Analytical and Numerical Aspects of Certain Nonlinear Evolution Equations. II. Numerical, Nonlinear Schrödinger Equation

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Various numerical methods are employed in order to approximate the nonlinear Schrödinger equation, namely: (i) The classical explicit method, (ii) hopscotch method, (iii) implicit-explicit method, (iv) Crank-Nicolson implicit scheme, (v) the Ablowitz-Ladik scheme, (vi) the split step Fourier method (F. Tappert), and (vii) pseudospectral (Fourier) method (Fornberg and Whitham). Comparisons between the Ablowitz-Ladik scheme, which was developed using notions of the inverse scattering transform, and the other utilized schemes are obtained.

Introduction

The nonlinear Schrödinger (NLS) equation describes a wide class of physical phenomena (e.g., modulational instability of water waves, propagation of heat pulses in anharmonic crystals, helical motion of a very thin vortex filament, nonlinear modulation of collisionless plasma waves, self-trapping of a light beam in a color-dispersive system [1]). The NLS equation was investigated numerically by Karpman and Krushkal [2], Yajima and Outi [3], and Satsuma and Yajima [4], Tappert [5] and Hardin and Tappert [6]. In the latter two works the NLS equation was integrated by the split-step Fourier method. As discussed in part I Ablowitz and Ladik [7] found nonlinear partial difference equations (based on the inverse scattering transform) which can be used as a numerical scheme for the NLS equation. This scheme has certain desirable properties [8] (see part I).

This work aims to compare the Ablowitz and Ladik scheme and other known numerical methods for the NLS equation

$$iq_t = q_{xx} + 2|q|^2 q.$$
 (1.1)

Roughly speaking numerical methods for obtaining solutions to initial value problems fall into two categories [9]: (1) finite difference methods and (2) function approx-

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imation methods. For the finite difference methods we seek approximation q_n^m to the original function q(x, t) at a set of points x_n , t_m on a rectangular grid in the x, t plane, where $x_n = hn$, $t_m = km$, t is the increment in x, and k is the increment in t. By expanding function values at grid points in a Taylor series, approximations to the differential equation involving algebraic relations between grid point values can be obtained. The function approximation method approximates the exact solution q(x, t) by an approximate solution defined on a finite dimensional subspace

$$q(x,t) \approx \tilde{q}(x,t) = \sum_{i=1}^{n} C_i(t) \, \Phi_i(x).$$

The $\Phi_i(x)$ are appropriately chosen basis functions. Common choices for these are the trigonometric functions, leading to a finite Fourier transform or pseudospectral method and piecewise polynomial functions with a local basis, giving the finite element method.

The following numerical methods were applied to the NLS equation.

- 1. Finite difference methods.
 - (a) Explicit methods.
 - (i) The classical explicit method.
 - (ii) The hopscotch method [10].
 - (b) Implicit methods.
 - (i) Implicit for the linear part and explicit for the nonlinear part (implicit-explicit).
 - (ii) Crank-Nicolson implicit scheme.
 - (iii) The Ablowitz and Ladik scheme.
- 2. Finite Fourier transform or pseudospectral methods.
 - (i) Split step Fourier method [6].
 - (ii) Pseudospectral method by Fornberg and Whitham [11].

In order to compare schemes, our approach for comparison is to (a) fix the accuracy (L_{∞}) for computations beginning at t=0 and ending at t=T; (b) leave other parameters free (e.g., Δt or Δx) and compare the computing time required to attain such accuracy for various choices of the parameters [12].

These methods are applied to the NLS equation (1.1) subject to the following conditions:

(A) THE INITIAL CONDITIONS

(i) 1-Soliton Solution

The exact solution of (1.1) on the infinite interval is

$$q(x,t) = 2\eta e^{-t(2\xi x - 4(\xi^2 - \eta^2)t + (\psi_0 + \pi/2))} \operatorname{sech}(2\eta x - 8\xi \eta t - x_0),$$

where x_0 , η , ξ and ψ_0 are constants.

For initial conditions, Eq. (1.3) is used at t = 0, and the constants are chosen to be $x_0 = 0$, $\psi_0 = 0$, $\xi = 1$, and $\eta = 0.5$, 1, 2, and 3.

(ii) Collisions of Two Solitons [13]

The exact solution of (1.1) on the infinite interval is

$$q(x, t) = G(x, t)/F(x, t),$$

where

$$F(x,t) = 1 + a(1, 1^*) \exp(\eta_1 + \eta_1^*) + a(1, 2^*) \exp(\eta_1 + \eta_2^*)$$

$$+ a(2, 1^*) \exp(\eta_2 + \eta_1^*) + a(2, 2^*) \exp(\eta_2 + \eta_2^*)$$

$$+ a(1, 2, 1^*, 2^*) \exp(\eta_1 + \eta_2 + \eta_1^* + \eta_2^*),$$

$$G(x,t) = \exp(\eta_1) + \exp(\eta_2) + a(1,2,1^*) \exp(\eta_1 + \eta_2 + \eta_1^*) + a(1,2,2^*) \exp(\eta_1 + \eta_2 + \eta_2^*),$$

$$a(i,j^*) = (P_i + P_j^*),$$

$$a(i,j) = (P_i - P_j)^2,$$
 (1.8)

$$a(i^*, j^*) = (P_i^* - P_i^*)^2, \tag{1.9}$$

$$a(i,j,k^*) = a(i,j) a(i,k^*) a(j,k^*),$$
 (1.10)

$$a(i, j, k^*, l^*) = a(i, j) a(i, k^*) a(i, l^*) a(j, k^*) a(j, l^*) a(k^*, l^*),$$
(1.11)

where * implies a complex conjugate, and

$$\eta_j = P_j x - \Omega_j t - \eta_j^{(0)}, \qquad \Omega_j = i P_j^2,$$

where P_j and $\eta_j^{(0)}$ are complex constants relating respectively to the amplitude and to the phase of the *i*th soliton.

For initial conditions, Eq. (1.4) is used at t = 0, and three different sets of parameters are studied:

(i)
$$P_1 = 1 - 0.25i$$
, $P_2 = 0.5 + 0.15i$, $\eta_1^{(0)} = -2$ and $\eta_2^{(0)} = 0$,

(ii)
$$P_1 = 2 - 0.5i$$
, $P_2 = 1 + 0.75i$, $\eta_1^{(0)} = -2$ and $\eta_2^{(0)} = 1.0$,

(iii)
$$P_1 = 4 - 2i$$
, $P_2 = 3 + i$, $\eta_1^{(0)} = -9.04$, $\eta_2^{(0)} = 2.1$.

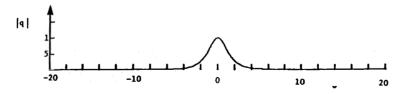


Fig. Initial condition (1.3), $\eta = 0.5$ (i.e., amplitude = 1).

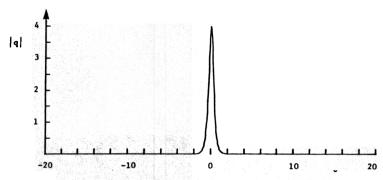


Fig. 2. Initial condition (1.3), $\eta = 2$ (i.e., amplitude = 4).

(B) BOUNDARY CONDITIONS

Periodic boundary conditions are used. The period is chosen to be -20, 20 in the case of small amplitudes and [-10, 10] in the case of relatively higher amplitudes. (See Figs. (1) and (2).)

The numerical solution is compared with the exact solution. In addition, two of the conserved quantities are computed, namely, $\int |q|^2 dx$, and $\int (|q|^4 - |\partial q/\partial x|^2) dx$.

2. THE REPRESENTATION OF THE NLS EQUATION USING NUMERICAL METHODS

1. FINITE DIFFERENCE METHODS

(A) EXPLICIT METHODS

(i) The Classical Explicit Method

Using the classical emplicit method with central difference in time (for stability), the finite difference representation of Eq. (1.1) is

$$\frac{q_n^{m+1} - q_n^{m-}}{2\Delta t} = \frac{q_{n+1}^m - 2q_n^m + q_{n-1}^m}{(\Delta x)^2} + 2(q^2)_n^m q_n^m, \qquad (2.1)$$

where |n| < p, and m > 0.

It is easily shown that this method is linearly (dropping the nonlinear term) stable for $\Delta t/(\Delta x)^2 \le 1/4$. The truncation error of this scheme is of order $(O((\Delta t)^2) + O((\Delta x)^2))$.

(ii) A Hopscotch Scheme

The NLS equation (1.1) can be approximated by

(a) an explicit scheme:

$$i\frac{q_n^{m+1}-q_n^m}{\Delta t}=\frac{q_{n-1}^m-2q_n^m+q_{n+1}^m}{(\Delta x)^2}+\left|\left(|q|_{n-1}^m\right)^2q_{n-1}^m+\left(|q|_{n+1}^m\right)^2q_{n+1}^m\right|,\quad(2.2)$$

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(b) an implicit scheme:

$$i\frac{q_n^{m+1}-q_n^m}{\Delta t} = \frac{q_{n+1}^{m+1}-2q_n^{m+1}+q_{n-1}^{m+1}}{(\Delta x)^2} + \left[(|q|_{n-1}^{m+1})^2 q_{n-1}^{m+1} + (|q|_{n+1}^{m+1})^2 q_{n+1}^{m+1} \right]. (2.3)$$

The hopscotch scheme applies Eq. (2.2) at odd values of (n+m) and (2.3) at even values of (n+m). This combination makes (2.3) explicit. If we write Eq. (2.3) for m=m-1, and substitute the resulting equation into (2.2), the explicit scheme (2.2) (after the first time step) may be replaced by

$$q_n^{m+1} = 2q_n^m - q_n^{m-1}. (2.4)$$

This scheme has truncation error of order $(O((\Delta t)^2) + O((\Delta x)^2))$, and it is unconditionally stable according to linear analysis.

(B) IMPLICIT METHODS

(i) Implicit-Explicit Method

The Crank-Nicolson scheme is used to approximate the linear part and an explicit average is used for the nonlinear part of the Eq. (1.1). The scheme is

$$i\frac{q_n^{m+1}-q_n^m}{\Delta t} \frac{1}{2(\Delta x)^2} \left[q_{n+1}^m - 2q_n^m + q_{n-1}^m + q_{n+1}^{m+1} - 2q_n^{m+1} + q_{n-1}^{m+1} \right] + (|q|_{n-1}^m)^2 q_{n-1}^m + (|q|_{n+1}^m)^2 q_n^m$$

The scheme is unconditionally stable according to linear analysis. The truncation error is of order $(O((\Delta t) + O((\Delta x)^2))$. To implement this scheme, a quasi-tridiagonal system of equations is required to be solved at each time step. An optimization of the Gaussian elimination method is introduced to solve this system. (See Appendix A.) We carry out the elimination procedure only once and use back substitution thereafter.

(ii) Crank-Nicolson Implicit Scheme

The difference scheme for representing Eq. (1.1) is

$$i\frac{q_n^{m+1} - q_n^m}{\Delta t} = \frac{1}{2(\Delta x)^2} \left[q_{n+1}^m - 2q_n^m + q_{n-1}^m + q_{n+1}^{m+1} - 2q_n^{m+1} + q_{n-1}^{m+1} \right] + (|q|_n^{m+1})^2 q_n^{m+1} + (|q|_n^m)^2 q_n^m$$
(2.6)

This scheme is also unconditionally stable according to linear analysis. The truncation error of this scheme is of order $(O((\Delta t)^2) + O((\Delta x)^2))$.

We briefly remark on how we solve (2.6). Rewrite Eq. (2.6) as

$$-\frac{\lambda}{2} q_{n-1}^{m+1} + (i+\lambda) q_n^{m+1} - \frac{\lambda}{2} q_{n+1}^{m+1}$$

$$= \frac{\lambda}{2} \{q_{n+1}^m + q_{n-1}^m\} + (i-\lambda) q_n^m + \Delta t \{(|q_n^{m+1}|)^2 q_n^{m+1} + (|q_n^m|)^2 q_n^m\},$$

$$n = -N, ..., N, \quad (2.7)$$

and

$$\lambda = \frac{\Delta t}{2(\Delta x)^2},$$

where the solution is sought in the region $(-N\Delta x \le x \le N\Delta x) \times (t > m\Delta t, m = 1, 2,...)$. From the periodic boundary conditions, we have $q_{-N}^m = q_N^m$ and $q_{N+1}^m = q_{-N+1}^m$ for all m. Therefore, by applying Eq. (2.7) at each mesh point (i.e., n = -N + 1,..., N), we can write the totality of equations as

$$AQ^{m+1} = F, (2.8)$$

where

$$A = \begin{bmatrix} i+\lambda & -\frac{\lambda}{2} & & -\frac{\lambda}{2} \\ -\frac{\lambda}{2} & i+\lambda & -\frac{\lambda}{2} & & \\ & & -\frac{\lambda}{2} & i+\lambda & -\frac{\lambda}{2} \\ -\frac{\lambda}{2} & & -\frac{\lambda}{2} & i+\lambda \end{bmatrix}, \qquad Q^{m+1} = \begin{bmatrix} q_{-N+} \\ q_{-N} \\ & & \\ & q_{N} \end{bmatrix}^{m+1}$$

and

$$F_{j} = \frac{\lambda}{2} \left\{ q_{j+1}^{m} + q_{j-1}^{m} \right\} + (i - \lambda) q_{j}^{m} + \Delta t \left\{ (|q_{j}^{m+1}|)^{2} q_{j}^{m+1} + (|q_{j}^{m}|)^{2} q_{j}^{m} \right\},$$

$$j = -N + 1, ..., N. \tag{2.9}$$

The right-hand side of Eq. (2.8) is a function of known values of q at the previous time level $(t = m\Delta t)$ and unknown values of q at the new time level $(t = (m+1)\Delta t)$. We use an iteration technique to solve the system (2.8), and we assume (only in the right-hand side) the values of $q_n^{m+1} = q_n^m$ to start with. Therefore the right-hand side

becomes known, and we use the same optimization of the Gaussian elimination method for (2.5) to solve the system (2.8). The resulting values of q at the new time level are substituted in the right-hand side of Eq. (2.8) to start the new iteration, and we solve the new version of (2.8) by the previous method. We iterate until the condition

max
$$|q_n^{m+1,k} - q_n^{m+1,k+1}| < \text{tolerance}$$

 $n = -N,..., N$

(where k is the number of iterations) is satisfied. The iteration procedure is repeated at each new time level. The $q_n^{m+1,k+1}$ will be the approximated solution at the point $(n\Delta x, (m+1)\Delta t)$.

(C) THE ABLOWITZ AND LADIK SCHEME

The scheme is

$$q_{n}^{m+1} - q_{n}^{m}$$

$$= \frac{1}{2(\Delta x)^{2}} \left[q_{n+1}^{m} - 2q_{n}^{m} + q_{n-1}^{m} \prod_{k=-\infty}^{n-1} \Lambda_{k}^{m} + q_{n+1}^{m+1} \prod_{k=-\infty}^{n} \Lambda_{k}^{m} - 2q_{n}^{m+1} + q_{n-1}^{m+1} + \frac{1}{4} \left[q_{n}^{m} (q_{n}^{m^{*}} q_{n+1}^{m} + q_{n+1}^{m+1^{*}} q_{n+1}^{m+1}) \right] + q_{n}^{m+1} (q_{n-1}^{m} q_{n}^{m^{*}} + q_{n-1}^{m+1} q_{n}^{m+1^{*}}) + 2q_{n}^{m} q_{n}^{m^{*}} q_{n+1}^{m+1} \prod_{k=-\infty}^{n} \Lambda_{k}^{m} + 2q_{n}^{m+1} q_{n}^{m+1^{*}} q_{n-1}^{m} \prod_{k=-\infty}^{n-1} \Lambda_{k}^{m} - q_{n}^{m} \sum_{k=-\infty}^{n} \Delta_{m} S_{k}^{m} - q_{n}^{m+1} \sum_{k=-\infty}^{n-1} \Delta_{m} S_{k}^{m^{*}} \right]$$

$$(2.10)$$

where

$$S_{k}^{m} = q_{k}^{m} q_{k-1}^{m^{*}} + q_{k+1}^{m} q_{k}^{m^{*}}, q_{n}^{m+1^{*}} = (q_{n}^{m+1})^{*},$$

$$A_{k}^{m} = (1 + (\Delta x)^{2} q_{k}^{m+1} q_{k}^{m+1^{*}})/(1 + (\Delta x)^{2} q_{k}^{m} q_{k}^{m^{*}}),$$

and

$$\Delta_m S_k^m = S_k^{m+1} - S_k^m$$

This is a global scheme, unconditionally and nonlinearly stable, and the truncation error is of order $(O((\Delta t)^2) + O((\Delta x)^2))$. A local scheme (with the same truncation error) from (2.10) can be obtained if the sum terms are zero and the product terms are equal to one.

It is convenient to implement (2.10) as follows. Write the new time level equation as

$$q_{n+1}^{m+1}$$
 $(2+\varepsilon)q_n^{m+1}+q_{n-1}^{m+1}=B_n$

where

$$\varepsilon = \frac{2i(\Delta x)^2}{\Delta t} \qquad |\varepsilon| \leqslant$$

 $(\Delta t$ is supposed to be of the same order as Δx)

and

$$\begin{split} B_{n} &= -q_{n+1}^{m} - q_{n-1}^{m} + (2 - \varepsilon) \, q_{n}^{m} \\ &- \left| q_{n-1}^{m} \left(\prod_{k=-\infty}^{n-1} A_{k}^{m} - 1 \right) + q_{n+1}^{m+1} \left(\prod_{k=-\infty} A_{k}^{m} - 1 \right) \right. \\ &- \frac{(\Delta x)^{2}}{2} \left| q_{n}^{m} (q_{n}^{m}, q_{n+1}^{m} + q_{n}^{m+1}, q_{n+1}^{m+1}) \right. \\ &+ q_{n}^{m+1} (q_{n-1}^{m} q_{n}^{m}, q_{n+1}^{m+1} \prod_{k=-\infty} A_{k}^{m} + 2q_{n}^{m+1} q_{n}^{m+1}, q_{n-1}^{m} \prod_{k=-\infty}^{n-1} A_{k}^{m} \\ &- q_{n}^{m} \sum_{k=-\infty}^{n} A_{m} S_{k}^{m} - q_{n}^{m+1} \sum_{k=-\infty}^{n-1} A_{m} S_{k}^{m} \right] \end{split}$$

(2.11) is solved by a version of the Crank-Nicolson back and forth sweep method for the heat equation [14, 15]. We seek an equation of the form (at the new time level)

$$q_{n+1} = aq_n + b_n \tag{2.13}$$

suitable for computing q explicitly by sweeping to the right. For stability we require $|a| \le 1$. Repeated substitution into (2.11) to eliminate q_{n+1} and q_n in favor of q_{n-1} gives

$$b_n + [a - (2 + \varepsilon)] b_{n-1} + [a^2 - (2 + \varepsilon) a + 1] q_{n-1} = B_n$$
 (2.14)

Requiring the q_{n-1} term to drop out determines a (uniquely since $|a| \le 1$) as a solution of

$$a^2 - (2 + \varepsilon) a + 1 = 0$$
 (2.15)

and leaves for b_n a first-order difference equation.

The corresponding homogeneous equation of (2.14) has a solution of the form

$$b_n = k^n$$

where the constant k satisfies

$$k + [a - (2 + \varepsilon)] = 0.$$

It can be shown that the solution k of (2.17) corresponds to the second root (other than $a \le 1$) of the quadratic equation (2.15) determining a above, and that |k| > 1. It follows that b can be computed explicitly by sweeping to the left,

$$b_{n-1} = ab_n - aB_n$$

To obtain the solution q_n , first solve for b_n from (2.18) then use (2.13) to calculate q_n . In order to calculate the b's, we use an iteration procedure. We assumed that $q_n^{m+1} = q_n^m$ in Eq. (2.12) and $b_N = 0$ to start with, and then we apply the Gauss-Seidel technique [16] (in which the improved values are used as soon as they are computed) to calculate the rest of the b's. The calculated value of the b_N (= b_{-N}) is used to start the new iteration, and the iteration procedure is repeated until the condition

$$\max |b_{n-1} - (ab_n - aB_n)| < \text{tolerance}$$

$$n = -N \dots N$$

is satisfied. Then we use the above procedure by sweeping to the right by means of (2.13) to obtain the q's. After the calculations of the q's, we substitute their values instead of q_n^{m+1} in Eq. (2.12), and repeat the same procedure to calculate the b's and then the q's. This procedure is repeated until the condition

max
$$|q_n^{m+1,k} - q_n^{m+1,k+1}| < \text{tolerance}$$

 $n = -N,..., N$

(where k is the number of iterations) is satisfied. The $q_n^{m+1,k+1}$ will be the approximated solution at the point $(n\Delta x, (m+1)\Delta t)$.

2. FINITE FOURIER TRANSFORM OR PSEUDOSPECTRAL METHODS

(i) Split Step Fourier Method [6]

For convenience the spatial period is normalized to $[0, 2\pi]$, then equation (1.1) becomes

$$iq_t = \frac{\pi^2}{p^2} q_{xx} + 2|q|^2 q,$$
 (2.19)

where P is half the length of the interval of interest, and $X = (x + P) \pi/P$. (Here we take P to be 20 or 10 depending on the calculation.) This interval is discretized by N equidistant points, with spacing $\Delta X = 2\pi/N$. The function q(X, t), numerically defined only on these points, can be transformed to the discrete Fourier space by

$$\hat{q}(k,t) = Fq = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} q(j\Delta X, t) e^{-2\pi i j k/N}$$

$$k = -\frac{N}{2}, ..., -1, 0, 1, ..., \frac{N}{2}$$
(2.20)

The inversion formula is

$$q(j\Delta X, t) = F^{-1}\hat{q} = \frac{1}{\sqrt{N}} \sum_{k} \hat{q}(k, t) e^{2\pi i j k/N}$$

$$k = -\frac{N}{2}, ..., -1, 0, 1, ..., \frac{N}{2}$$
(2.21)

These transforms can be performed, efficiently with the fast Fourier transform (FFT) algorithm [17]. Following [6] in order to apply the split step Fourier method for Eq. (2.19) we (a) advance the solution using only the nonlinear part:

$$i\tilde{q}_i = 2 |\tilde{q}|^2 \tilde{q}. \tag{2.22}$$

This can be solved exactly,

$$\tilde{q}(X,t) = e^{-2i|q(X,0)|^2 t} q(X,0), \tag{2.23}$$

where $\tilde{q}(X, t)$ is a solution of Eq. (2.22) and q(X, 0) is the solution of Eq. (2.19) at t = 0. (b) advance the solution according to

$$iq_t = \frac{\pi^2}{P^2} q_{XX} \tag{2.24}$$

by means of the discrete Fourier transform

$$q(X_i, t + \Delta t) = F^{-1}(e^{ik^2 \Delta t \pi^2 / P^2} F(\tilde{q}(X_i, t))). \tag{2.25}$$

This method is second order accurate in Δt and all order in Δx , and is unconditionally stable according to linear analysis.

(ii) Pseudospectral Method (Fornberg and Whitham) [11]

This is a Fourier (pseudospectral) method in which q(x, t) is transformed into Fourier space with respect to x, and derivatives (or other operators) with respect to x are then made algebraic in the transformed variable. Again for convenience the spatial period is normalized to $[0, 2\pi]$. With this scheme, q_{xx} can be evaluated as

 $F^{-1}\{i^2k^2F(q)\}$. Combined with a leap frog time step the NLS equation (2.19) is then approximated by

$$q(X, t + \Delta t) = q(X, t - \Delta t) + 2i\Delta t \frac{\pi^2}{P^2} F^{-1}(k^2 F(q(X, t)))$$
$$-4i\Delta t |q|^2 q. \tag{2.26}$$

Using the ideas of Fornberg and Whitham we make a modification in approximating Eq. (2.19),

$$q(X, t + \Delta t) = q(X, t - \Delta t) + 2iF^{-1} \left(\sin \left(\frac{k^2 \pi^2}{P^2} \Delta t \right) F(q(x, t)) \right)$$
$$-4i\Delta t |q|^2 q. \tag{2.27}$$

The difference between Eqs. (2.26) and (2.27) is in the approximation of the linear Eq. (2.24). The linear part of Eq. (2.27) will be exactly satisfied for any solution of Eq. (2.24) (see [11]). Also it turns out that Eq. (2.26) is linearly (dropping the nonlinear term) stabe for $\Delta t/(\Delta x)^2 < 1/\pi^2$, while Eq. (2.27) is unconditionally stable according to linear analysis.

3. Conclusions

Various numerical methods are used in order to approximate the NLS equation (1.1), namely; (i) The classical explicit method (2.1), (ii) hopscotch method (2.2), (2.3), (iii) implicit—explicit method (2.5), (iv) Crank—Nicolson implicit scheme (2.6), (v) The Ablowitz and Ladik scheme (2.10), (vi) The split step Fourier method (2.23), (2.25) and the (vii) pseudospectral method of Fornberg and Whitham (2.27). We obtain a comparison between the Ablowitz—Ladik scheme and the other utilized schemes. Our approach for comparison is to (a) fix the accuracy (L_{∞}) for computations beginning at t = 0 and ending at t = T; (b) leave other parameters free (e.g. Δt , or Δx), and compare the computing time required to attain such accuracy for various choices of the parameters. For the comparison two sets of initial conditions are studied: (A) 1-soluton solution with different values of the amplitude, (B) Collisions of two solitons with different values of the parameters. According to this approach we have made the following conclusions:

(1) The schemes explicit (i), implicit—explicit (iii), and the hopscotch (ii) take more computing time than the other schemes ((iv, (v), (vi), (vii)) and the difference in the computing time increases as the amplitude increased. The hopscotch method (ii) takes less computing time than the other two methods ((i), (iii)) for the 1-soliton cases, while the explicit (i) method took less computing time than the hopscotch (ii) and the implicit—explicit (iii) methods for the 2-soliton cases.

TABLE I

Comparison of the Computing Time (E) Which IS Required to Attain an Accuracy (L_{∞}) < 0.006 for Computations Beginning at t = 0 and Ending at t = 1.0, for the Numerical Methods Utilized in Solving the NLS Equation⁴

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Vo.	Method	Mesh size	min	sec	t = T	L_s	$\mathbf{P}_{\mathbf{t}}$	v_2	E
No.	Explicit	$\Delta x = 0.05$ $\Delta t = 0.000625$	E: 7	33	0.25 0.5 1.0	0.00159 0.00308 0.00564	0.00000 0.00000 0.00000	-0.00554 -0.00555 -0.00556	41.2
ž.,	Implicit- explicit.	$\Delta x = 0.05$ $\Delta t = 0.001$	E; 11	45	0.25 0.5 1.0	0.00146 0.00287 0.00577	-0.00099 -0.00197 -0.00393	-0.00719 -0.00882 -0.01205	64.1
3.	Implicit (Crank- Nicolson).	$\Delta x = 0.05$ $\Delta t = 0.005$	E: 5	39	0.25 0.5 1.0	0.00165 0.00320 0.00585	0.00000 0.00000 -0.00001	-0.00555 -0.00556 -0.00557	30.8
4.	Hopscotch	$\Delta x = 0.08$ $\Delta t = 0.002$	E: 1	4	0.25 0.5 1.0	0.00209 0.00321 0.00538	0.00000 0.00003 0.00003	-0.01409 -0.01408 -0.01407	5.8

	Split step Fourier method	$\Delta x = 0.3125$ $\Delta t = 0.02$	E: 0		0.25 0.5 1.0	0.00463 0.00502 0.00466	0.00000 0.00000 0.00000	0.00000 0.00001 0.00005	
6.	The Ablowitz and Ladik local scheme	$\Delta x = 0.06$ $\Delta t = 0.0165$	E: 2		0.25 0.5 1.0	0.00157 0.00306 0.00580	0.00001 0.00002 0.00004	-0.00791 -0.00798 -0.00797	11.
7.	The Ablowitz and Ladik global scheme	$\Delta x = 0.05$ $\Delta t = 0.04$	E: 2	10	0.25 0.5 1.0	0.00136 0.00272 0.00561	0.00001 0.00002 0.00003	0.00554 0.00553 0.00550	11.8
8.	Pseudospectral (Fornberg- Whitham)	$\Delta x = 0.3125$ $\Delta t = 0.0026$	E: 0	50	0.25 0.5 1.0	0.00513 0.00505 0.00513	0.00000 0.00000 0.00001	-0.00003 0.00001 -0.00003	4.5

a Two conserved quantities are shown. 1-soliton as an initial condition with amplitude = 1 on the interval [-20, 20].

 $[\]Delta x =$ The increment in x.

 $[\]Delta t =$ The increment in t.

 $v_1 = (q_1 - q_{10})/q_{10}$, $q_{10} =$ The exact value of the the $\int |q|^2 dx$. $v_2 = (q_2 - q_{20})/q_{20}$, $q_{20} =$ The exact value of the $\int (|q|^4 - |\partial q/\partial x|^2) dx$. $q_1 =$ The calculated value of the conserved quantity of the NLS equation which is $\int |q^2| dx$.

 q_2 = The calculated value of the conserved quantity of the *NLS* equation which is $\int (|q|^4 - |\partial q/\partial x|^2) dx$. $L_{\infty} = \max |\vec{q}_n^m - q_n^m|, \vec{q}_n^m$ is the numerical solution and q_n^m is the exact solution at the point $(\Delta x \cdot n, \Delta t \cdot m)$ for all n, m.

TABLE II

Comparison of the Computing Time (E) Which Is Required to Attain an Accuracy $(L_{\infty}) < 0.01$ for Computations Beginning at t = 0 and Ending at t = 1.0, for the Numerical Methods Utilized in Solving the NLS Equation.^a

				T	ime					
No.	Method	Mesh size	ı	nin	sec	t = T	L_{α}	v_{i}	v_2	Normalized E
L	Explicit	dx = 0.02 $dt = 0.0001$	<i>E</i> :	116	50	0.25 0.5 1.0	0.00205 0.00304 0.00931	-0.00219 -0.00221 -0.00437	-0.00293 -0.00292 -0.00284	81.5
2.	Implicit- explicit	$\Delta x = 0.03$ $\Delta t = 0.00022$	E:	82	18	0.25 0.5 1.0	0.00768 0.00938 0.00759	0.00001 0.00002 0.00003	-0.01022 -0.01424 -0.02243	57.4
3.	Implicit (Crank- Nicolson	$\Delta x = 0.02$ $\Delta t = 0.011$	E:	16	44	0.25 0.5 1.0	0.00329 0.00522 0.00971	0.00000 0.00000 0.00000	-0.00277 -0.00276 -0.00273	11.7
4.	Hopscotch	Ax = 0.02 $At = 0.0004$	E:	19	42	0.25 0.5 1.0	0.00420 0.00744 0.00963	0.00002 0.00002 0.00002	-0.00283 -0.00286 -0.00284	13.7
5.	Split step Fourier method	dx = 0.1563 $dt = 0.0048$	E:	1	26	0.25 0.5 1.0	0.00893 0.00594 0.00464	0.00000 0.00000 0.00000	0.00044 0.00030 0.00034	- 1
6.	The Ablowitz and Ladik local scheme	$\Delta t = 0.06$ $\Delta t = 0.03$	E:	2	28	0.25 0.5 1.0	0.00731 0.00886 0.00695	-0.00001 -0.00001 -0.00001	-0.02531 -0.02541 -0.02526	1.7
7.	The Ablowitz and Ladik global scheme	$\Delta x = 0.07$ $\Delta t = 0.012$	E:	7	33	0.25 0.5 1.0	0.00600 0.0100 0.00937	-0.00003 -0.00006 -0.00004	-0.03311 -0.03311 -0.03324	5.3
3.	Pseudospectral (Fornberg- Whitham)	dx = 0.1563 dt = 0.0011	E:	4	6	0.25 0.5 1.0	0.00860 0.00860 0.00840	0.00000 0.00000 0.00000	0.00005 -0.00013 0.00005	2.9

Two conserved quantities are shown. I-soliton as an initial condition with amplitude = 2 on the interval [-20, 20]

TABLE III

Comparison of the Computing Time (E) Which Is Required to Attain an Accuracy $(L_{\infty}) < 0.08$ for Computations Beginning at t = 0 and Ending at t = 1.0, for the Numerical Methods Utilized in Solving the NLS Equation^a

			Tir	ne					Normalize
No.	Method	Mesh size		sec	t = T	L_{∞}	v_{i}	v_2	Normanzeo E
	Implicit (Crank- Nicolson)	$\Delta x = 0.02$ $\Delta t = 0.004$	E: 18	29	0.25 0.5 1.0	0.01922 0.03751 0.07380	0.00002 0.00004 0.00008	-0.02658 -0.02725 -0.02725	37
2.	Split step Fourier method	$\Delta x = 0.15625$ $\Delta t = 0.007$	<i>E</i> : 0	30	0.25 0.5 1.0	0.06552 0.03703 0.05859	-0.00032 0.00179 -0.00093	-0.14279 0.12066 -0.18904	
3.	The Ablowitz and Ladik local scheme	$\Delta x = 0.02$ $\Delta t = 0.004$	<i>E</i> : 16	20	0.25 0.5 1.0	0.01852 0.03676 0.07270	0.00002 0.00003 0.00006	-0.02625 -0.02638 -0.02674	37.7
4.	The Ablowitz and Ladik global scheme	$\Delta x = 0.06$ $\Delta t = 0.02$	E: 4	25	0.25 0.5 1.0	0.04613 0.05490 0.07835	-0.00044 -0.00043 -0.00037	0.21209 0.21162 0.21266	8.8
5.	Pseudospectral (Fornberg- Whitham)	$\Delta x = 0.15625$ $\Delta t = 0.0021$	E: 1	2	0.25 0.5 1.0	0.05980 0.03765 0.06619	-0.00179 0.00341 0.01620	-0.16379 0.37022 0.22311	2.1

^a Two conserved quantities are shown. 1-soliton as an initial condition with amplitude = 4 on the interval [-10, 10].

TABLE IV

Comparison of the Computing Time (E) Which Is required to Attain an Accuracy $(L_{\alpha}) < 0.15$ for Computations Beginning at t = 0 and Ending at t = 0, for the Numerical Methods Utilized in Solving the NLS Equation^a

			Ti	me					
No.	Method	Mesh size	min	sec	t = T	L_{σ}	v,	v ₂	Normalized E
1.	Implicit (Crank- Nicolson)	Ax = 0.015 $At = 0.00125$	E: 56	59	0.25 0.5 1.0	0.03858 0.07309 0.14176	-0.00003 -0.00005 -0.00010	0.00844 0.00830 0.00830	37.2
	Split step Fourier method	$\Delta x = 0.078$ $\Delta t = 0.0045$	E: 1	32	0.25 0.5 1.0	0.14704 0.12475 0.13180	0.00018 -0.00010 0.00008	-0.07642 -0.07051 -0.07854	1
3,	The Ablowitz and Ladik local scheme	$\Delta x = 0.015$ $\Delta t = 0.00125$	E: 57	39	0.25 0.5 1.0	0.03977 0.07745 0.15498	-0.00005 -0.00009 -0.00018	0.00814 0.00796 0.00748	37.6
4.	The Ablowitz and Ladik global scheme	dx = 0.06 $dt = 0.01$	E: 11	12	0.25 0.5 1.0	0.10067 0.12484 0.14704	-0.00211 -0.00135 -0.00133	0.09536 0.10340 0.10210	7.3
5.	Pseudospectral (Fornberg- Whitham)	$\Delta x = 0.078$ $\Delta t = 0.00079$	E: 5	39	0.25 0.5 1.0	0.04890 0.03489 0.12482	-0.00046 -0.00041 0.00599	-0.02629 0.02385 -0.01356	3.7

Two conserved quantities are shown. 1-soliton as an initial condition with amplitude = 6 on the interval [-10, 10]

- (2) The previous three methods; explicit (i), hopscotch (ii), and implicit-explicit (iii) do not appear in Tables I, IV, and VII since extremely long computing time would be required.
- (3) The Crank-Nicolson implicit method (iv) takes more computing time than the Ablowitz-Ladik (local and global) method, the split step Fourier method and Fornberg-Whitham method in the case of 1-soliton, and it becomes comparable with the Ablowitz-Ladik local scheme for high amplitudes. In the case of 2-solitons, Crank-Nicolson takes less computing time than the Ablowitz-Ladik local scheme.
- (4) The Ablowitz-Ladik global scheme takes more computing time than the local scheme in the case of small amplitudes, but for high amplitudes it is roughly five times faster than the local, and the Crank-Nicolson schemes.
- (5) The pseudospectral method is roughly two times faster than the Ablowitz-Ladik local scheme for small amplitudes, but it is much faster for high amplitudes. This method is roughly two times faster than the Ablowitz-Ladik global scheme for high amplitudes. This method only proves to be faster than the split step Fourier method for small amplitude 2-soliton cases.
- (6) The split step Fourier method is faster than all the utilized methods for small and large amplitudes for the 1-soliton case. In the average it is three times faster than the Fornberg-Witham method. Also it proves to be faster than the Fornberg-Whitham method for high amplitude 2-soliton cases. The tables and figures exhibit the results.

As a conclusion we find that the split step Fourier method is the best method for the NLS equation, followed by the pseudospectral method then the Ablowitz-Ladik global scheme. However we believe that if we were able to go to very high amplitudes (our machine capability prevented this) the Ablowitz-Ladik global scheme would improve dramatically and would prove to be better than the other methods. However it should be noted that the NLS equation is quite unusual in the sense that the nonlinearity is especially simple. This has a dramatic effect in the split step Fourier method—see Eq. (2.22)—which means that both steps admit to essentially exact methods. Generally this will not be true (see paper III). We also note that whereas the Ablowitz-Ladik scheme is $O((\Delta t)^2, (\Delta x)^2)$ the split step Fourier and Fornberg-Whitham methods are of order $O((\Delta t)^2, (\Delta x)^p)$ for all p. (See also the calculations for the KdV equation in paper III.) It is also worth mentioning that we have tried the sweeping technique in implementing the implicit-explicit and the Crank-Nicolson methods, and found that it did not affect the overall conclusions.

All the numerical calculations are inspected at every step by using the conserved quantities $\int |q|^2 dx$, and $\int (|q|^4 - |\partial q/\partial x|^2) dx$ (Tables I-VII). The two conserved quantities are calculated by means of Simpson's rule [18]. In the finite difference schemes we have discretized U_x by using a central difference approximation. In the Fourier methods the derivatives are calculated using Fourier method. The Ablowitz-Ladik global scheme is the only utilized scheme which has an infinite number of conserved quantities. It is worth mentioning that we calculated the L_2 error norm and found that it reflects the same conclusions as the L_∞ norm.

TABLE V Comparison of the Computing Time (E) Which Is Required to Attain an Accuracy (L_{∞}) < 0.003 for Computations Beginning at t=0 and Ending at t=2.5, for the Numerical Methods Utilized in Solving the NLS Equations^a

			Ti	me					
No.	Method	Mesh size	min	sec	I = T	L_{∞}	ν_1	v_j	Normalized E
1.	Explicit	$\Delta x = 0.13$ $\Delta t = 0.0036$	E: 1	1	0.5 1.0 1.6 1.8 2.5	0.00116 0.00141 0.00175 0.00189 0.00265	0.00000 0.00000 0.00000 0.00000	0.00619 0.00483 0.00415 0.00415 0.00659	1.2
2.	Implicit— explicit	dx = 0.05 $dt = 0.0025$	E: 9	14	0.5 1.0 1.6 1.8 2.5	0.00084 0.00096 0.00124 0.00133 0.00250	0.00084 0.00150 0.00215 0.00235 0.00314	0.00372 0.00563 0.00777 0.00863 0.01434	10.9
3,	Implicit (Crank- Nicolson)	Ax = 0.13 $At = 0.04$	E: 1	15	0.5 1.0 1.6 1.8 2.5	0.00116 0.00148 0.00182 0.00198 0.00272	0.00001 0.00002 0.00002 0.00001 -0.00009	0.00622 0.00495 0.00423 0.00420 0.00619	1.5



4.	Hopscotch	$\Delta x = 0.05$ $\Delta t = 0.001$	E: 5	58	0.5 1.0 1.6 1.8 2.5	0.00099 0.00141 0.00173 0.00188 0.00251	0.00002 0.00004 0.00005 0.00005 0.00001	0.00008 0.00060 0.00093 0.00088 0.00063	7
5.	Split step Fourier method	$\Delta x = 0.625$ $\Delta t = 0.005$	E: 0	51	0.5 1.0 1.6 1.8 2.5	0.00086 0.00097 0.00116 0.00125 0.00251	-0.00028 -0.00022 -0.00007 -0.00004 0.00071	-0.01117 -0.00895 -0.00184 0.00032 0.03595	
6.	The Ablowitz and Ladik local scheme	$\Delta x = 0.07$ $\Delta t = 0.07$	E: 1	36	0.5 1.0 1.6 1.8 2.5	0.00053 0.00095 0.00142 0.00158 0.00282	-0.00017 -0.00028 0.00031 0.00028 0.00000	0.00037 -0.00090 -0.00144 -0.00128 0.00156	1.9
7.	The Ablowitz and Ladik global scheme	$\Delta x = 0.08$ $\Delta t = 0.045$	E: 2	13	0.5 1.0 1.6 1.8 2.5	0.00055 0.00104 0.00156 0.00170 0.00278	-0.00021 0.00034 0.00041 0.00039 0.00012	0.00050 -0.00113 -0.00196 -0.00189 0.00148	2.6
8.	Pseudospectral (Fornberg- Whitham)	$\Delta x = 0.625$ $\Delta t = 0.0071$	E: 0	26	0.5 1.0 1.6 1.8 2.5	0.00136 0.00122 0.00149 0.00166 0.00266	-0.00028 -0.00022 -0.00007 -0.00005 0.00073	-0.01125 -0.00963 -0.00342 -0.00158 0.03247	0.5

^a Two conserved quantities are shown. Two solitons as an initial condition with amplitudes 1 and 0.5 respectively, and they are allowed to interact, on the interval [-20, 20].

TABLE VI

Comparison of the Computing Time (E) Which Is Required to Attain an Accuracy (L_{∞}) < 0.0062 for Computations Beginning at t=0 and Ending at t=1.0, for the Numerical Methods Utilized in Solving the NLS Equation^a

			Tir	ne					
No.	Method	Mesh size	min	sec	t = T	L_{∞}	v_1 .	v_2	Normalized E
	Explicit	$\Delta x = 0.032$			0.1	0.00071	0.00000	0.00345	
		$\Delta t = 0.000256$	E: 19	4	0.25	0.00111	0.00000	0.00281	
					0.5	0.00192	0.00000	0.00229	2.8
					0.8	0.00615	0.00000	0.01640	-
					1.0	0.00500	0.00000	0.01237	
2.	Implicit-	$\Delta x = 0.03$			0.1	0.00321	0.00027	0.00498	
	explicit	$\Delta t = 0.0002$	E: 68	9	0.25	0.00576	0.00068	0.00764	
					0.5	0.00712	0.00135	0.01225	9.9
					0.8	0.00615	0.00203	0.01698	
					1.0	0.00467	0.00272	0.02154	
	Implicit (Crank-	$\Delta x = 0.03$			0.1	0.00067	-0.00003	0.00285	
	Nicolson)	$\Delta t = 0.012$	E: 6	58	0.25	0.00093	-0.00005	0.00214	
					0.5	0.00188	-0.00012	0.00110	
					0.8	0.00601	-0.00124	0.00435	
					1.0	0.00605	-0.00094	0.00377	

4.	Hopscotch	$\Delta x = 0.015$ $\Delta t = 0.0001$	E: 73	44	0.1 0.25 0.5 0.8 1.0	0.00086 0.00149 0.00250 0.00855 0.00704	0.00000 0.00001 0.00001 -0.00005 -0.00004	0.00052 0.00000 -0.00033 0.01091 0.00777	10.7
5.	Split step Fourier method	$\Delta x = 0.156$ $\Delta t = 0.001$	E: 6	55	0.1 0.25 0.5 0.8 1.0	0.00157 0.00168 0.00221 0.00613 0.00598	0.00000 0.00000 0.00000 0.00001 -0.00004	-0.00054 -0.00012 0.00194 0.01595 -0.02103	
6.	The Ablowitz and Ladik local scheme	$\Delta x = 0.02$ $\Delta t = 0.01$	E: 13	24	0.1 0.25 0.5 0.8 1.0	0.00029 0.00072 0.00156 0.00617 0.00381	-0.00003 -0.00009 -0.00012 0.00081 0.00065	0.00099 0.00014 0.00042 0.01801 0.01348	9
7.	The Ablowitz and Ladik global scheme	$\Delta x = 0.03$ $\Delta t = 0.03$	E: 6	47	0.1 0.25 0.5 0.8 1.0	0.00057 0.00139 0.00265 0.00620 0.00632	-0.00004 -0.00011 -0.00014 0.00119 0.00087	0.00247 0.00085 -0.00032 0.03656 0.02689	
8.	Pseudospectral (Fornberg- Whitham)	$\Delta x = 0.156$ $\Delta t = 0.0012$	E: 3	56	0.1 0.25 0.5 0.8 1.0	0.00202 0.00228 0.00378 0.00612 0.00564	0.00000 0.00000 0.00000 0.00002 0.00003	-0.00028 0.00007 0.00002 0.00041 -0.00987	0.6

^a Two conserved quantities are shown. Two solitons as an initial condition with amplitudes 2 and 1 respectively, and they are allowed to interact, n the interval [-20, 20].

TABLE VII

Comparison of the Computing Time (E) Which Is Required to Attain an Accuracy (L_{∞}) < 0.013 for Computations Beginning at t=0 and Ending at t=1,0, for the Numerical Methods Utilized in Solving the NLS Equation^a

			Tin	ne					NI1'
No.	Method	Mesh size	min	sec	t = T	L_{∞}	v_{i}		Normalize E
	Implicit (Crank-	$\Delta x = 0.0085$			0.1	0.00150	-0.00001	0.00288	
	Nicolson)	$\Delta t = 0.0001$	E: 98	25	0.25	0.00276	-0.00002	0.00276	
					0.5	0.01296	-0.00020	0.00736	5.7
					0.75	0.00667	-0.00006	0.00215	
					1.0	0.00797	-0.00008	0.00190	
2.	Split step	$\Delta x = 0.078$			0.1	0.00503	0.00000	0.00069	
	Fourier method	$\Delta t = 0.0004$	E: 17	9	0.25	0.00416	0.00000	0.00031	
					0.5	0.01363	0.00039	0.19676	
					0.75	0.00393	0.00000	0.00002	
					1.0	0.00512	0.00000	0.00031	
3.	The Ablowitz	$\Delta x = 0.007$			0.1	0.00083	0.00000	0.00210	
	and Ladik local	$\Delta t = 0.0007$	E: 168	59	0.25	0.00162	-0.00001	0.00211	
	scheme				0.5	0.01283	0.00027	-0.02727	9.9
					0.75	0.00460	-0.00002	0.00185	
					1.0	0.00637	-0.00002	0.00175	
4.	The Ablowitz	$\Delta x = 0.01$			0.1	0.00150	0.00001	0.00407	
	and Ladik global	$\Delta t = 0.005$	E: 49	55	0.25	0.00193	0.00003	0.00435	
	scheme				0.5	0.01348	0.00059	0.03407	2.9
					0.75	0.00289	0.00003	0.00404	
					1.0	0.00406	0.00007	0.00430	
5.	Pseudospectral	$\Delta x = 0.078$			0.1	0.00641	0.00000	0.00088	
	(Fornberg-	$\Delta t = 0.0002$	E: 22	45	0.25	0.00630	0.00000	0.00043	
	Whitham)				0.5	0.01301	0.00039	0.12960	1.3
	•				0.75	0.00758	0.00000	-0.00018	. 5
					1.0	0.01024	0.00000	0.00050	

^a Two conserved quantities are shown. Two solitons as an initial condition with amplitudes 4 and 3 respectively, on the interval [-10, 10].

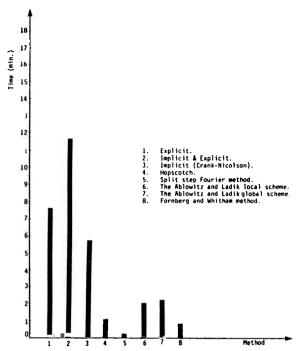


Fig. 3. Displays the computing time (E) which is required by each utilized method given in Table I. 1-soliton, amplitude = 1.

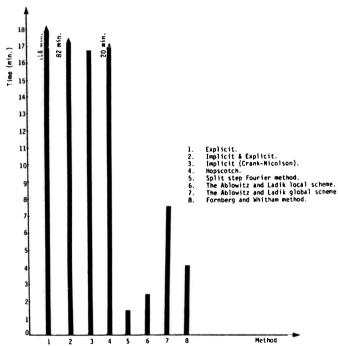


Fig. 4. Displays the computing time (E) which is required by each utilized method given in Table II. 1-soliton, amplitude = 2.

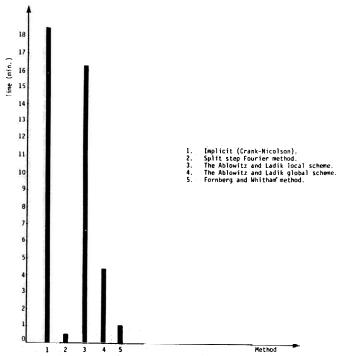


FIG. 5. Displays the computing time (E) which is required by each utilized method given in Table III. soliton, amplitude = 4.

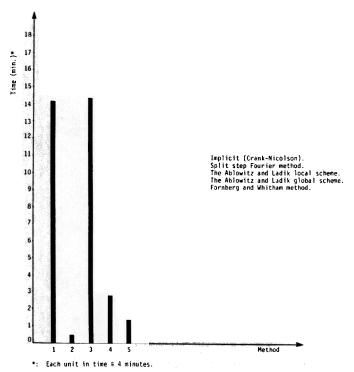


FIG. 6. Displays the computing time (E) which is required by each utilized method given in Table IV. 1-soliton, amplitude = 6.

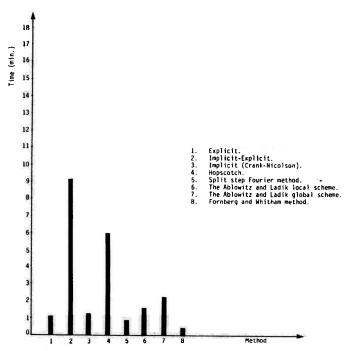


FIG. 7. Displays the computing time (E) which is required by each utilized method given in Table V. Two solitons with amplitudes 0.5 and 1.

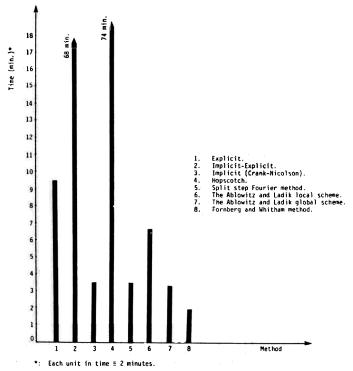


FIG. 8. Displays the computing time (E) which is required by each utilized method given in Table VI. Two solitons with amplitudes 1 and 2.

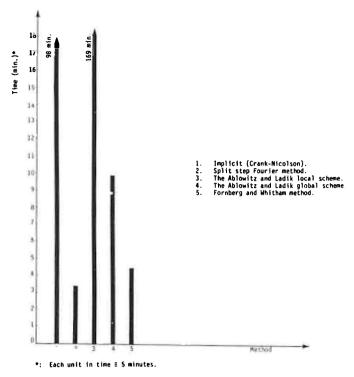


Fig. 9. Displays the computing time (E) which is required by each utilized method given in Table VII. Two solitons with amplitudes 3 and 4.

APPENDIX A: AN OPTIMIZATION OF GAUSSIAN ELIMINATION

This method seeks to optimize Gaussian elimination by eliminating unnecessary storage and multiplication by zeros. To begin we have the following quasi-tridiagonal system

Instead of storing the $N \times N$ matrix, we store the augmented matrix in an $N \times 4$ matrix whose elements are the tridiagonal elements and the b_i 's. We then perform Gaussian elimination on the $N \times 4$ matrix keeping in mind their original locations in the matrix. When this is done we have an upper triangular matrix and an original system is of the form

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where * values are the updated elements. Using back substitution we obtain the solution. The total number of operations required to obtain the solution using this method is (11N-15). The same idea can be applied to quasi-pentagonal system of equations and so on.

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