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A Self Adaptive Difference Scheme for the Nonlinear Schrödinger Equation

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ABSTRACT. An idea of Sanz-Serna [1982] suggested for the numerical solution of the Korteweg de Vries equation is applied to the numerical solution of the Nonlinear Schrödinger Equation. The approximating method is an explicit scheme where the time step is chosen at each stage to exactly conserve the L_2 'energy' of the theoretical solution of the discretised procedure. The algorithm is applied to the case of a single soliton and to the interaction of two solitons.

1. Introduction

In the past few years interest has substantially increased in the solution of nonlinear time dependent partial differential equations governing nonlinear waves in dispersive media – see for example Scott *et al.* (1973), Whitham (1974), Lamb (1980), ... etc.

The development of mathematical techniques like inverse scattering for analysing these equations has been accompanied by a similar development and study of numerical algorithms for their approximate solution.

Most of these numerical studies have been devoted to the Korteweg de Vries equation (Zabusky and Kruskal 1965, Greig and Morris 1976, Alexander and Morris 1979, Sanz Serna and Christie 1981 and Mitchell and Schoombie 1981) although other 'soliton producing' equations such as the Sine Gordon equation (Manoranjan 1981) and the nonlinear Schrödinger equation (Griffiths *et al.* 1982) have received some attention. In all these publications, however, the computed solution is ob-

tained by methods which do not conserve energy and so the threat of nonlinear instabilities is always present in the calculation in time. A simple idea introduced by Sanz Serna (1982) for the Korteweg de Vries equation, where the time step is adjusted in order to conserve the discrete energy of the computed solution, is tried out on the nonlinear Schrödinger (N.L.S.) equation in the present paper. Although conservative numerical schemes have been developed in the past for a variety of partial differential equations (Arakawa 1966, Morton 1977 and Navon 1981), we believe that Sanz Serna is the first to describe a *self adaptive* time procedure based on the conservation of the discrete energy.

The N.L.S. equation is given by

$$i\frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} + u|u|^2 = 0, \; i = \sqrt{-1}, \tag{1.1}$$

where u(x,t) is a complex field governing the evolution of any weakly nonlinear strongly dispersive almost monochromatic wave. This problem posed as a pure initial value problem was solved exactly by Zakharov and Shabat (1972), using the inverse scattering method for initial data u(x,0) which vanishes for sufficiently large |x|. For more general initial conditions, the theoretical solution is not known. Consequently, in Griffiths *et al.* (1982) an investigation is carried out into methods for the numerical solution of the N.L.S. These methods based on finite differences and finite elements use a constant time step and give only an approximate conservation of the energy. Thus, the question of constructing self adaptive conservative schemes remains; a situation remedied in the present paper.

2. An Explicit Energy Conserving Scheme

Consider the N.L.S. equation (1.1) together with the initial condition

$$u(x,0) = g(x), \qquad x_L \leqslant x \leqslant x_R$$

and the homogeneous Neumann boundary conditions

$$\frac{\partial u}{\partial x} = 0 \qquad x = x_L; x = x_R \qquad t > 0$$

where $x_L < x_R$. Let

$$u(x,t) = v(x,t) + iw(x,t)$$

and so (1.1) leads to the system

$$\frac{\partial \mathbf{u}}{\partial t} + A \frac{\partial^2 \mathbf{u}}{\partial x^2} + \mathbf{f}(\mathbf{u}) = \mathbf{0} \tag{2.1}$$

where $\mathbf{u} = [v,w]^T$, $A = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$ and $\mathbf{f}(\mathbf{u}) = [w(v^2 + w^2), -v(v^2 + w^2)]^T$ subject to

$$v(x,0) = g_k(x) \; ; \; w(x,0) = g_I(x)$$

and

$$\frac{\partial v}{\partial x} = 0 \, , \, \frac{\partial w}{\partial t} = 0 \quad \text{at} \quad x = x_L, x_R,$$

where $g(x) = g_k(x) + ig_I(x)$. We construct the weak form of (2.1) by taking the L_2-inner product with elements of the space $H^1(x_L,x_R)$. Integrating by parts and utilizing the boundary conditions yields

$$\left(\frac{\partial \mathbf{u}}{\partial t} \, , \, \psi\right) - A\left(\frac{\partial \mathbf{u}}{\partial x} \, , \, \frac{\partial \psi}{\partial x}\right) + (\mathbf{f},\psi) = \mathbf{0}, \quad \forall \, \psi \in H^1(x_L,x_R). \tag{2.2}$$

In the above, $H^1(x_L,x_R)$ is the space of functions in the range $x_L \leq x \leq x_R$ with the integrable function value and first derivative.

Introduce a uniform grid with $x_L = x_1 < x_2 < \cdots < x_N = x_R$ and $x_j - x_{j-1} = h$ ($j = 2, 3, \ldots, N$). Let S^h be an N dimensional subspace of H^1 and choose elements of S^h to be piecewise linear hat functions denoted by $\{\psi_j\}_{j=1}^N$. Suppose an approximation $\mathbf{U}$ is given by

$$\mathbf{U}(x,t) = \sum_{j=1}^{N} \boldsymbol{\alpha}_j(t)\psi_j(x) \tag{2.3}$$

where $\boldsymbol{\alpha}_j(t) = (\boldsymbol{\alpha}_{j^1}(t),\boldsymbol{\alpha}_{j^2}(t))^T$, $j = 1, 2, \ldots, N$ are time dependent coefficients to be determined. The discrete form of (2.2) is

$$\sum_{j=1}^{N} \boldsymbol{\alpha}_j(\psi_j,\psi_k) - A \sum_{j=1}^{N} \boldsymbol{\alpha}_j(\psi_j',\psi_k') + (\underline{f},\psi_k) = 0 \qquad k = 1, 2, \ldots, N \tag{2.4}$$

where a dot denotes differentiation with respect to t and a dash with respect to x. Product Approximation (see Christie *et al.* 1981) is used to simplify $(\mathbf{f},\psi_k)$ so that

$$(\mathbf{f},\psi_k) = (\sum_{j=1}^{N} f(\boldsymbol{\alpha}_j)\psi_j,\psi_k).$$

Since $\{\psi_j\}$ are chosen to be linear 'hat' basic functions,

$$\psi_j(x) = \begin{cases} (x - x_{j-1})/h & x_{j-1} \leqslant x \leqslant x_j \\ (x_{j+1} - x)/h & x_j \leqslant x \leqslant x_{j+1} \end{cases} \qquad j = 2, 3, \ldots, N-1$$

and

$$\psi_1(x) = (x_2 - x)/h \qquad x_1 \leqslant x \leqslant x_2$$

$$\psi_N(x) = (x - x_{N-1})/h \qquad x_{N-1} \leqslant x \leqslant x_N$$

Direct calculation of the inner products in (2.4) leads to

$$M \frac{d\boldsymbol{\alpha}}{dt} + S\boldsymbol{\alpha} + M\mathbf{F} = 0 \tag{2.5}$$

where

$$M = \frac{1}{6}\begin{bmatrix} 2I & I & & & \\ I & 4I & I & & \\ & I & 4I & I & \\ & & I & 4I & I \\ & & & I & 2I \end{bmatrix}$$

and $S = \dfrac{1}{h^2}\begin{bmatrix} -A & A & & & \\ A & -2A & A & & \\ & A & -2A & A & \\ & & A & -2A & A \\ & & & A & -A \end{bmatrix}$

are the mass and stiffness matrices respectively.
$\mathbf{F} = (\mathbf{F}_1, \mathbf{F}_2, \ldots, \mathbf{F}_N)^T$ is the load vector where
$\mathbf{F}_j = \mathbf{f}(\boldsymbol{\alpha}_j)$ and $\boldsymbol{\alpha} = (\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \ldots, \boldsymbol{\alpha}_N)^T$.

In order to solve the system of ordinary differential equations (2.5), the following time discretisation is proposed. Suppose at time level t_m a time step τ_m is used to advance the solution $\boldsymbol{\alpha}$ from t_m to t_{m+1} where

$$t_m = \sum_{j=0}^{m-1} \tau_j \qquad m = 1, 2, \ldots$$

$$= t_{m-1} + \tau_{m-1}$$

and τ_0 is a given starting time step. Replace $\frac{d\boldsymbol{\alpha}}{dt}$ by $(\boldsymbol{\alpha}_{m+1} - \boldsymbol{\alpha}_{m-1})/(\tau_m + \tau_{m-1})$ and $\boldsymbol{\alpha}$ by $\boldsymbol{\alpha}_m$ in (2.5), where $\boldsymbol{\alpha}_m = \boldsymbol{\alpha}(t_m)$ etc.
There results the time stepping scheme

$$\mathbf{M}\boldsymbol{\alpha}_{m+1} = \mathbf{M}\boldsymbol{\alpha}_{m-1} - (\tau_m + \tau_{m+1})[\mathbf{S}\boldsymbol{\alpha}_m + \mathbf{M}\mathbf{F}_m) \qquad m = 1, 2, \ldots \quad (2.6)$$

where $\boldsymbol{\alpha}_0$ and $\boldsymbol{\alpha}_1$ are obtained from the initial data.

It is easy to show that the L_2 'energy' of the solution $\mathbf{u}$ of (1.2) is conserved, *i.e.*

$$\frac{d}{dt}\int_{x_L}^{x_R} \mathbf{u}^T\mathbf{u}dx = 0.$$

The initial 'energy' is given by

$$\int_{x_L}^{x_R} \mathbf{u}_0^T\mathbf{u}_0 dx = (\mathbf{u}_0,\mathbf{u}_0)$$

where $\mathbf{u}_0 = (g_k(x),g_l(x))$. The discrete approximation $\mathbf{U}$ has initial 'energy'

$$\int_{x_L}^{x_R} \mathbf{U}^T(x,0)\mathbf{U}(x,0)dx = h\boldsymbol{\alpha}_0^T\mathbf{M}\boldsymbol{\alpha}_0$$

which converges to $(\mathbf{u}_0,\mathbf{u}_0)$ as $h \to 0$. For a given value of h, therefore, we wish to construct $\{\boldsymbol{\alpha}_m\}$ for increasing m so that

$$\boldsymbol{\alpha}_m^T\mathbf{M}\boldsymbol{\alpha}_m = \boldsymbol{\alpha}_0^T\mathbf{M}\boldsymbol{\alpha}_0, \quad (2.7a)$$

or with *mass lumping*, $\mathbf{M} = \mathbf{I}$, (Mitchell and Griffiths 1980).

$$\boldsymbol{\alpha}_m^T\alpha_m = \boldsymbol{\alpha}_0^T\boldsymbol{\alpha}_0. \quad (2.7b)$$

Now premultiply (2.6) by $\boldsymbol{\alpha}_{m+1}^T$ and eliminate $\boldsymbol{\alpha}_{m+1}^T$ from the right hand side of the expression obtained. This leads to

$$\boldsymbol{\alpha}_{m+1}^T\mathbf{M}\boldsymbol{\alpha}_{m+1} = \boldsymbol{\alpha}_{m-1}^T\mathbf{M}\boldsymbol{\alpha}_{m-1} - (\tau_m + \tau_{m-1})\{(\mathbf{M}^{-1}\mathbf{S}\boldsymbol{\alpha}_m + \mathbf{F}_m)^T\mathbf{M}\boldsymbol{\alpha}_{m-1}$$

$$+ \boldsymbol{\alpha}_{m-1}^T(\mathbf{S}\boldsymbol{\alpha}_m + \mathbf{M}\mathbf{F}_m) - (\tau_m + \tau_{m-1})(\mathbf{M}^{-1}\mathbf{S}\boldsymbol{\alpha}_m + \mathbf{F}_m)^T(\mathbf{S}\boldsymbol{\alpha}_m + \mathbf{M}\mathbf{F}_m)\}$$

and to obtain (2.7a) we require

$$\tau_m = \frac{2\,\boldsymbol{\alpha}_{m-1}^{T}(S\alpha_m + M\mathbf{F}_m)}{(S\boldsymbol{\alpha}_m + M\mathbf{F}_m)^{T}M^{-1}(S\boldsymbol{\alpha}_m + M\mathbf{F}_m)} - \tau_{m-1} \tag{2.8a}$$

Iff mass lumping is employed, (2.8a) is replaced by

$$\tau_m = \frac{2\,\boldsymbol{\alpha}_{m-1}^{T}(S\boldsymbol{\alpha}_m + \mathbf{F}_m)}{||S\boldsymbol{\alpha}_m + \mathbf{F}_m||_2^2} - \tau_{m-1}. \tag{2.8b}$$

where $||\cdot||_2$ is the discrete L_2 norm. The recommended numerical scheme for the N.L.S. is thus (2.6) with $(\tau_m + \tau_{m-1})$ given by (2.8a), or with mass lumping, (2.6) with $M = I$ and $(\tau_m + \tau_{m-1})$ given by (2.8b). The order of accuracy of these schemes in time is discussed by Sanz Serna (1982).

3. Stability

The algorithm with a time step adapted to conserve 'energy' (see section 2) is a nonlinear difference equation and consequently does not lend itself to regular von Neumann analysis. If, however, we assume a constant time step τ and linearise the nonlinear function $\mathbf{F}$ we get the algorithm

$$\mathbf{V}_{m+1} = \mathbf{V}_{m-1} - 2\,\tau[S\mathbf{V}_m + B\mathbf{V}_m] \tag{3.1}$$

where

$$B = \begin{bmatrix} 2vw & (v^2 + 3w^2) \\ -(3v^2 + w^2) - 2vw & \end{bmatrix}$$

is the locally constant Jacobian matrix of $\mathbf{f}$ with respect to $\mathbf{u}$. If λ and $\mathbf{c}$ are an eigenvalue and corresponding eigenvector of the amplification matrix (see Mitchell and Griffiths 1980) corresponding to (3.1), then

$$\lambda^{m+1}\mathbf{c} = \lambda^{m-1}\mathbf{c} - 2\,\lambda^{m}[-4\,A\,r\sin^2\frac{\theta}{2} + \tau B]\mathbf{c} \tag{3.2}$$

where θ is the Fourier frequency and $r = \tau/h^2$ is constant. Consequently λ satisfies the equation

$$\begin{vmatrix} \lambda^2 - 1 + 4\,\tau v w \lambda & -8\,r\lambda \sin^2\frac{\theta}{2} + 2\,\tau(v^2 + 3\,w^2)\lambda \\ 8\,r\lambda \sin^2\frac{\theta}{2} - 2\,\tau(3\,v^2 + w^2)\lambda & \lambda^2 - 1 - 4\,\tau v w \lambda \end{vmatrix} = 0,$$

which leads to

$$\mu^2 + [12\,\tau^2|u|^4 + 64\,r \sin^2\frac{\theta}{2}(r \sin^2\frac{\theta}{2} - \tau|u|^2) - 2]\mu + 1 = 0 \tag{3.3}$$

where $\mu = \lambda^2$. For stability, we require the discriminant of (3.3) to be non positive, and so after a certain amount of manipulation we get

$$0 \leqslant 16\,r \sin^2\frac{\theta}{2}[r \sin^2\frac{\theta}{2} - \tau|u|^2] + 3\,\tau^2|u|^4 \leqslant 1.$$

which leads to

$$0 \leqslant \tau^2\left(\frac{4\,s^2}{h^2} - 3|u|^2\right)\left(\frac{4\,s^2}{h^2} - |u|^2\right) \leqslant 1 \tag{3.4}$$

where $s^2 = \sin^2\frac{\theta}{2}$ .If we put $S = 4\,s^2/h$, then the segment of the positive quadrant of the $(S,|\mu|^2)$ plane lying between $S = |u|^2$ and $S = 3|u|^2$ contains values which cannot be satisfied by the inequality (3.4). This is not surprising in view of the fact that N.L.S. equation (1.1) is unstable itself, although depending on the initial condition, this may not show up for a long time, if at all. (Yuen and Ferguson 1978).

4. Numerical Results

We now investigate the performance of the algorithm (2.6) with M = I and $(\tau_m + \tau_{m-1})$ given by (2.8b) by solving the following two problems.

(1) Single Soliton

The theoretical solution of (1.1) (see Whitham 1974) is given by

$$u(x,t) = \sqrt{2\alpha}\exp\{i(\tfrac{1}{2}cx - \tfrac{1}{4}(c^2 - \alpha))\}\operatorname{sech}(\sqrt{\alpha}(x - ct)) \tag{4.1}$$

where α and c are positive constants. From (4.1) we choose our initial condition to be

$$u(x,0) = \sqrt{2\alpha}\exp(\tfrac{1}{2}icx)\operatorname{sech}(\sqrt{\alpha}\,x) \tag{4.2}$$

and note that it is exponentially small for $|x| \to \infty$. We use a natural boundary condition

$$\frac{\partial u}{\partial x} = 0 \text{ at } x = x_L \text{ and } x = {}_R \textbf{ for all } t > 0$$

and choose $x_L = -30$, $x_R = 70$ for convenience. The solution (4.1) is a complex valued function whose maximum modulus is $\sqrt{2\alpha}$. The modulus $|u|$ represents a soliton which travels with velocity c in the positive x-direction. The amplitude and velocity are independent parameters and so two initial wave profiles with the same value of α can propagate with different wave speeds.

(2) Collision of Two Solitons

Waves which collide in an elastic manner are considered to be solitons. We now investigate the ability of our numerical scheme to follow such waves and to preserve initial profiles after collision. For the collision of two solitons we choose our initial condition to be

$$u(x,0) = \sqrt{2\alpha}[\exp(\tfrac{1}{2}ic_1x_1)\operatorname{sech}(\sqrt{\alpha}\,x_1) + \exp(\tfrac{1}{2}ic_2x_2)\operatorname{sech}(\sqrt{\alpha}\,x_2)] \tag{4.3}$$

where $c_1 > c_2$, $x_1 = x$, and $x_2 = x - 25$. This initial condition represents two wave forms separated by a distance equal to 25 units. The faster wave is situated at $x = 0$ and the slower wave at $x = 25$. As time evolves, the faster wave (speed c_1) catches the slower wave (speed c_2) passing through it with only a phase shift. Natural boundary conditions are assumed at $x_L = -30$, and $x_R = 70$.

Figure 1 shows the single soliton solution using the adaptive scheme with mass lumping for $h = 0.5$ and an initial time step $\tau_0 = 0.01$. This corresponds to the results in Table 1, row 1. The dashed curve indicates the theoretical solution at $t = 0$ (the left most peak) and at $t = 30.0$ (the right most peak). The numerical

Table 1.

No. of Solitons	h	Initial τ	Max. τ	Min. τ
1	0.5	.0100	.0103	.0018
	0.25	.0100	.0101	.0086
2	0.5	.0100	.0100	.0010
	0.25	.0100	.0100	.0063

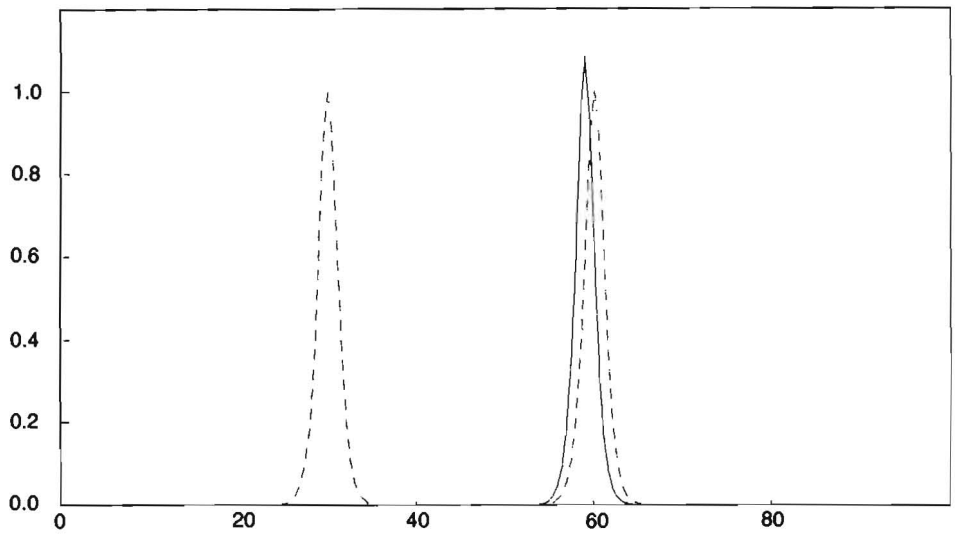

Fig. 1. h = 0.5, τ_0 = 0.01.

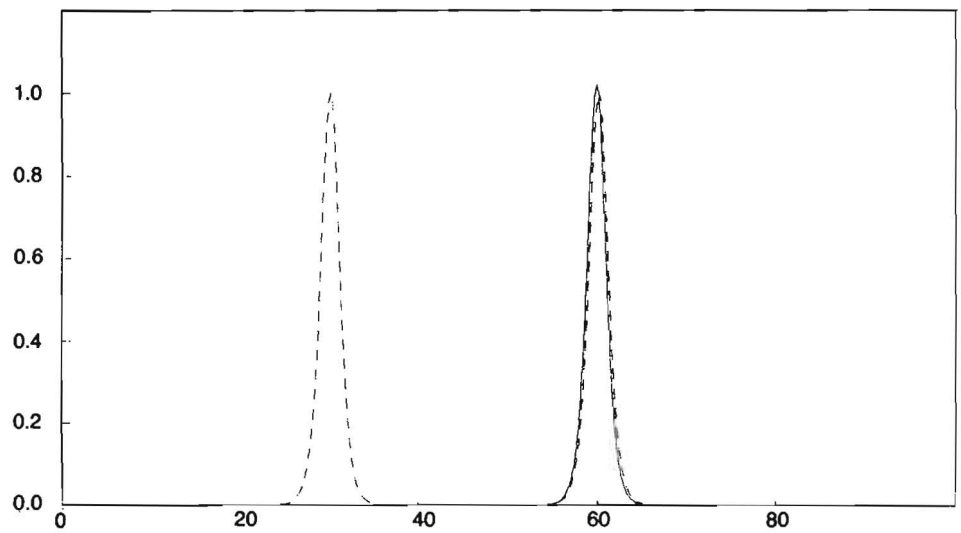

Fig. 2. h = 0.25, τ_0 = 0.01.

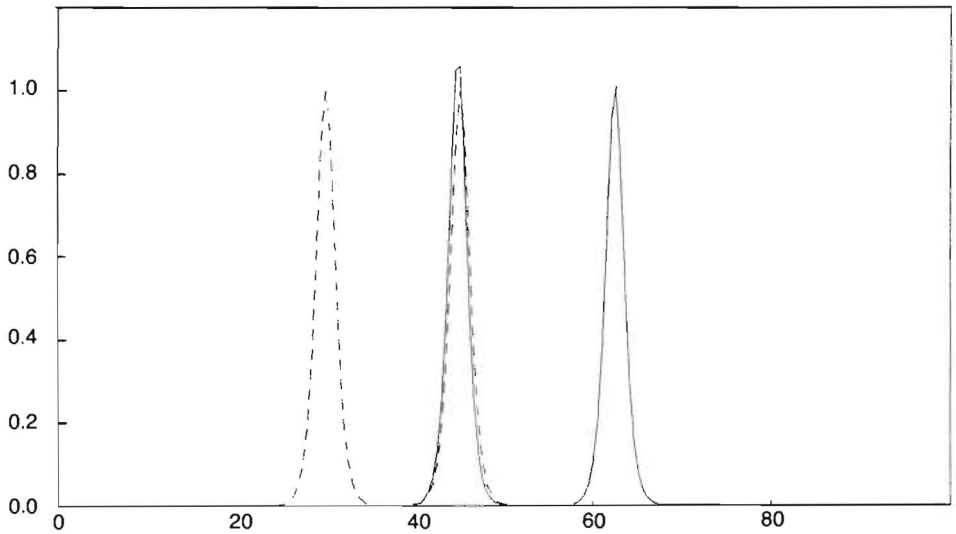

Fig. 3. h = 0.5, τ_0 = 0.01.

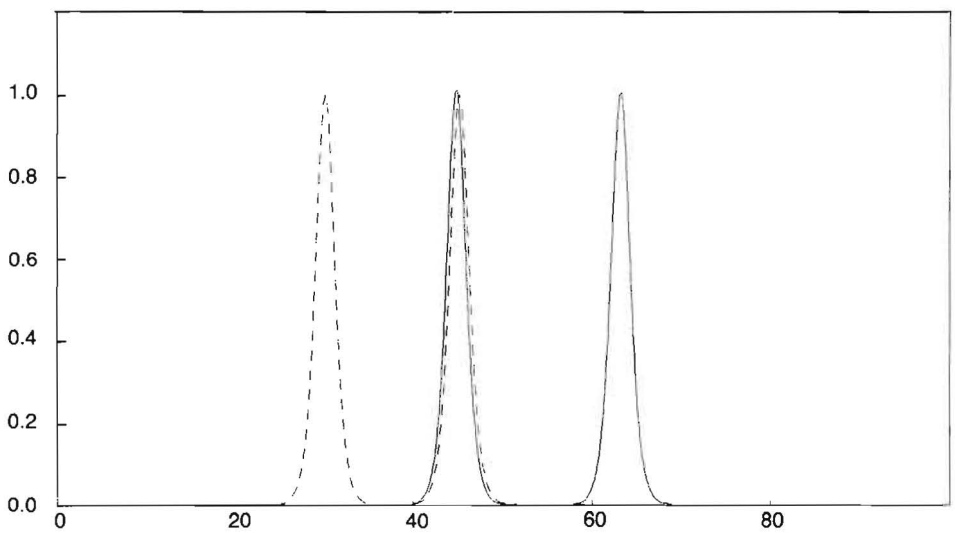

Fig. 4. h = 0.25, τ_0 = 0.01.

solution at t = 30.0 using the theoretical solution at t = 0 and t = τ_0 as initial data is depicted as the continuous curve. The computed solution both lags behind and has amplitude greater than the theoretical solution. By reducing h to 0.25, the computed results are much improved as can be seen from Fig. 2. In all cases, the velocity c is taken to be 1.0 and α to be 0.5.

In Fig. 3 and 4, we show the results obtained for two solitons. The broken lines show the initial positions of the two solitons with the faster soliton (c = 1.0) on the left of the slower soliton (c = 0.1). Both solitons have unit amplitude. After interaction (t = 30), the solitons are in the positions shown by the continuous lines with the faster soliton now on the right of the slower soliton. It is obvious from the positions of the slower soliton that a phase shift has taken place. Once again, the results for h = 0.25 (Fig. 4) are much better than those for h = 0.5 (Fig. 3).

The above results are in contrast with the standard leap frog (mid-point) method with equal grid spacing in time which exhibits blow-up when used to solve the N.L.S. equation.

5. Concluding Remarks

We have intorduced a simple mechanism for adjusting the time step in order to conserve the L_2 'energy' of the computed solution of the Nonlinear Schrödinger Equation. In the problem of the single soliton where the solution is maintaining its shape and velocity, there seems no reason why the time step should not remain constant. From Table 1, we see that for h = 0.25 the time step lies in the range $.0086 \leqslant \tau \leqslant .0101$. The evidence is that this range will decrease as h becomes smaller. In the two soliton problem, the time step to conserve energy will reduce during the interaction of the solitons. This is illustrated by the range $.0063 \leqslant \tau \leqslant .0100$ when h = 0.25 for the second problem.

The numerical results presented in this paper are obtained using double precision. With single precision the results are much poorer suggesting that round-off error is playing a major role in the present method. It appears, therefore, that for the adaptive time algorithm to be successful we require not only a fine grid in space but also a high degree of numerical precision. This way, the computed energy conservation is close to its theoretical counterpart.

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مخطط فرقي ذاتيّ التهايؤ لمعادلة شرودنجر اللاخطية

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قسم الرياضيات ـ جامعة دندى ـ اسكتلنده ؛ وقسم علم الحاسبات ـ جامعة ووترلو ـ كندا

تستخدم في هذا البحث فكرة سانز سيرنا (١٩٨٢) التى إقترحها للحل العددى لمعادلة كورتفج دي فريز في الحل العددى لمعادلة شرودنجر اللاخطية . تعتبر طريقة التقريب مخطط صريح فيه تختار الخطوة الزمنية في كل مرحلة لتحفظ تماماً « طاقة » L_2 للحل النظرى للأسلوب المنفصل . تطبق الطريقة في حالة سوليتون منفرد وفي حالة سوليتونين .