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NOTE

Linearized Crank–Nicholson Scheme for Nonlinear Dirac Equations

Since the pioneering work in [1], split-step spectral (SSS) methods have sometimes used for nonlinear wave computation. In a recent paper, De Frutos and Sanz-Serna [2] have applied these methods to nonlinear Dirac systems in $(1+1)$-dimensions. As a result of their numerical experiments, they conclude that SSS methods are clearly better than standard finite-difference schemes for these nonlinear systems.

Because long evolution times are required in the study of solitary wave dynamics in nonlinear Dirac systems, speed and accuracy are essential properties for a practical code. These requirements rule out some standard schemes as, for example, the Crank–Nicholson (CN) one, although it is convergent and stable for nonlinear Dirac systems [3]. The drawback of this scheme is its slowness because of the required iterations by the solution of its nonlinear algebraic equations.

In this note, we present a finite-difference method for nonlinear Dirac systems, already used some time ago [4], which is more accurate and orders of magnitude faster than the above-mentioned SSS methods. This finite-difference algorithm is a linearized Crank–Nicholson (LCN) scheme. The lack of iterations in this algorithm, without decreasing its accuracy, is the principal difference with the CN scheme. The LCN algorithm has been used in $(1+3)$-dimensions with spherical [5] and cylindrical [6] symmetry with satisfactory results. In the latter case the LCN scheme was completed with Strang's splitting [7].

Before proceeding any further, it is convenient to say something about the nonlinearity of the Dirac systems. The numerical properties of the LCN scheme, and also of the CN one, for nonlinear Dirac systems are based on the existence of a discrete norm which is constant. This corresponds to charge conservation in the continuum model and it is independent of the nonlinear terms. Therefore the numerical properties of the LCN scheme for a nonlinearity are valid, with some changes, for other ones. In order to compare with the numerical experiments of [2] and for the sake of simplicity, we shall analyse the Dirac equation with a scalar self-coupling. For numerical results with other more complicated nonlinearities see [8].

We begin with the following Dirac system in $(1+1)$-dimensions

$$u_t = \mathscr{A} u, \tag{1}$$

with the initial condition

$$u(x, 0) = \phi(x), \qquad -\infty < x < \infty,$$

where

$$\mathscr{A} = -\sigma_1 \frac{\partial}{\partial x} + i(|u_1|^2 - |u_2|^2 - 1)\,\sigma_3,$$

$u = u(x, t)$ is the spinor unknown, represented as a two-dimensional complex vector $u = [u_1, u_2]^{\mathrm{T}}$, where T stands for transpose, i is the imaginary unit, and σ_i $(i = 1, 2, 3)$ denote the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

We suppose that $|\phi_i(x)| \to 0$ as $|x| \to \infty$ and therefore $|u_i(x, t)| \to 0$ as $|x| \to \infty$.

Let h and k be respectively the space and time discretization mesh sizes. We denote by u_j^n the approximation to the unknown u at the space point $x_j = jh$ and at time $t_n = nk$. The LCN scheme for the system (1) is given by

$$(u_j^{n+1} - u_j^n)/k = A_j^{n+1/2}(u_j^{n+1} + u_j^n)/2, \tag{2}$$

where $A_j^{n+1/2}$ is the following linearization of the operator $\mathscr{A}$

$$A_j^{n+1/2} = -\sigma_1 D_0 + i(|u_{1j}^n|^2 - |u_{2j}^n|^2 - 1)\,\sigma_3 + ik(|u_{1t}|^2 - |u_{2t}|^2)_j^n\,\sigma_3/2.$$

Here u_{1t} and u_{2t} are, respectively, the first and second row

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of the right-hand side of Eq. (1) and D_0 is the central spatial difference operator

$$D_0 u_j^n = (u_{j+1}^n - u_{j-1}^n)/2h.$$

Substituting this difference operator into the spatial derivatives of the last term of $A_j^{n+1/2}$, we obtain

$$A_j^{n+1/2} = -\sigma_1 D_0 - i f_j^n \sigma_3$$

with

$$f_j^n = -1 + |u_{1j}^n|^2 - |u_{2j}^n|^2 + k\,\mathrm{Re}(u^+ \sigma_2 D_0 u)_j^n,$$

where $\mathrm{Re}(z)$ denotes the real part of z and u^+ stands for the complex-conjugate transpose of u. After rearrangement, the LCN scheme reads in the following tridiagonal form

$$-k\sigma_1 v_{j-1}/4h + a_j^n v_j + k\sigma_1 v_{j+1}/4h = u_j^n, \tag{3}$$

with

$$v_j = (u_j^{n+1} + u_j^n)/2$$

and

$$a_j^n = \begin{pmatrix} 1 + ikf_j^n/2 & 0 \\ 0 & 1 - ikf_j^n/2 \end{pmatrix}.$$

For the purpose of comparison, we shall consider the theoretical solution

$$\psi(x, t) = [M(x), iN(x)]^{\mathrm{T}} e^{-i\Lambda t},$$

$$M(x) = 2^{1/2}(1-\Lambda^2)^{1/2}(1+\Lambda)^{1/2} \times \frac{\cosh((1-\Lambda^2)^{1/2} x)}{1 + \Lambda \cosh(2(1-\Lambda^2)^{1/2} x)}$$

$$N(x) = 2^{1/2}(1-\Lambda^2)^{1/2}(1-\Lambda)^{1/2} \times \frac{\sinh((1-\Lambda^2)^{1/2} x)}{1 + \Lambda \cosh(2(1-\Lambda^2)^{1/2} x)}$$

with frequency $\Lambda = 0.75$. As $\psi_1(-x, t) = \psi_1(x, t)$, $\psi_2(-x, t) = -\psi_2(x, t)$, and the LCN scheme preserves this symmetry, we implemented this scheme in the x half-line $x \geqslant 0$. Besides, as the solution is exponentially small away from $x = 0$, we have introduced a cutoff at $x = 8$ in the initial condition. The LCN method was implemented in $0 \leqslant x \leqslant 16$ and $0 \leqslant t \leqslant 8$, the same subset of the spacetime as in [2].

Since the numerical initial condition was zero for $x > 8$, we have found it expedient to introduce a right moving boundary in order to solve the tridiagonal system (3) by the Thomas method [9]. This moving boundary works in the following way:

(i) Let us suppose that we want to know the solution of (3) at the first time step, that is at $t = k$. We introduce $u(8 + 2h, k) = 0$ as input in the Thomas algorithm and we calculate the auxiliary matrix coefficients of the algorithm.

(ii) The value of $u(0, k)$ is obtained from (i) and from the above-mentioned symmetry properties of the solution. Now, $u(x, k)$ is calculated in $0 \leqslant x \leqslant 8 + h$ by the Thomas method.

(iii) For later times, the points (i) and (ii) are recursively applied by increasing the range of x one step at a time. When the right moving boundary overtakes the value $x = 16$, we have put $u(16, t) = 0$.

(iv) The calculation accuracy was monitored against the conservation of the discrete L^2-norm

$$\|u^n\| = \left[h \sum_{j=0}^{J} (|u_{1j}^n|^2 + |u_{2j}^n|^2) \right]^{1/2}$$

with $J = 16/h$.

TABLE I

L^2-Errors for the LCN Scheme

k \ h	0.5 ($J = 32$)	0.25 ($J = 64$)	0.125 ($J = 128$)
0.5	0.7459E−02 (129)	0.7778E−03 (133)	0.4852E−04 (160)
0.25	0.7286E−02 (145)	0.7541E−03 (161)	0.6687E−04 (184)
0.125	0.7251E−02 (170)	0.7460E−03 (193)	0.7152E−04 (264)
0.0625	0.7233E−02 (205)	0.7356E−03 (298)	0.7069E−04 (439)

Note. The numbers in brackets represent CPU times in hundredths of a second.

TABLE II

L^2-Errors for the SSS Scheme with Simple Splitting

k \ h	0.5 ($J = 64$)	0.25 ($J = 128$)	0.125 ($J = 256$)
0.5	0.2242E+00 (128)	0.2242E+00 (283)	0.2242E+00 (616)
0.25	0.1120E+00 (254)	0.1120E+00 (561)	0.1120E+00 (1209)
0.125	0.5614E−01 (501)	0.5615E−01 (1111)	0.5614E−01 (2424)
0.0625	0.2813E−01 (993)	0.2814E−01 (2192)	0.2814E−01 (4796)

Note. The numbers in brackets represent CPU times in hundredths of a second.

TABLE III

L^2-Errors for the SSS Scheme with Strang's Splitting

k \ h	0.5 ($J=64$)	0.25 ($J=128$)	0.125 ($J=256$)
0.5	0.2917E−01 (138)	0.2917E−01 (295)	0.2917E−01 (633)
0.25	0.7066E−02 (364)	0.7067E−01 (576)	0.7068E−02 (1214)
0.125	0.1767E−02 (510)	0.1770E−02 (1127)	0.1772E−02 (2410)
0.0625	0.4816E−03 (1108)	0.4874E−03 (2212)	0.4927E−03 (4761)

Note. The numbers in brackets represent CPU times in hundredths of a second.

The LCN scheme was implemented in single precision complex arithmetic on the same type of machine of Ref. [2], that is a VAX 11/780 computer, with VMS as operating system and with a VAX-11 FORTRAN compiler.

The results of the runs are summarized in Table I. The numbers in brackets represent CPU times in hundredths of a second and the entries without brackets give the L^2-errors. In order to facilitate the comparison of the methods, we report in Tables II and III the results shown in [2] for SSS schemes. From these results, we deduce that the LCN is clearly more accurate and faster than the SSS method with simple or Strang's splitting. Likewise, we note the different behaviour of the L^2-errors as a function of h and k: for the LCN scheme, the error is nearly independent of the time mesh size and varies with the mesh size in space, whereas for the SSS methods it is the opposite. This is qualitatively the same error behaviour as for the CN scheme (see Table II in [2]). For other solutions of Eq. (1), less smooth than (4), and for long evolution times the LCN scheme shows the same good performance [4]. We conclude that for nonlinear Dirac models the LCN is reliable, with easy coding, and more efficient than the split-step schemes used for comparison.

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A. ALVAREZ

Departamento de Física Teórica and
Instituto de Física Fundamental
Universidad Complutense
28040 Madrid, Spain