

# Padé numerical schemes for the sine-Gordon equation

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## Abstract

The sine-Gordon equation turn up in several problems in science and engineering. Although it is integrable, in practical applications, its numerical solution is powerful and versatile. Four novel implicit finite difference methods based on  $(q, s)$  Padé approximations with  $(q + s)$ -th order in space have been developed and analyzed for this equation; all share the same treatment for the nonlinearity and integration in time. Concretely,  $(0, 4)$ ,  $(2, 2)$ ,  $(2, 4)$ , and  $(4, 4)$  Padé methods; additionally, the energy conserving, Strauss–Vázquez scheme has been considered in a  $(0, 2)$  Padé implementation. These methods have been compared among them for both the kink–antikink and breather solutions in terms of global error, computational cost and energy conservation. The  $(0, 4)$  and  $(2, 4)$  Padé methods are the most cost-effective ones for small and large global error, respectively. Our results indicate that spatial order of accuracy is more relevant to effectiveness of a method than energy conservation even in very long time integrations.

*Keywords:* Sine-Gordon equation, Padé numerical methods, Implicit time integration, Solitons

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## 1. Introduction

The sine-Gordon equation (sGE) arises in many branches of mathematical physics. It was discovered in the study of surfaces of constant negative curvature. It is also a continuum model for waves in coupled-pendulum, mechanical systems, the magnetic-flux propagation in large Josephson junctions, the study of the domain wall dynamics in magnetic crystals, the propagation of crystal dislocations in solids, the propagation of ultra-short optical pulses in optical fibers, and as a nonlinear, effective, field theory for strong interactions in particle physics, among others [1, 2, 3]. The sGE is exactly solvable by the inverse scattering method [4, 5, 6, 7], however it still continues to provide mathematical surprises and new physical applications [3], such in graphene superlattices [8].

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Let us briefly review the current state of the numerical solution of the sGE. The first two numerical methods for the sGE were developed by Perring and Skyrme (PS), a method of characteristics and a leapfrog finite difference scheme [9]. A staggered-leapfrog scheme was introduced by Ablowitz, Kruskal, and Ladik (AKL) with the goal of stabilizing the PS scheme [10]. An energy-conserving, implicit, leapfrog finite difference scheme was developed by Strauss and Vázquez (SV) for the Klein–Gordon equation [11], first used for the sGE in Ref. [12]. A comparison of four leapfrog numerical schemes, the PS, AKL, SV, and a new fully-explicit method shows that, for long-time integration, the SV scheme is the best one [13]. Several generalizations of the SV scheme, also energy-conserving and second-order in both space and time, have been published [14, 15, 16, 17, 18]; the comparison among these methods shows that implicitness is the key property for long-time stability, instead of energy conservation [19]. However, a general procedure for the development of energy-conserving methods based on the nonlinear treatment of the SV scheme [20] and starting from a discrete energy [21] have been developed.

Finite difference schemes based on  $(q, s)$  Padé approximants, with  $(q + s)$ -th order in space, are also referred to as compact operator methods. Bratsos and Twizell [22] used  $(0, 2)$ ,  $(1, 1)$ , and  $(1, 2)$  Padé methods, Duncan [23] and Bratsos [24] a  $(2, 2)$  one, and Sari and Güarslan [25] a  $(2, 4)$  one, all with the nonlinearity treatment of the PS scheme; a comparison of some of the Padé methods with PS, AKL, and SV schemes shows that high-order methods are more efficient for high accuracy [23]. Other Padé methods up to fourth-order have been developed in Refs. [26, 27, 28], however, up to these authors’ knowledge, Padé methods with the nonlinearity treatment of the SV scheme have not been either developed or analyzed.

Apart from finite differences, other numerical methods have also been used for the sGE. Pseudospectral methods, like the split-step Fourier scheme [29, 30, 31], and spectral methods like an energy-conserving, Fourier scheme [32], a Legendre spectral element method [33], a wavelet spectral method [34, 35], and a multiresolution analysis method based on Legendre wavelets [36]. Finite element methods based on a Petrov–Galerkin scheme [37], and on a collocation scheme using Legendre–Gauss–Lobatto points [38], or cubic B-splines [39]. Multisymplectic methods [40, 41], including a systematic method for discretizing Hamiltonian partial differential equations preserving their energy exactly [32, 42], even for arbitrary boundary conditions [43]. Moreover, meshless methods based on multiquadric quasi-interpolation [44, 45], on radial basis functions [46, 47], and on an optimal nodal distribution determined by the so-called optimal sampling density of kernel interpolation time variables [48]. Even, exponentially-fitted and piecewise analytical methods [49], boundary element methods [50], local discontinuous Galerkin methods [51, 52], and numerical implementations of the inverse scattering transform have been developed for the sGE [53, 54]. Finally, note that many of these methods have been extended to two and three dimensions [55].

Previous studies [23, 31, 35] pointed out that the spatial order of accuracy is more important for accuracy than either the symplectic or the energy conser-

60 vation property; although some authors have results that do not seem to agree with it [49]. Hence, high-order methods must be explored. The goal of this paper is to develop Padé methods with the nonlinearity treatment of the SV scheme.

The contents of this paper are as follows. Section 2 presents the five numerical Padé approximation schemes for the sGE; their linear stability is studied in Subsection 2.1. A detailed comparison of these methods is presented in Section 3, for the propagation of both a kink-antikink solution in Subsection 3.1, and a breather in Subsection 3.2. Finally, the last section is devoted to some conclusions.

## 2. Numerical schemes

70 The initial-value problem for the sine-Gordon equation is written in non-dimensional form as

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + \frac{dF(u)}{du} = 0, \quad x \in \mathbb{R}, \quad t \geq 0, \quad (1)$$

$$u(x, 0) = u_0(x), \quad \frac{\partial u}{\partial t}(x, 0) = u_1(x), \quad (2)$$

where  $F(u) = 1 - \cos(u)$  is the potential energy, with  $F_u(u) \equiv dF(u)/du = \sin(u)$ , and  $u(x, t)$  denotes the amplitude of the solution,  $x$  is the spatial coordinate, and  $t$  is time. The existence, uniqueness, and regularity of the solutions of the initial-boundary value problem for the sGE can be proved by using the same approach as for the inhomogeneous, linear wave equation; it is sufficient to show the contractivity of Duhamel's formula as a nonlinear integral operator. In fact, Theorem B.5 in Ref. [56, Appendix B] states that for  $u_0(x) \in L^p(\mathbb{R})$ ,  $\partial u_0(x)/\partial x \in L^p(\mathbb{R})$ , and  $u_1(x) \in L^p(\mathbb{R})$ , the unique weak solution of the sGE for  $t \in [0, T]$  is  $u(x, t) \in L^p(\mathbb{R}) \times L^\infty[0, T]$ . Hence, high-order numerical methods can be applied without concern for consistency, since for enough regularity in the initial condition, the classical solution achieves the same regularity.

85 The sGE is integrable in the sense of Liouville, having an infinite set of conservation laws. In order to assess the accuracy of the numerical methods, let us use the momentum and the energy, given by

$$P(t) = - \int_{-\infty}^{\infty} \left( \frac{\partial u}{\partial t} \right) \left( \frac{\partial u}{\partial x} \right) dx = P(0), \quad (3)$$

$$90 \quad E(t) = \int_{-\infty}^{\infty} \left( \frac{1}{2} \left( \frac{\partial u}{\partial t} \right)^2 + \frac{1}{2} \left( \frac{\partial u}{\partial x} \right)^2 + F(u) \right) dx = E(0), \quad (4)$$

respectively. Since  $F(u)$  is positive definite, it can be shown that  $|P(t)| \leq E$ ; moreover, the speed of the kinks (antikinks) can be calculated as  $v(t) = P(t)/E(t)$ , thanks to the negative sign in the definition of the momentum.

Let us consider five numerical methods for the solution of Eq. (1) by using  
 95 Padé approximants in space, all with the same central, second-order differences  
 in time, and an approximation of the nonlinear term inspired in the conservative  
 method of Strauss–Vázquez [11]. The resulting scheme can be written as

$$\mathcal{A}_i(\mathbf{E}) \frac{U_m^{n+1} - 2U_m^n + U_m^{n-1}}{\Delta t^2} - \mathcal{B}_i(\mathbf{E}) U_m^n + \mathcal{A}_i(\mathbf{E}) H(U_m^{n+1}) = 0, \quad (5)$$

with

$$100 \quad H(U_m^{n+1}) \equiv \frac{F(U_m^{n+1}) - F(U_m^{n-1})}{U_m^{n+1} - U_m^{n-1}}, \quad (6)$$

where  $U_m^n \approx u(x_m, t^n) = u_m^n$ , with  $x_m = m \Delta x$ ,  $m \in \mathbb{Z}$ , with  $\Delta x$  as the grid  
 size, and  $t^n = n \Delta t$ ,  $n \in \mathbb{N}$ , with  $\Delta t$  as the time step, and  $\mathcal{A}_i^{-1}(\mathbf{E}) \mathcal{B}_i(\mathbf{E}) u_m^n$  is  
 the  $i$ -th Padé approximation for the second-order spatial derivative of  $u(x_m, t^n)$   
 in Method  $i$ , with  $\mathbf{E}$  being the shift operator, i.e.,  $\mathbf{E} U_m^n = U_{m+1}^n$ . Hereon, for  
 105 the numerical solution of the initial-value problem of Eq. (1), periodic boundary  
 conditions are used in the finite interval  $x \in (-L/2, L/2]$ , with  $x_m = -L/2 +$   
 $m \Delta x$ ,  $m = 1, 2, \dots, M$ , and  $\Delta x = L/M$  (note that  $x_0 \equiv x_M$ ), and a finite time  
 interval  $t \in [0, T]$ , with  $t^n = n \Delta t$ ,  $n = 0, 1, \dots, N$ , and  $\Delta t = T/N$ .

Method (5) is implicit, since the calculation of  $U_m^{n+1}$  from  $U_m^n$  and  $U_m^{n-1}$   
 110 requires the solution of a nonlinear equation. Let us use Newton's iterative  
 method given by

$$\begin{aligned} & \mathcal{A}_i(\mathbf{E}) \left( U_m^{(k+1)} - 2U_m^k + U_m^{k-1} \right) - \Delta t^2 \mathcal{B}_i(\mathbf{E}) U_m^k \\ & + \Delta t^2 \mathcal{A}_i(\mathbf{E}) \left( H(U_m^{(k)}) + H_u(U_m^{(k)}) (U_m^{(k+1)} - U_m^{(k)}) \right) = 0, \end{aligned} \quad (7)$$

with

$$115 \quad H_u(U_m^{(k)}) \equiv \frac{F_u(U_m^{(k)}) (U_m^{(k)} - U_m^{k-1}) - (F(U_m^{(k)}) - F(U_m^{k-1}))}{(U_m^{(k)} - U_m^{k-1})^2}. \quad (8)$$

Our stopping criterion for Newton's iteration convergence is based on the relative  
 error using the infinite norm, i.e.,  $\|U_m^{(k+1)} - U_m^{(k)}\|_\infty \leq \text{Tol} \|U_m^{(k+1)}\|_\infty$ , with  
 $\|U_m^{(k)}\|_\infty = \max_m |U_m^{(k)}|$ , and Tol being a small enough tolerance.

There are catastrophic cancellations in the numerical evaluation of Eq. (6)  
 120 for  $H(U)$ , and Eq. (8) for  $H_u(U)$ , when  $|U - U_m^{n-1}| \ll 1$ . For the sGE, they  
 can be avoided by rearranging the expression of  $H(U)$  by means of the exact  
 formula [17, 32, 42]

$$H(U) = \frac{\cos(U) - \cos(U_m^{n-1})}{U - U_m^{n-1}} = \frac{2 \sin((U + U_m^{n-1})/2) \sin((U - U_m^{n-1})/2)}{U - U_m^{n-1}},$$

and that of  $H_u(U)$  by means of

$$125 \quad H_u(U) = \frac{\sin(U)}{U - U_m^{n-1}} - \frac{2 \sin((U + U_m^{n-1})/2) \sin((U - U_m^{n-1})/2)}{(U - U_m^{n-1})^2}.$$

The local truncation error terms  $\mathcal{L}_i(u)$  of Method  $i$  can be easily calculated as follows; note that for smooth initial conditions the solution is smooth in both space and time. By using Taylor series expansion after the substitution of  $U_m^n$  by the exact solution  $u(x_m, t^n)$  in Eq. (5) for the  $i$ -th method results in

$$130 \quad \mathcal{M}_i(u) \equiv \mathcal{G}(u) + \mathcal{L}_i(u) = 0, \quad (9)$$

where  $\mathcal{G}(u)$  is the sGE, cf.

$$\mathcal{G}(u) \equiv \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + \sin(u),$$

and the local truncation error is

$$\mathcal{L}_i(u) = \mathcal{T}(u) \Delta t^2 + \mathcal{S}_i(u) \Delta x^{p_i} + \text{h.o.t.}, \quad (10)$$

135 where h.o.t. stands for higher-order terms depending on  $u$  and its partial derivatives,  $p_i$  is the approximation order of the Padé operator for  $i$ -th method, and

$$\mathcal{T}(u) = -\frac{1}{6} \sin(u) \left( \frac{\partial u}{\partial t} \right)^2 + \frac{1}{2} \cos(u) \frac{\partial^2 u}{\partial t^2} + \frac{1}{12} \frac{\partial^4 u}{\partial t^4}.$$

**Method 1.** The finite difference method developed by Strauss and Vázquez [11] is interpreted as a (0,2)-Padé method by using

$$140 \quad \mathcal{A}_1(\mathbf{E}) = \mathcal{I},$$

$$\mathcal{B}_1(\mathbf{E}) = \frac{\mathbf{E}^{-1} - 2 + \mathbf{E}^1}{\Delta x^2},$$

where  $\mathcal{I}$  is the identity operator. Method 1 is second-order accurate in space ( $p_1 = 2$ ) since

$$145 \quad \frac{\mathcal{B}_1(\mathbf{E})}{\mathcal{A}_1(\mathbf{E})} u(x_m, t^n) = \frac{\partial^2 u}{\partial x^2} + \frac{\Delta x^2}{12} \frac{\partial^4 u}{\partial x^4} + \mathcal{O}(\Delta x^4).$$

The local truncation error for the Strauss–Vázquez method,  $\mathcal{L}_1(u)$  in Eq. (10), is given by

$$\mathcal{L}_1(u) = \mathcal{T}(u) \Delta t^2 - \frac{\Delta x^2}{12} \frac{\partial^4 u}{\partial x^4} + \text{h.o.t.} \quad (11)$$

150 **Method 2.** A novel (0,4)-Padé method of fourth-order in space, inspired in the method of lines developed by Duncan [23, section 2.5] using symplectic and Dormand–Prince, Runge–Kutta methods, but with the SV scheme for the nonlinearity, given as

$$155 \quad \mathcal{A}_2(\mathbf{E}) = \mathcal{I},$$

$$\mathcal{B}_2(\mathbf{E}) = \frac{-\mathbf{E}^{-2} + 16 \mathbf{E}^{-1} - 30 + 16 \mathbf{E}^1 - \mathbf{E}^2}{12 \Delta x^2}.$$

By using Taylor series expansion, the Padé operator yields

$$\frac{\mathcal{B}_2(\mathbb{E})}{\mathcal{A}_2(\mathbb{E})} u(x_m, t^n) = \frac{\partial^2 u}{\partial x^2} - \frac{\Delta x^4}{90} \frac{\partial^6 u}{\partial x^6} + \mathcal{O}(\Delta x^6).$$

The local truncation error for this method is given by

$$\mathcal{L}_2(u) = \mathcal{T}(u) \Delta t^2 + \frac{\Delta x^4}{90} \frac{\partial^6 u}{\partial x^6} + \text{h.o.t.} \quad (12)$$

160 **Method 3.** A novel (2,2)-Padé method of fourth-order in space, inspired in the compact operator methods used by Duncan [23, section 2.4], but incorporating the SV scheme for the nonlinearity, which can written as

$$\mathcal{A}_3(\mathbb{E}) = \frac{\mathbb{E}^{-1} + 10 + \mathbb{E}^1}{12},$$

$$165 \quad \mathcal{B}_3(\mathbb{E}) = \frac{\mathbb{E}^{-1} - 2 + \mathbb{E}^1}{\Delta x^2},$$

which approximates the second-order derivative up to the fourth-order, as shown by Taylor series expansion,

$$\frac{\mathcal{B}_3(\mathbb{E})}{\mathcal{A}_3(\mathbb{E})} u(x_m, t^n) = \frac{\partial^2 u}{\partial x^2} - \frac{\Delta x^4}{240} \frac{\partial^6 u}{\partial x^6} + \mathcal{O}(\Delta x^6).$$

The local truncation error for this method is given by

$$170 \quad \mathcal{L}_3(u) = \mathcal{T}(u) \Delta t^2 + \frac{\Delta x^4}{240} \frac{\partial^6 u}{\partial x^6} + \text{h.o.t.} \quad (13)$$

**Method 4.** A novel (2,4)-Padé method of sixth-order in space, with the SV scheme for the nonlinearity, given by

$$\mathcal{A}_4(\mathbb{E}) = \frac{2\mathbb{E}^{-1} + 11 + 2\mathbb{E}^1}{3},$$

$$175 \quad \mathcal{B}_4(\mathbb{E}) = \frac{\mathbb{E}^{-2} + 16\mathbb{E}^{-1} - 34 + 16\mathbb{E}^1 + \mathbb{E}^2}{4\Delta x^2},$$

which can be easily checked by Taylor series expansion yielding

$$\frac{\mathcal{B}_4(\mathbb{E})}{\mathcal{A}_4(\mathbb{E})} u(x_m, t^n) = \frac{\partial^2 u}{\partial x^2} + \frac{23\Delta x^6}{75600} \frac{\partial^8 u}{\partial x^8} + \mathcal{O}(\Delta x^8).$$

In this case, the local error is

$$\mathcal{L}_4(u) = \mathcal{T}(u) \Delta t^2 - \frac{23\Delta x^6}{75600} \frac{\partial^8 u}{\partial x^8} + \text{h.o.t.} \quad (14)$$

180 **Method 5.** A novel (4,4)-Padé method of eighth-order in space, with the SV scheme for the nonlinearity, which can be written as

$$\mathcal{A}_5(E) = \frac{23 E^{-2} + 688 E^{-1} + 2358 + 688 E^1 + 23 E^2}{15},$$

$$\mathcal{B}_5(E) = \frac{31 E^{-2} + 128 E^{-1} - 318 + 128 E^1 + 31 E^{-2}}{\Delta x^2},$$

185 whose accuracy can be verified by Taylor series expansion resulting in

$$\frac{\mathcal{B}_5(E)}{\mathcal{A}_5(E)} u(x_m, t^n) = \frac{\partial^2 u}{\partial x^2} - \frac{79 \Delta x^8}{4762800} \frac{\partial^{10} u}{\partial x^{10}} + \mathcal{O}(\Delta x^{10}).$$

In this case, the local error is

$$\mathcal{L}_5(u) = \mathcal{T}(u) \Delta t^2 + \frac{79 \Delta x^8}{4762800} \frac{\partial^{10} u}{\partial x^{10}} + \text{h.o.t.} \quad (15)$$

For a fair comparison of the five methods the discrete analogue of the energy (4) given by

$$E^n = \Delta x \sum_m \left[ \frac{1}{2} \left( \frac{U_m^{n+1} - U_m^n}{\Delta t} \right)^2 + \frac{1}{2} \left( \frac{U_{m+1}^{n+1} - U_m^{n+1}}{\Delta x} \right) \left( \frac{U_{m+1}^n - U_m^n}{\Delta x} \right) \right]$$

$$+ \Delta x \sum_m \left[ \frac{F(U_m^{n+1}) + F(U_m^{n-1})}{2} \right], \quad (16)$$

is used; this discrete energy is exactly conserved ( $E^n = E^0$ ) by the SV method [11]. Neither of the Methods 2–5 exactly conserve it.

195 In order to numerically estimate the speed of the kinks (antikinks) by means of  $v(t) = P(t)/E(t)$ , a discrete analogue of the momentum (3) given by

$$P^n = -\Delta x \sum_m \left[ \left( \frac{U_m^{n+1} - U_m^{n-1}}{2 \Delta t} \right) \left( \frac{U_{m+1}^n - U_{m-1}^n}{2 \Delta x} \right) \right], \quad (17)$$

has been used [11]. Note that neither of the Methods 1–5 exactly conserve this discrete momentum.

### 200 2.1. Stability analysis

The linear stability of Methods 1–5 can be easily studied by means of using the von Neumann analysis. The computational error  $Z_m^n = U_m^n - U_m^{n*}$ , with respect to a given solution  $U_m^{n*}$ , can be Fourier expanded as  $Z_m^n = \exp(i m \beta \Delta x) \xi^n$ , where  $i = \sqrt{-1}$ ,  $\beta$  is the spatial frequency, and  $\xi$  is the amplification factor, and substituted into Eq. (5) with  $F \equiv 0$ . After cancelling common factors, the

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$$p_i(\xi) = A_i \xi^2 - 2 B_i \xi + A_i = 0, \quad (18)$$

whose two roots  $\xi_1$  and  $\xi_2$  have modulus smaller than or equal to unity for every  $\xi$  if and only if  $|B_i| \leq A_i$ , i.e.,  $-A_i \leq B_i \leq A_i$ . These two inequalities yield  
 210 necessary condition for linear stability on both  $\Delta x$  and  $\Delta t$ .

**Method 1.** The (linear) stability polynomial (18) for the Strauss–Vázquez method has coefficients

$$A_1 = 1, \quad B_1 = 1 - 2r^2 \sin^2(\omega), \quad (19)$$

where  $r = \Delta t/\Delta x$ , and  $\omega = \beta \Delta x/2$ . For stability, the condition  $B_1 \leq A_1$  is  
 215 always true, and the condition  $-A_1 \leq B_1$  gives

$$2r^2 \sin^2(\omega) \leq 2,$$

$$\left(\frac{\Delta t}{\Delta x}\right)^2 \leq 1, \quad \Delta t \leq \Delta x. \quad (20)$$

Note that this is the CFL condition.

220 **Method 2.** The stability polynomial (18) for this method is given by

$$A_2 = 1, \quad B_2 = 1 - \frac{8r^2}{3} \sin^2(\omega) + \frac{r^2}{6} \sin^2(2\omega). \quad (21)$$

In this case, the condition  $B_2 \leq A_2$  yields

$$0 \leq \frac{8}{3} \sin^2(\omega) - \frac{1}{6} \sin^2(2\omega) \leq \frac{8}{3},$$

being always true, and the condition  $-A_2 \leq B_2$  gives

$$225 \quad r^2 \left( \frac{8}{3} \sin^2(\omega) - \frac{1}{6} \sin^2(2\omega) \right) \leq 2,$$

$$\left(\frac{\Delta t}{\Delta x}\right)^2 \leq \frac{3}{4}, \quad \Delta t \leq \frac{\sqrt{3}}{2} \Delta x \leq \Delta x. \quad (22)$$

**Method 3.** This method has a stability polynomial (18) with coefficients

$$A_3 = 1 - \frac{1}{3} \sin^2(\omega), \quad (23)$$

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$$B_3 = 1 - \frac{1}{3} \sin^2(\omega) - 2r^2 \sin^2(\omega). \quad (24)$$

In this case, the condition  $B_3 \leq A_3$  is always true, and the condition  $-A_3 \leq B_3$  gives

$$2r^2 \sin^2(\omega) \leq 2 - \frac{2}{3} \sin^2(\omega),$$



$$2 r^2 \sin^2(\omega) \leq 2 - \frac{2}{3} = \frac{4}{3},$$

$$\left(\frac{\Delta t}{\Delta x}\right)^2 \leq \frac{2}{3}, \quad \Delta t \leq \frac{\sqrt{6}}{3} \Delta x \leq \Delta x. \quad (25)$$

**Method 4.** The stability polynomial (18) of this method is given by

$$A_4 = 5 - \frac{8}{3} \sin^2(\omega), \quad (26)$$

$$B_4 = 5 - \frac{8}{3} \sin^2(\omega) - 8 r^2 \sin^2(\omega) - \frac{r^2}{2} \sin^2(2\omega). \quad (27)$$

In this case, the condition  $B_4 \leq A_4$  is always true, and the condition  $-A_4 \leq B_4$  gives

$$r^2 \left( 8 \sin^2(\omega) + \frac{1}{2} \sin^2(2\omega) \right) \leq 10 - \frac{16}{3} \sin^2(\omega), \quad (245)$$

$$\left(\frac{\Delta t}{\Delta x}\right)^2 \leq \frac{7}{12}, \quad \Delta t \leq \frac{\sqrt{21}}{6} \Delta x \leq \Delta x. \quad (28)$$

**Method 5.** The stability polynomial (18) of this method is given by

$$A_5 = 252 - \frac{2752}{15} \sin^2(\omega) - \frac{92}{15} \sin^2(2\omega), \quad (29)$$

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$$B_5 = 252 - \frac{2752}{15} \sin^2(\omega) - \frac{92}{15} \sin^2(2\omega) \quad (30)$$

$$- 504 r^2 \sin^2(\omega) + 248 r^2 \sin^4(\omega). \quad (31)$$

In this case, the condition  $B_5 \leq A_5$  is always true, and the condition  $-A_5 \leq B_5$  gives

$$r^2 (504 \sin^2(\omega) - 248 \sin^4(\omega)) \leq \left( 504 - \frac{5504}{15} \sin^2(\omega) - \frac{184}{15} \sin^2(2\omega) \right), \quad (255)$$

$$\left(\frac{\Delta t}{\Delta x}\right)^2 \leq \frac{257}{480}, \quad \Delta t \leq \frac{\sqrt{7710}}{120} \Delta x \leq \Delta x. \quad (32)$$

Nonlinear stability theorems are direct by-products of the discrete conservation properties. Method 1 exactly conserves the discrete energy  $E^n$ , however

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it is not positive definite (the product  $(U_{m+1}^{n+1} - U_m^{n+1})(U_{m+1}^n - U_m^n)$  is not necessarily greater than zero). Hence no strong nonlinear stability theorem can be proved [17]. However, under the CFL condition,  $\Delta t \leq \Delta x$ , the discrete energy is positive definite and Method 1 is nonlinearly stable, as proved by Comech and Komech [57]. The nonlinear stability of Methods 2–5 has not yet been studied in the literature.

The nonlinear stability and consistency of Method 1 ensures its convergence thanks to the Lax equivalence theorem. However, in long-time integrations of solutions growing in amplitude, like the kink-antikink collisions under periodic boundary conditions, nonconvergent results have been observed [58, 40]; such problems have not been observed with bounded solutions, like breathers. In the case of Methods 2–5, the linear stability and consistency ensures local convergence thanks to the Lax equivalence theorem. The behaviour of these methods in long-time integrations should be explored.

### 3. Numerical results

Let us summarize the results obtained for the behaviour in space of Methods 1–5 after an extensive set of simulations for both kink-antikink and breather solution for the sGE. The five methods are compared in terms of global error, energy conservation, computational cost, and behaviour in long-time integrations. Subsection 3.1 presents the results for a kink-antikink collision solution, and Subsection 3.2 for the breather solution.

#### 3.1. Kink-antikink

Let us consider the analytical solution of the sGE given by

$$u_{ka}(x, t) = 4 \tan^{-1} \frac{\sinh(v(t-10)/r_-)}{v \cosh(x/r_-)}, \quad (33)$$

where  $r_- = \sqrt{1-v^2}$ , and  $v = 1/2$ , corresponding to a kink-antikink collision. For the validation and comparison of Methods 1–5, the initial conditions (2) are approximated by means of  $U_m^0 = u_{ka}(x_m, 0)$ , and  $U_m^{-1} = u_{ka}(x_m, -\Delta t)$ , and the numerical solution  $U_m^n$  for  $n = 2, 3, \dots, N$ , is calculated for different values of  $\Delta t$  and  $\Delta x$ , always with  $T = 20$ ,  $L = 50$ , and  $\text{Tol} = 10^{-14}$ .

Figure 1 (left plot) shows the numerical error  $\|U_m^N - u_{ka}(x_m, 20)\|_\infty$  for Methods 1–5 with  $\Delta t = 0.001$  as a function of  $\Delta x \in [0.001, 1]$ . The linear stability conditions in Section 2.1 for  $\Delta t = 1/1000$  requires that  $\Delta x \geq 1/1000$ ,  $\gtrsim 1/866$ ,  $\gtrsim 1/816$ ,  $\gtrsim 1/764$ , and  $\gtrsim 1/731$ , for Methods 1–5, resp.; hence, in Fig. 1 the plots only show the results when  $\Delta x \geq 1/800$ ,  $\geq 1/800$ ,  $\geq 1/700$ , and  $\geq 1/700$  for Methods 2–5, respectively. The spatial order of the methods can be validated by means of linear fitting of the logarithm of the error versus the logarithm of the grid size when the error in time is smaller than the error in space; in our case, for  $\Delta x \in \{0.2, 0.3, \dots, 1.0\}$ , the resulting slopes are given by 2.8, 4.7, 5.0, 7.2, and 8.7, for Methods 1–5, respectively, in agreement with the theoretical consistency order, cf. 2, 4, 4, 6, and 8, resp. Hence, for  $\Delta x > 0.1$  the

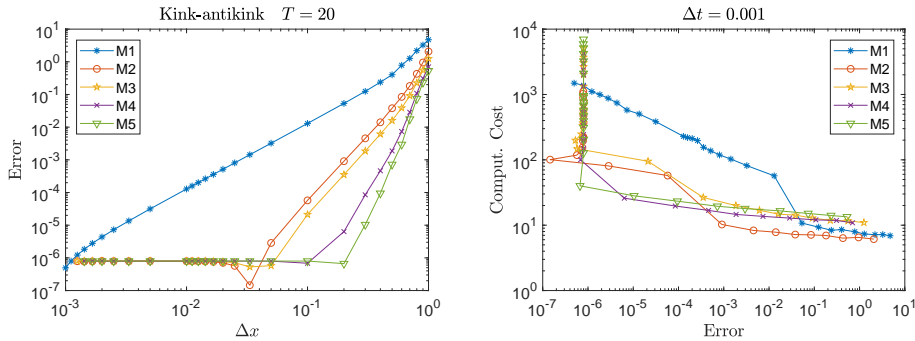


Figure 1: Numerical error (left plot) and computational cost (right plot) for the kink-antikink solution with  $T = 20$  and  $\Delta t = 1/1000$  as a function of  $\Delta x \in \{1/1000, 1/900, 1/800, \dots, 1/100, 1/90, 1/80, \dots, 1/10, 2/10, 3/10, \dots, 1\}$ , for Methods 1–5.

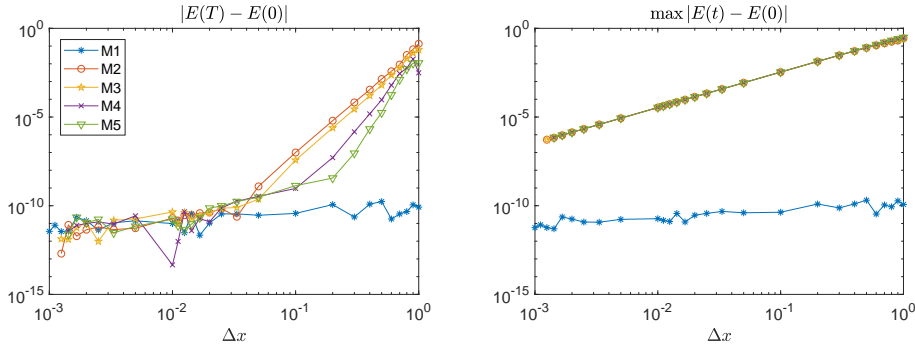


Figure 2: Numerical error of the discrete analogue of the energy (16) for the kink-antikink solution with  $T = 20$  and  $\Delta t = 0.001$  as a function of  $\Delta x \in \{1/1000, 1/900, 1/800, \dots, 1/100, 1/90, 1/80, \dots, 1/10, 2/10, 3/10, \dots, 1\}$ , for Methods 1–5. The left plot shows  $|E^N - E^0|$ , the numerical approximation of  $|E(T) - E(0)|$ , and right plot shows  $\|E^n - E^0\|_\infty$ .

high-order methods are more accurate than the lower order ones. However, for  $\Delta x \lesssim 0.03$  for Method 2,  $\Delta x \lesssim 0.05$  for Method 3, and  $\Delta x \lesssim 0.1$  for Methods 4 and 5, the error for Methods 2–5 reaches a constant value  $\approx 8.0 \times 10^{-7}$ , due to the error in time; such a plateau error can be reduced by using values of  $\Delta t < 0.001$ .

Figure 1 (right plot) shows the computational cost, estimated by using the run-time in seconds, for Methods 1–5 with  $\Delta t = 0.001$  as a function of the numerical error. Method 2 is the most efficient one for errors larger than  $10^{-3}$ , but its cost is similar in magnitude to that of high-order methods. For errors smaller than  $10^{-3}$ , Methods 4 and 5 are the most cost-effective ones, being about tens of times more efficient than Method 1.

The energy of Methods 1–5 is illustrated in Figure 2, where the discrete analogue of the energy (16), exactly conserved by Method 1, has been used instead

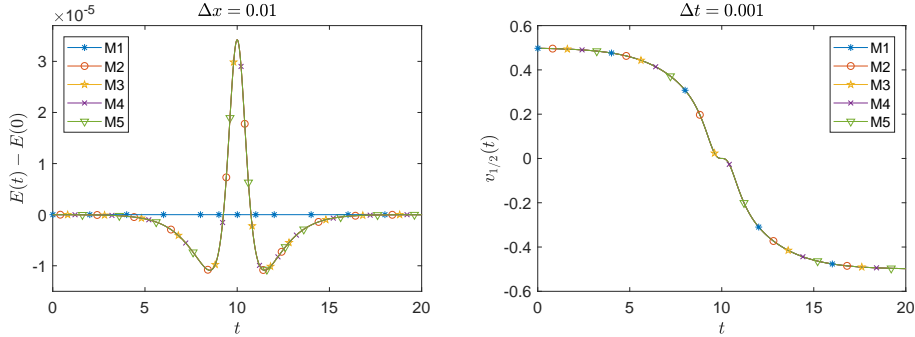


Figure 3: Evolution in time of the energy  $E^n - E^0$  (approximation to  $E(t) - E(0)$ ), left plot, and of the speed  $V(t)$ , right plot, of the kink-antikink solution with  $T = 20$ ,  $\Delta t = 0.001$ , and  $\Delta x = 0.01$ , for Methods 1–5.

of a high-order approximation for the exact energy (4); this choice has been  
 315 motivated by the aim of making a fair comparison of the energy conservation  
 properties among all the methods. Figure 2 shows the value of  $|E^N - E^0|$  (left  
 plot) and  $\|E^n - E^0\|_\infty$  (right plot) for Methods 1–5 with  $T = 20$  and  $\Delta t = 0.001$   
 as a function of  $\Delta x \in [0.001, 1]$ .

Figure 2 (left plot) shows that, as expected, Method 1 conserves the energy  
 320 for all  $\Delta x$ , but Methods 2–5 only show good conservation properties for very  
 accurate solutions, when  $\Delta x$  is smaller than  $\sim 0.04$ ; for larger values of  $\Delta x$  the  
 error in the energy decreases as the grid size does, with a slope that increases  
 with the order of the method.

Figure 2 (right plot) shows that the maximum error in the energy is constant  
 325 for Method 1, but its value decreases with  $\Delta x$  for Methods 2–5; surprisingly, it  
 coincides among them, being independent of the spatial order of the method.  
 Moreover, this value is  $O(\Delta x^2)$ , the order of approximation in space of the  
 discrete energy (16). Figure 3 (left plot) shows that the maximum error in  
 330 the energy is reached at  $t = T/2$ , where the solution and its spatial derivative  
 becomes null, but its time derivative has a local maximum; in such a point the  
 error in the discrete energy is dominated by the method of integration in time,  
 which is exactly the same for Method 2–5. In our opinion, this is the origin of  
 the features observed in Fig. 2 (right plot).

The speed  $v(t) = P(t)/E(t)$  of the exact kink-antikink solution is zero. How-  
 335 ever, the speed of the kink (antikink) before (after) the collision can be estimated  
 by using the half-interval speed  $v_{1/2}(t) = 2P_{1/2}(t)/E(t)$ , where  $P_{1/2}(t)$  is the  
 half-momentum calculated by means of the integration of Eq. (3) in  $x \in (-\infty, 0)$ ;  
 note that, the factor 2 is necessary because the energy is calculated in the whole  
 real line. Figure 3 (right plot) shows the evolution in time of  $v_{1/2}(t)$ , numerically  
 340 calculated by the discrete half-momentum, summing for  $m \in \{1, 2, \dots, M/2\}$  in  
 Eq. (17); Methods 1–5 conserve the half-momentum with an error smaller than  
 the resolution of the plot, so the corresponding curves shows overlapped in the

figure. Before the collision,  $v_{1/2}(t)$  is the speed of the kink, decreasing monotonically from  $v_{1/2}(0) = 1/2$  to  $v_{1/2}(T/2) = 0$ ; during the collision,  $v_{1/2}(t)$  shows a tiny plateau, but a careful analysis shows that it is only apparent; after the collision,  $v_{1/2}(t)$  is negative, as expected for the speed of the antikink, decreasing monotonically from  $v_{1/2}(T/2) = 0$  to  $v_{1/2}(T) = -1/2$ .

Following Ablowitz et al. [58] and Marsden et al. [40] long-time integration of the kink-antikink solution have been executed for both odd ( $M = 255$ ) and even ( $M = 256$ ) number of spatial nodes, with  $v = 1/10$ ,  $L = 40$ ,  $\Delta x = L/M$ ,  $\Delta t = \Delta x/8$ , and  $T = 200000$ , corresponding to an exact solution undergoing 1297 kink-antikink collisions. The results show that the solution of the high-order methods at  $t = T$  is not a kink-antikink solution, but it is degraded by the accumulation of round-off errors. Specifically, Method 4 results in unreliable solutions in both even and odd  $M$ , but Method 3 only for even  $M$ , and Method 5 only for odd  $M$ . Ablowitz et al. [58] explained this behaviour depending on the parity of the number of spatial points is due to homoclinic crossings induced by the numerical errors since the initial solution is near a homoclinic orbit. Methods 1 and 2 are stable, but there are errors in the speed of the numerical solitons that result in an incorrect number of collisions with respect to the exact solution. In summary, our best long-time integration results are obtained with Method 2 for both even and odd  $M$ , and also with Method 5 but only for even  $M$ .

### 3.2. Breather

The breather solution of the sGE is given by

$$u_{br}(x, t) = 4 \tan^{-1}(\sin(v(t - 10)/r_+) \operatorname{sech}(x/r_+)/v), \quad (34)$$

where  $r_+ = \sqrt{1 + v^2}$ , and  $v = 1/2$ . Let us compare Methods 1–5 with the initial conditions (2) approximated by means of  $U_m^0 = u_{br}(x_m, 0)$ , and  $U_m^{-1} = u_{br}(x_m, -\Delta t)$ , and the numerical solution  $U_m^n$  for  $n = 2, 3, \dots, N$ , is calculated for different values of  $\Delta t$  and  $\Delta x$ , always with  $T = 20$ ,  $L = 50$ , and  $\text{Tol} = 10^{-14}$ .

Figure 4 (left plot) shows the numerical error  $\|U_m^N - u_{br}(x_m, 20)\|_\infty$  for Methods 1–5 with  $\Delta t = 0.001$  as a function of  $\Delta x \geq \Delta t$ . The estimation of the spatial order of the methods by means of linear fitting for  $\Delta x \in \{0.3, 0.4, \dots, 1.0\}$ , results in 2.0, 4.3, 4.8, 6.8, and 8.7, for Methods 1–5, respectively, similar to the expected values of the theoretical consistency order. Hence, for  $\Delta x > 0.2$  the high-order methods are more accurate than the lower order ones. However, for  $\Delta x \lesssim 0.03$  for Method 2,  $\Delta x \lesssim 0.05$  for Method 3,  $\Delta x \lesssim 0.1$  for Method 4, and  $\Delta x \lesssim 0.2$  for Method 5, the error for Methods 2–5 is dominated by error in time, reaching a constant value  $\approx 7.0 \times 10^{-7}$ ; as expected, using values of  $\Delta t < 0.001$ , the plateau error can be reduced.

Figure 4 (right plot) shows the run-time (in seconds) for Methods 1–5 with  $\Delta t = 0.001$  as a function of the numerical error. Method 2 is the most efficient one for errors larger than  $10^{-4}$ , but its cost is similar in magnitude to that of high-order methods; for errors smaller than  $10^{-4}$ , Method 4 is the most cost-effective one, but Methods 2, and 5 have similar cost.

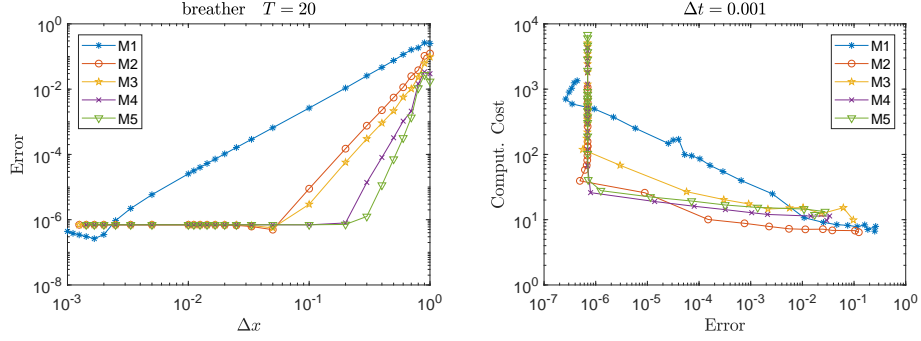


Figure 4: Numerical error (left plot) and computational cost (right plot) for the breather solution with  $T = 20$  and  $\Delta t = 1/1000$  as a function of  $\Delta x \in \{1/1000, 1/900, 1/800, \dots, 1/100, 1/90, 1/80, \dots, 1/10, 2/10, 3/10, \dots, 1\}$ , for Methods 1–5.

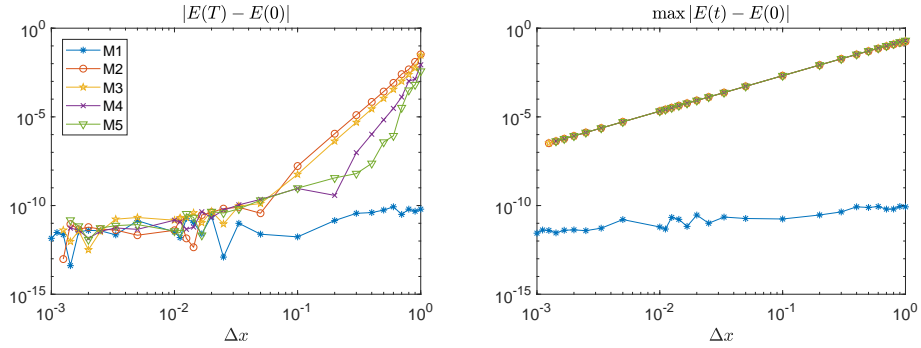


Figure 5: Numerical error of the discrete analogue of the energy (16) for the breather solution with  $T = 20$  and  $\Delta t = 0.001$  as a function of  $\Delta x \in \{1/1000, 1/900, 1/800, \dots, 1/100, 1/90, 1/80, \dots, 1/10, 2/10, 3/10, \dots, 1\}$ , for Methods 1–5. The left plot shows  $|E^N - E^0|$ , the numerical approximation of  $|E(T) - E(0)|$ , and right plot shows  $\|E^n - E^0\|_\infty$ .

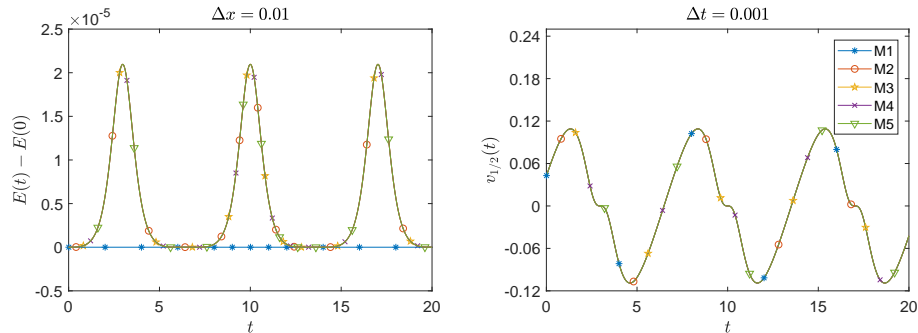


Figure 6: Numerical energy (left plot) and speed (right plot) of the breather solution with  $T = 20$ ,  $\Delta t = 0.001$ , and  $\Delta x = 0.01$ , for Methods 1–5.

Figure 5 (left plot) shows that, as expected, Method 1 conserves the energy for all  $\Delta x$ , but Methods 2–5 only show good conservation properties for very accurate solutions, when  $\Delta x$  is smaller than  $\sim 0.05$ ; for larger values of  $\Delta x$  the error in the energy decreases as the grid size does, with a slope that increases with the order of the method. Figure 5 (right plot) shows that the maximum error in the energy is constant for Method 1, but its value decreases with  $\Delta x$  for Methods 2–5, as previously observed for the kink-antikink solution in Section 3.1. The maximum error in the energy is of the order of approximation in space of the discrete energy (16), i.e.,  $O(\Delta x^2)$ .

Figure 6 (left plot) shows that the maximum error in the energy for Methods 1–5. It is constant for Method 1, but it oscillates at the same frequency that the breather solution does, for Methods 2–5, with three maxima at  $t = 2.98, 10.0$ , and  $17.0$ . At these maxima, the breather solution and its spatial derivative becomes null, hence the maximum error in the discrete energy is dominated by the method of integration in time, which is exactly the same for Method 2–5.

Figure 6 (right plot) shows the evolution in time of  $v_{1/2}(t)$ , cf. Section 3.1, for the numerical breather solution; note that the exact breather has a speed  $v(t) = 0$ . Methods 1–5 show the same oscillatory behaviour for  $v_{1/2}(t)$ , thanks to their good conservation properties for the momentum. The value of  $v_{1/2}(t)$  oscillates at the same frequency that the breather, with local maxima at  $t = 1.33, 8.36$ , and  $15.4$ , and local minima at  $t = 4.62, 11.6$ , and  $18.7$ . Between the maxima and minima there is a tiny plateau, at the same position of the maxima in Fig. 6 (left plot); its origin is similar to the one observed in the kink-antikink solution in Section 3.1.

#### 4. Conclusions

Five numerical schemes for the sGE have been developed and analyzed. All use the same second-order differences in time and the same approximation to the nonlinearity, with a proper rearrangement to avoid catastrophic cancellations in

its numerical evaluation; they are implicit, so Newton’s iterative method has  
 415 been used. Method 1 is the classical Strauss–Vázquez method, interpreted as  
 a (0,2)-Padé numerical method; this method conserves a discrete analog of the  
 energy of the sGE and it is of second-order in space. Methods 2–5 are (0,4)-,  
 (2,2)-, (2,4)-, and (4,4)-Padé methods which fourth-, fourth-, sixth-, and eighth-  
 order of accuracy in space. The local truncation error terms of the five methods  
 420 have been calculated by using Taylor series expansion. The linear stability of  
 Methods 1–5 has been studied by using the von Neumann analysis, showing  
 that  $(\Delta t/\Delta x)^2 \leq 1, 3/4, 2/3, 7/12,$  and  $257/480,$  for Methods 1–5, resp.

Methods 1–5 have been compared for both the kink–antikink and breather  
 solutions of the sGE with  $\Delta t = 0.001$  and  $\Delta x \in [1/1000, 1]$ . The results are  
 425 similar in both cases. For large enough  $\Delta x$  with respect to  $\Delta t$ , the spatial order  
 of the methods has been validated; however, for small  $\Delta x$  the global error is  
 dominated by the contribution of the common method of integration in time.  
 The computational cost (the run-time in seconds) for Methods 1–5 shows that  
 Method 2 is the most efficient one for errors larger than  $10^{-3}$  and  $10^{-4}$  for the  
 430 kink–antikink and breather solutions, resp.; but for smaller errors Method 4  
 and 5 are the most cost-effective ones.

Method 1 exactly conserves a discrete energy analogous to the energy of  
 the sGE, but Methods 2–5 shows good conservation properties for accurate  
 solutions, with the error in the energy decreasing as the grid size does, with  
 435 a slope that increases with the order of the method. In fact, the maximum  
 error in the energy is constant for Method 1, but it is  $O(\Delta x^2)$ , the order of  
 approximation in space of the discrete energy, for Method 2–5; for the kink-  
 antikink solution this maximum is located at the center of the collision, but  
 for the breather solution oscillates at the same frequency as the breather; in  
 440 both cases, the maximum is reached where the amplitude and spatial derivative  
 of the solution are null. The speed of the kink (antikink) before (after) the  
 collision in the kink-antikink solution has been estimated using the half-interval  
 speed calculated by the half-interval momentum; the results coincide among  
 Methods 1–5, decreasing monotonically from  $1/2$  before the collision to  $-1/2$   
 445 after it, for the kink-antikink solution. The half-interval speed has also been  
 calculated for the breather solution, showing an oscillatory behaviour at the  
 same frequency that the breather.

In long-time integrations, the best results have been obtained by using  
 Method 2, and also Method 5 but only for an even number of spatial points.  
 450 Method 1 exactly conserves an analogue of the energy, but this property it is  
 not enough to avoid the accumulation of error in the speed of the solitons, that  
 degrades the solution with large amounts of noise (contradicting the theoretical  
 results of convergence published in the literature). For an initial solution near a  
 homoclinic orbit, Method 4 yields noisy solutions for both even and odd number  
 455 of spatial nodes, Method 3 only for even  $M$ , and Method 5 only for odd  $M$ .

In summary, our analysis indicates that Method 2 and Method 4 are the most  
 cost-effective ones for small and large error, resp., in short-time integrations, and  
 Method 2 and Method 5, the last one with an even number of spatial points, are  
 the best ones for long-time integrations. Comparing the fourth-order methods,



460 Method 2 is better than Method 3, even if its local truncation error term is  
smallest (the sixth-order spatial derivative is multiplied by a smaller number).  
Comparing the higher-order methods, Method 5 is better than Method 4 for  
long-time integrations. Except in terms of linear stability, it turns out that the  
widely used Method 1 is the worst among the other methods studied in this  
465 paper, in spite of his energy conservation property.

Our results indicate that to attain a very small global error our high-order  
methods in space require a high-order scheme in time. There are several possibil-  
ities to be explored in the future, either Richardson extrapolation, or diagonally  
implicit Runge–Kutta–Nyström methods, or even modified equation techniques.  
470 The theoretical analysis of the nonlinear stability and convergence of the four  
novel methods developed in this paper is also an open problem requiring further  
research.

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