

respectively, in which the relative error δ_2 in discrete approximation of I_2 is roughly 13%. However, the numerical results on Table 4 of the present study show that each of the conserved quantities is very well preserved by the present split-step schemes. Therefore the observations made in both [9] and [10] about the behavior of the numerical approximation of I_2 are not valid for the present split-step schemes.

3.2. Interacting solitons

In the second numerical experiment we study the interaction of two solitons for the integrable case of GNLS equation, in which the coefficients are $q_1 = 1$, $q_2 = 1$, $q_3 = -2$, $q_4 = 0$. The initial condition [9] (there are some misprints in Eqs. (3.3.1) and (3.3.2) of [9]) is given by

$$w(x,0) = 1/\sqrt{2}\,\mathrm{sech}[\tfrac{1}{2}(x-15)]\exp \mathrm{i}\{\tfrac{1}{4}(x-15) + \tanh[\tfrac{1}{2}(x-15)]\} + 1/2\sqrt{2}\,\mathrm{sech}[\tfrac{1}{4}(x-35)]$$
$$\times \exp \mathrm{i}\{-\tfrac{1}{2}(x-35) + \tfrac{1}{2}\tanh[\tfrac{1}{4}(x-35)]\}.$$

This equation corresponds to two solitons, the one initially located at $x = 15$ and moving to the right with speed 1/2, the one initially located at $x = 35$ and moving to the left with speed 1. The exact values of the conserved quantities for this problem are $I_1 = 3$, $I_2 = 3/16$, and $I_3 = 0$. The problem is solved on the interval $-60 \le x \le 110$ for times up to $t = 20$ using the fourth-order split-step scheme. The modulus of the numerical solution obtained using $N = 1024$ spatial grid points and a time step of $\Delta t = 2.7573 \times 10^{-4}$ is presented in Fig. 4. As in Fig. 3 of [9], Fig. 4 shows that the solitary waves are stable under the collision in the sense that the solitary waves do not leave dispersive oscillations and their amplitudes are not altered after the collision. In Fig. 5(a)–(c) we present the conservation errors δ_1, δ_2 and δ_3, respectively, as functions of time. The fourth-order split-step Fourier scheme preserves each of the conserved quantities very well (up to 10^{-12} for I_1 and I_2 and up to 10^{-10} for I_3). This behavior provides a valuable check on our numerical results. Also it is contrary to that observed in Fig. 4 of [9], where the conserved quantities calculated using the first-order split-step scheme by Pathria and Morris are not conserved under the collision. We observe from Fig. 5(a)–(c) that the conservation error δ_1 is a

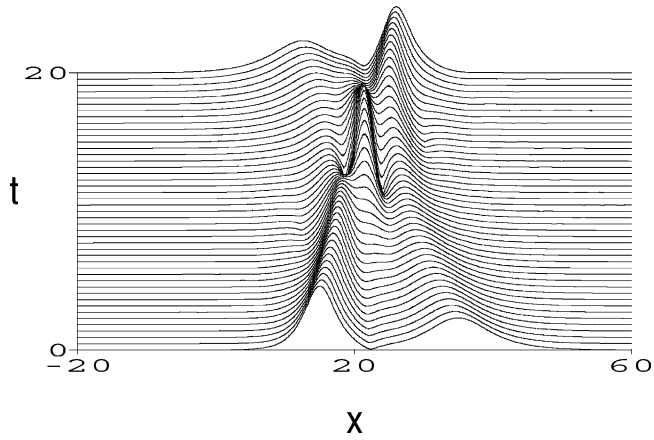

Fig. 4. The modulus of the numerical solution obtained for the interacting solitons with $N = 1024$ and $\Delta t = 2.7573 \times 10^{-4}$.

strictly increasing function of t, while the conservation errors δ_2 and δ_3 are non-monotonic functions of t. In addition, note how the results for δ_1, δ_2, δ_3 in Fig. 5 differ from those given in Table 4 in terms of order of magnitude, showing that the interacting solitons problem is computationally more difficult than the single solitary wave problem treated above. This implies that further spatial resolution is needed to capture the dynamics related to the interaction of two solitary waves.

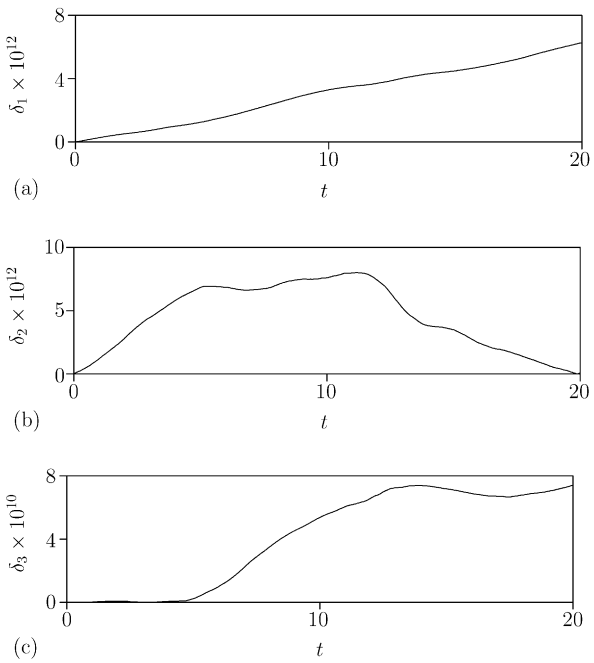

Fig. 5. The conservation errors as functions of time for interacting solitons problem: (a) δ_1; (b) δ_2; (c) δ_3 (the fourth-order split-step Fourier scheme with $N = 1024$, $\Delta t = 2.7573 \times 10^{-4}$, $-60 \leq x \leq 110$).

Table 5
Variation of discrete approximations of the conserved quantities, I_1, I_2 and I_3, and $|\, w(0,t)\,|$ with time for the fourth-order split-step Fourier scheme in the case of the blow-up ($N = 432$, $-7.5 \le x \le 7.5$, $\Delta t = 0.266 \times 10^{-4}$)

t	$\bar{I}_1$	$\bar{I}_2$	$\bar{I}_3$	$\lvert W(0,t)\rvert$
0.00	1.25331413731550	−2.684467300953	−9.79328637E−17	1.000000000
0.01	1.25331413731505	−2.684467300949	−6.65191731E−13	1.007348147
0.06	1.25331413731279	−2.684467299107	−4.67361424E−12	1.526254353
0.07	1.25331413731807	−2.684448736528	−4.39563753E−12	2.376429075
0.08	1.25335259643817	−2.829258617167	−6.08510830E−10	3.430374335

3.3. Blow-up

For certain values of the coefficients and certain initial conditions, solutions to the GNLS equation experience finite time blow-up [8]. We now apply the fourth-order split step scheme to a case of the GNLS equation in which the exact solution blows up in finite time. The initial condition is the Gaussian function $w(x,0) = \exp(-x^2)$ and the coefficients are $q_1 = -2, q_2 = 20, q_3 = 0, q_4 = 0$. The exact values of the conserved quantities I_1, I_2 and I_3 are $I_1 = \sqrt{\pi/2}$, $I_2 = \sqrt{\pi}(9\sqrt{2} + 9 - 20\sqrt{6})/18$ and $I_3 = 0$ for this problem. In [8], it has been shown analytically that the exact solution $w(x,t)$ for this problem will blow up in finite time and furthermore, an upper bound on the blow-up time is $t \approx 1.7$. Using a first-order split-step Fourier method, Pathria and Morris have shown numerically that the blow-up becomes pronounced near $t = 0.07$. They have concluded the above upper bound appears to be quite loose. The question arises whether the upper bound derived in [8] is sharp. The same problem has been also investigated numerically using an orthogonal spline collocation method in [10] by Robinson. Robinson has pointed out that the blow-up is quite evident at $t = 0.08$ and that this result is consistent with the result obtained using the first-order split-step Fourier method in [8]. Robinson has also observed that "the blow-up is accompanied by a radical change in the value of $\bar{I}_2$ although $\bar{I}_1$ and $\bar{I}_3$ experience little change."

In the present study, the above problem is solved on the interval $-7.5 \le x \le 7.5$ for times up to $t = 0.08$. We present the numerical results obtained using the fourth-order scheme on Table 5. Although a formal proof of the existence of the blow-up is not presented here, the numerical results strongly indicate that a blow-up is well underway by time $t = 0.08$. This is consistent with the numerical results in [8] and [10]. The fact that the three results about the predicted time of blow-up, which were obtained using totally different methods, are in complete agreement makes one believe in their correctness. Following Pathria and Morris [8], we conclude that the upper bound given in [8] is not sharp.

A comparison of the numerical results corresponding to I_1 and I_3 shows good qualitative agreement between the numerical results in the present study and those given in Table 8 of [10]. The only difference between the present results and those given in Table 8 of [10] is the presence of a discrepancy regarding the value of discrete approximation of I_2. In other words, the variation in discrete approximation of I_2 with increasing time is not as much as that observed in [10]. This is consistent with the observations made in the single solitary wave problem of the present study, regarding the value of discrete approximation of I_2. The reason of this discrepancy remains an open question. The fact that different numerical integration techniques have been used to calculate the conservation integrals in these studies may be an explanation of this discrepancy.

4. Conclusions

In this study we have applied the well-known split-step Fourier method to the GNLS equation. We have presented three split-step schemes in which the main difference among the three schemes is in the order of the splitting approximation used. The method is easy to implement on a computer and one can easily introduce higher-order splitting formulae to increase greatly the accuracy of split-step method. It should be stressed that the latter is done at the cost of increasing computation time. A proper choice of the splitting approximation is a compromise between these competing effects. Naturally, for a fixed number of spatial grid points, the algorithm for the fourth-order scheme is more expensive than the ones for the first-order and the second-order schemes. However, the numerical experiments reported here for the case of one solitary wave show that the fourth-order split-step Fourier scheme is computationally more efficient than the first-order and second-order schemes. Also the numerical experiments indicate that the proposed split-step schemes exhibit the expected rates of convergence. We have found that the numerical results are in a good agreement with the results reported in the literature and that the schemes have remarkable conservation properties for global invariants. The results obtained when the same initial datum is considered over different domains are also compared. We conclude that as the order of splitting is increased, the integration must be carried out over a larger interval to keep both the error due to boundary effects and the error due to insufficient inner resolution at the same level.

Moreover, the collision of two solitons and a finite time blow-up problem are investigated numerically and particular attention is paid to the behavior of the conserved quantities as an indicator of numerical difficulties. We observe that the only difference between the present numerical results and those given in both [9] and [10] is the absence of a radical change in the value of discrete approximation of I_2.

The approaches presented in some previously published papers related to numerical solutions of the GNLS equation have been mostly limited to the absence of the nonlinear derivative terms [2,3,13]. The numerical results presented here show that the nonlinear derivative terms do not create any special difficulties in the split-step Fourier method. It is hoped that the presentation will be useful to those who might be involved in the numerical solution of the GNLS equation with a great accuracy, even though a convergence proof of the proposed schemes is lacking at this stage.

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