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Symplectic integration of Sine–Gordon type systems

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Abstract

We construct a class of symplectic integration schemes to general Sine–Gordon type systems. We also conduct several numerical tests for these symplectic schemes. Our numerical results demonstrate the effectiveness of these schemes for numerical computation of the solutions to the general Sine–Gordon type systems. © 1999 IMACS/Elsevier Science B.V. All rights reserved.

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1. Introduction

Symplectic integration techniques have attracted more and more attention during the recent years. In numerical computations for Hamiltonian systems, most standard numerical methods cannot produce excellent results simply because these methods usually neglect the important features of the dynamics in the Hamiltonian system and fail to preserve the symplectic property of the solution. The symplectic integration schemes have lots of advantages over these standard numerical methods. They can approximate the map of the exact dynamics in time direction to any desired order and still maintain the symplectic property for numerical solutions. Therefore, the symplectic integration schemes are clean schemes, free from all kinds of non-Hamiltonian pollutions. They actually give outstanding performance, far superior than the conventional non-symplectic methods, especially in the aspects of global, structural properties and long-term tracking capabilities.

In this paper, we discuss how to implement the symplectic integration techniques for general Sine–Gordon type systems [9]. The general Sine–Gordon type system can be described as

$$\partial_t^2 u - \partial_x^2 u + g(u) = 0, \tag{1}$$

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for all $(x,t) \in \mathbf{R} \times (0,\infty)$, where $g(u)$ is a smooth function of u. This system has lots of applications. It also can be put within the Hamiltonian framework [3]. In fact, Eq. (1) can be written as an infinite dimensional Hamiltonian system by letting $v = \partial_t u$:

$$\partial_t u = -\frac{\delta H}{\delta v}(u,v), \ \partial_t v = \frac{\delta H}{\delta u}(u,v), \tag{2}$$

with Hamiltonian functional $H(u,v) = \int_R [\frac{1}{2}(-v^2 + u_x^2) + G(u)]\,\mathrm{d}x$, where $G'(u) = -g(u)$. The solution $(u(x,t),\ v(x,t))$, as a time-t map in the phase space, is symplectic.

Our paper is organized as follows: In Section 2, we give a brief overview of the generating function method, which is used to design the symplectic integration method. In Section 3, we present the general symplectic integration method for infinite dimensional Hamiltonian system and construct two types of explicit symplectic numerical schemes for system (1). The numerical results are presented in Section 4, followed by a brief conclusion in Section 5.

2. Hamiltonian systems and generating functions

Symplectic schemes for both finite and infinite dimensional Hamiltonian systems have been widely discussed in the literature [4–8,12]. It is well-known that for a general infinite dimensional Hamiltonian systems:

$$\frac{\partial}{\partial t}\begin{pmatrix} u \\ v \end{pmatrix} = J \cdot \begin{pmatrix} \delta H/\delta u(u,v) \\ \delta H/\delta v(u,v) \end{pmatrix}, \quad J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \tag{3}$$

where $u = u(x,t),\ v = v(x,t)$ are two real functions, and $H(u,v)$ is the Hamiltonian (energy) functional, the symplectic scheme can be constructed via its time-dependent generating functional $\Phi(W,t) = \Phi(u,v,t)$ [4,6,10,11]. The following two lemmas illustrate the property of the generating functional Φ. Due to the limitation of the length of the paper, we just list the results. The interested reader may consult the literature [4,6,10,11] for details.

Definition 1. A 4×4 real matrix T is called **Darboux** matrix if:

$$T^* \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix} T = \begin{pmatrix} J & 0 \\ 0 & -J \end{pmatrix}, \tag{4}$$

where I is the 2×2 identity matrix.

It is convenient to use the following block representation for a 4×4 **Darboux** matrix T and its inverse T^{-1}

$$T\begin{pmatrix} A & B \\ C & D \end{pmatrix}, \quad T^{-1} = \begin{pmatrix} A_1 & B_1 \\ C_1 & D_1 \end{pmatrix}, \tag{5}$$

where A, B, C, D, A_1, B_1, C_1 and D_1 are all 2×2 real matrices.

Lemma 1. *For any Hamiltonian functional H in* (3) *and* **Darboux** *matrix T of form* (5) *which satisfies* $|C+D|\neq 0$, *a generating functional* $\Phi(W,t)$ *can be defined. This generating functional satisfies the Hamilton–Jacobi equation*:

$$\frac{\mathrm{d}\Phi(W,t)}{\mathrm{d}t} = -H(A_1\nabla\Phi(W)+B_1W). \tag{6}$$

Lemma 2. *For a sufficiently small t, the generating functional* $\Phi(W,t)$ *can be expressed by the Taylor series in t as*:

$$\Phi(W,t) = \sum_{k=1}^{\infty}\phi^{(k)}(W)t^k, \quad |t| \text{ small.} \tag{7}$$

The coefficients $\phi^{(k)}(W)$ *in* (7) *can be determined recursively*:

$$\phi^{(1)}(W) = -H(W), \tag{8}$$

and for $k=2,3,\ldots$

$$\phi^{(k)}(W) = -\frac{1}{k}\sum_{m=1}^{k-1}\frac{1}{m!}\sum_{i_1,\ldots,i_m=1}^{2} H_{i_1,\ldots,i_m}(W)\sum_{j_1+\ldots+j_m=k-1,j_l\geq 1}(A_1\nabla\phi^{(j_1)}(W))_{i_1}\ldots(A_1\nabla\phi^{(j_m)}(W))_{i_m}, \tag{9}$$

where the notation $H_{i_1,\ldots,i_m}$ *denotes the mth order partial derivative of H(W) with respect to variables* $w_{i_1},w_{i_2},\ldots,w_{i_m}$, A_1 *is the upper-left sub-block of* T^{-1}, *and the* $(\,)_{i_1}$ denotes the i_1th component of a vector.

3. Symplectic schemes for Sine–Gordon type systems

The generating functional is closely related to the symplectic scheme of the infinite dimensional Hamiltonian system (3). We consider the solution of the system (3) on a discrete time mesh $\{n\Delta t,\ n=0,1,\ldots\}$, where Δt is the time step, and denote $u^n=u(x,n\Delta t)$ and $v^n=n(x,n\Delta t)$. Then, based on the generating functional Φ, we have

Theorem 1. *A mth order accuracy symplectic scheme for general infinite dimensional Hamiltonian system* (3) *can be constructed as*:

$$\bar{W}^{n+1} = \sum_{k=1}^{m}\nabla\phi^{(k)}(W^n)\Delta t^k, \quad n=1,2,\ldots, \tag{10}$$

where the functions $\phi^{(k)},\ k=1,2,\ldots,m$ *are defined as in (8) and (9), and the two vectors* $\bar{W}^{n+1},\ W^n$ *are defined as*:

$$\bar{W}^{n+1} = \begin{pmatrix}\bar{W}_1^{n+1}\\ \bar{W}_2^{n+1}\end{pmatrix} = A\begin{pmatrix}u^{n+1}\\ v^{n+1}\end{pmatrix} + B\begin{pmatrix}u^n\\ v^n\end{pmatrix}, \tag{11}$$

$$W^n = \begin{pmatrix}W_1^n\\ W_2^n\end{pmatrix} = C\begin{pmatrix}u^{n+1}\\ v^{n+1}\end{pmatrix} + D\begin{pmatrix}u^n\\ v^n\end{pmatrix}. \tag{12}$$

Since the general Sine–Gordon type system (1) can also be written as an infinite dimensional Hamiltonian system, thus we can apply Theorem 1 directly and construct symplectic numerical schemes to this system. According to Theorem 1, the choices of Darboux matrices during the construction of the scheme are very flexible. In this paper, however, we select the following types of Darboux matrices:

$$T = \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} J & -J \\ 1/2(I+JL) & 1/2(I-JL) \end{pmatrix}, \tag{13}$$

and

$$T^{-1} = \begin{pmatrix} A_1 & B_1 \\ C_1 & D_1 \end{pmatrix} = \begin{pmatrix} 1/2(JLJ-J) & I \\ 1/2(JLJ+J) & I \end{pmatrix}, \tag{14}$$

with a real symmetric matrix $L = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. The two vectors $\bar{W}^{n+1}$ and W^n in Theorem 1 can be computed explicitly based on the matrix T in (13):

$$\bar{W}^{n+1} = \begin{pmatrix} v^n - v^{n+1} \\ u^{n+1} - u^n \end{pmatrix}, \quad W^n = \begin{pmatrix} u^n \\ v^{n+1} \end{pmatrix}. \tag{15}$$

Furthermore, the first two terms of the generating functional Φ for this specific Hamiltonian H in (2) can be computed as:

$$\phi^{(1)}(W^n) = \phi^{(1)}(u^n, v^{n+1}) = -H(u^n, v^{n+1}), \tag{16}$$

$$\phi^{(2)}(W^n) = \phi^{(2)}(u^n, v^{n+1}) = \tfrac{1}{2} v^{n+1}(g(u^n) - \partial_{xx} u^n). \tag{17}$$

Then the gradients $\nabla\phi^{(1)}(W^n)$ and $\nabla\phi^{(2)}(W^n)$ can be calculated as:

$$\nabla\phi^{(1)}(W^n) = \begin{pmatrix} \dfrac{\delta}{\delta(u^n)}\phi^{(1)}(u^n, v^{n+1}) \\[2ex] \dfrac{\delta}{\delta(v^{n+1})}\phi^{(1)}(u^n, v^{n+1}) \end{pmatrix} = \begin{pmatrix} -\dfrac{\delta}{\delta(u^n)} H(u^n, v^{n+1}) \\[2ex] -\dfrac{\delta}{\delta(v^{n+1})} H(u^n, v^{n+1}) \end{pmatrix} = \begin{pmatrix} g(u^n) - \partial_{xx} u^n \\ v^{n+1} \end{pmatrix}, \tag{18}$$

$$\begin{aligned} \nabla\phi^{(2)}(W^n) &= \begin{pmatrix} \dfrac{\delta}{\delta(u^n)}\phi^{(2)}(u^n, v^{n+1}) \\[2ex] \dfrac{\delta}{\delta(v^{n+1})}\phi^{(2)}(u^n, v^{n+1}) \end{pmatrix} = \begin{pmatrix} \dfrac{\delta}{\delta(u^n)}[\tfrac{1}{2} v^{n+1}(g(u^n) - \partial_{xx} u^n)] \\[2ex] \dfrac{\delta}{\delta(v^{n+1})}[\tfrac{1}{2} v^{n+1}(g(u^n) - \partial_{xx} u^n)] \end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix} v^{n+1} \cdot \dfrac{\delta}{\delta(u^n)} g(u^n) - \dfrac{\delta}{\delta(u^n)}[v^{n+1}\partial_{xx} u^n] \\[2ex] [g(u^n) - \partial_{xx} u^n]\dfrac{\delta}{\delta(v^{n+1})} v^{n+1} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} v^{n+1} g'(u^n) - \partial_{xx} v^{n+1} \\ g(u^n) - \partial_{xx} u^n \end{pmatrix}. \end{aligned} \tag{19}$$

Substituting (15), (18) and (19) back into (10), we derive the following two semi-discrete symplectic schemes:

Scheme I:

$$\begin{cases} u^{n+1} = u^n + \Delta t v^{n+1} \\ v^{n+1} = v^n + \Delta t \partial_{xx} u^n - \Delta t g(u^n). \end{cases} \tag{20}$$

Scheme II:

$$\begin{cases} u^{n+1} = u^n + \Delta t v^{n+1} + \dfrac{\Delta t^2}{2}(g(u^n) - \partial_{xx} u^n) \\ v^{n+1} = v^n + \Delta t(\partial_{xx} u^n - g(u^n)) + \dfrac{\Delta t^2}{2}[\partial_{xx} v^{n+1} - v^{n+1} g'(u^n)]. \end{cases} \tag{21}$$

Both Eqs. (20) and (21) need to be further discretized in the space direction. We have to decide how to discretize the spatial derivatives. The most naive way would be to use the forward or central difference, i.e., $\partial_x u^n = u^n(x + \Delta x) - u^n(x)/\Delta x$ or $\partial_x u^n = u^n(x + \Delta x) - u^n(x - \Delta x)/2\Delta x$, however, this choice is non-specific. We require that the discretization of (20) and (21) in the space variable also retain the Hamiltonian property. Therefore, we will use the central difference:

$$\partial_{xx} u_j^n \approx \frac{1}{\Delta x^2}(u_{j-1}^n - 2u_j^n + u_{j+1}^n). \tag{22}$$

Applying the approximation (22) to Eqs. (20) and (21), we get the $\mathrm{O}(\Delta t) + \mathrm{O}(\Delta x^2)$ accurate scheme:

$$u_j^{n+1} = u_j^n + \Delta t v_j^{n+1}, \qquad v_j^{n+1} = v_j^n + \frac{\Delta t}{\Delta x^2}(u_{j-1}^n - 2u_j^n + u_{j+1}^n) - \Delta t g(u_j^n), \tag{23}$$

and the $\mathrm{O}(\Delta t^2) + \mathrm{O}(\Delta x^2)$ accurate scheme:

$$u_j^{n+1} = u_j^n + \Delta t v_j^{n+1} - \frac{\Delta t^2}{2\Delta x^2}(u_{j-1}^n - 2u_j^n + u_{j+1}^n) + \frac{\Delta t^2}{2} g(u_j^n),$$

$$\left(1 + \frac{\Delta t^2}{2} g'(u_j^n) + \frac{\Delta t^2}{\Delta x^2}\right) v_j^{n+1} - \frac{\Delta t^2}{2\Delta x^2}(v_{j+1}^{n+1} + v_{j-1}^{n+1}) = v_j^n - \Delta t g(u_j^n) + \frac{\Delta t}{\Delta x^2}(u_{j-1}^n - 2u_j^n + u_{j+1}^n). \tag{24}$$

4. Numerical results

To illustrate the effectiveness of our method, we report three numerical examples in this section. These examples include a wave propagation in a fixed domain, single solitary wave propagation and interaction of double solitary waves.

4.1. Wave propagation in a fixed domain

We consider the IBV problem for system (1) with $g(u) = (\pi^2 - 1)u$ on the domain $[0, 1] \times (0, \infty)$. The initial and boundary value conditions are set to:

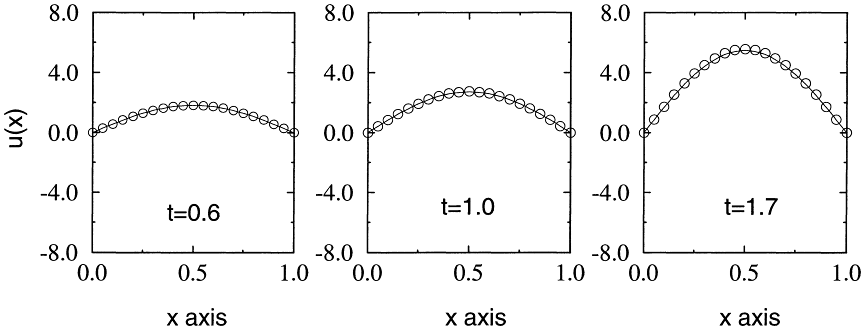

Fig. 1. Numerical results for wave propagation in the fix domain.

$$u(x,0) = \sin(\pi x), \; u_t(x,0) = \sin(\pi x), \tag{25}$$

$$u(0,t) = 0, \; u(1,t) = 0. \tag{26}$$

This problem has an analytic solution $u(x,t) = \exp(t)\sin(\pi x)$. We use Eqs. (23) and (24) to solve the wave propagation at different time. The time and spatial steps are selected as $\Delta x = 0.05, \; \Delta t = 0.02$ through all the computations. The numerical results obtained using Eqs. (23) and (24) are all precise enough and essentially indistinguishable from each other. Fig. 1 shows several snapshots of the numerical solution at $t = 0.6$, 1.0 and 1.7 given by Eq. (23). The analytic solutions are also plotted in the same pictures for comparison. It should be pointed out that the scheme has relatively high resolution and low dissipation.

4.2. Single solitary wave propagation

In this example, we consider the Sine–Gordon and the Φ^4 equation by choosing $g(u) = \sin u$ and $g(u) = -u + u^3$ in (1), respectively. Both equations possess kink-like solitary waves, which can be expressed as $u(x,t) = \tanh\left((x - \nu t)/\sqrt{2(1-\nu^2)}\right)$ for the Φ^4 equation and $u(x,t) = 4\arctan\left\{\exp\left((x-\nu t)/\sqrt{1-\nu^2}\right)\right\}$ for the Sine–Gordon equation, where the parameter ν is a real number with $0 < \nu < 1$.

First we simulate the motion of a single kink in the Sine–Gordon and the Φ^4 equations by using the discrete model (24). In Fig. 2 we present the plots of a single kink with $\nu = 0.3$ in both Sine–Gordon and Φ^4 equation at $t = 800$, 1600 and 2400. Our results were obtained on the grid stretching from -800 to 800 with step size 0.5; the time step of the calculation was 0.01. Note that all the kinks are described by essentially 10–12 grid points, the others differ very little from their asymptotic values. During the computation, the structure of the numerical solitary wave are well-preserved.

4.3. Interaction of two solitary waves

We use these schemes to simulate the solitary wave collisions in the Sine–Gordon and the Φ^4 equations. It is well-known theoretically, that in the Sine–Gordon equation, these two solitary waves

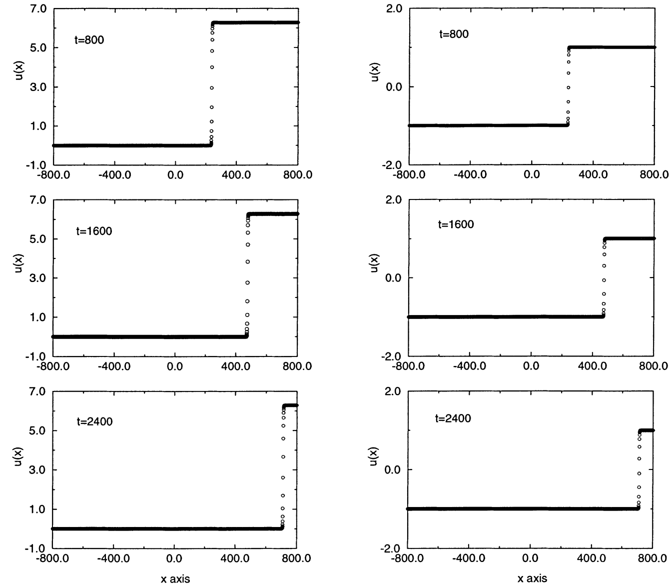

Fig. 2. The plots of single solitary wave for the Sine–Gordon and the Φ^4 equation at t = 800, 1600, and 2400.

will pass through each other without any interaction (with only a phase shift), however, it is not possible for the two solitary waves to pass through each other in the Φ^4 equation [1,2]. Our numerical results demonstrate these phenomena. In the numerical calculation, a kink with $v=-0.5$ and anti-kink with

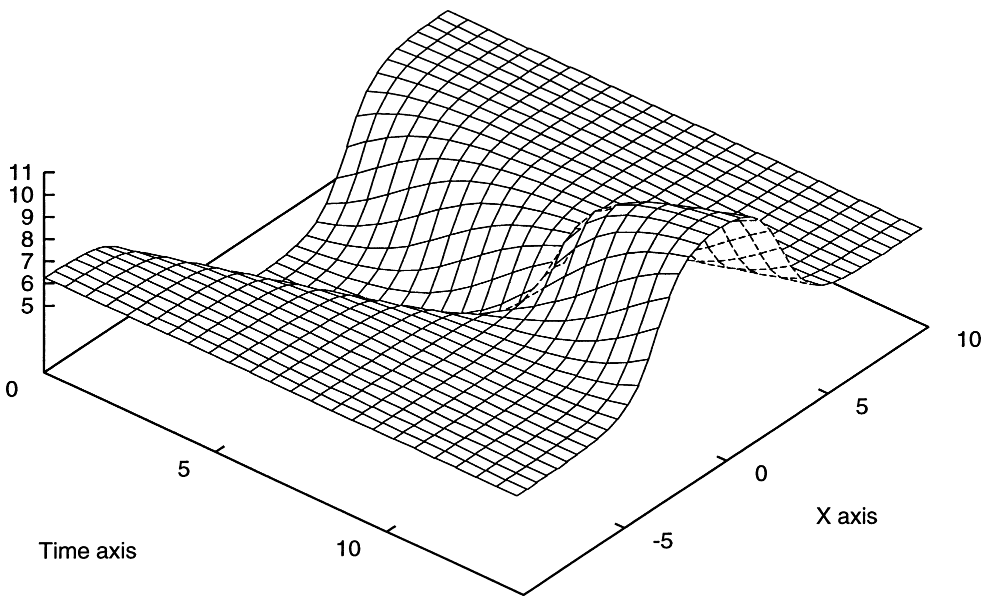

Fig. 3. The two solitary waves collision in the Sine–Gordon equation for $\nu=0.5$. Two solitary waves pass through each other without any intervention (only a phase shift). The choice of parameter ν is not significant.

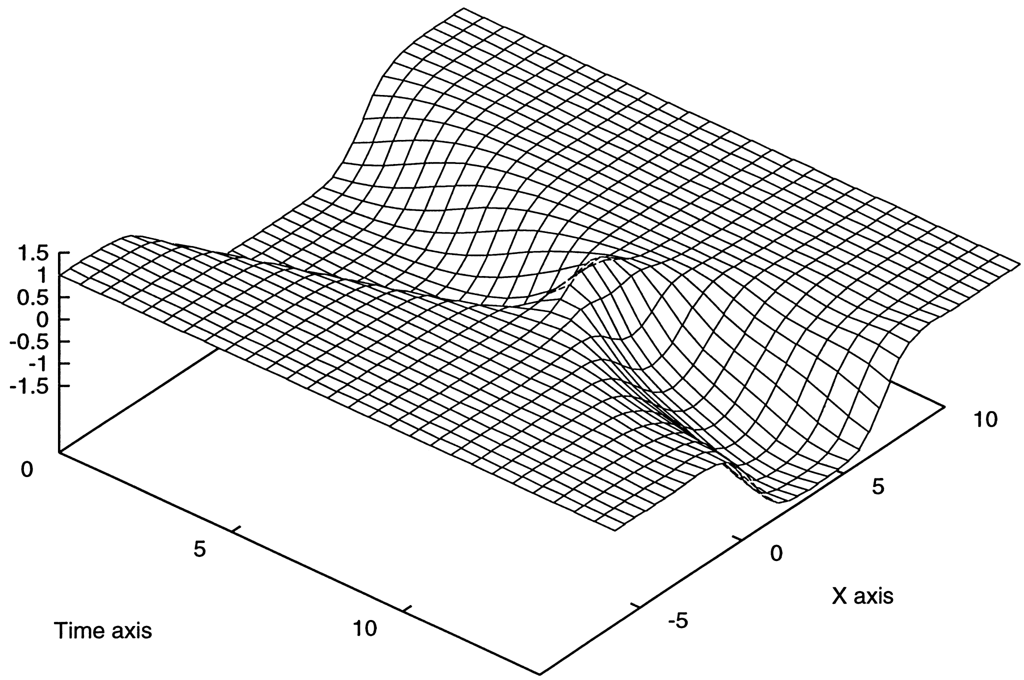

Fig. 4. The two solitary waves collision in the Φ^4 equation for $\nu = 0.3$.

$v = 0.5$ are initially placed at positions $x = 5.0$ and $x = -5.0$, respectively. The calculation domain is $[-10, 10]$ with time step $\Delta t = 0.05$ and spatial step $\Delta x = 0.5$. The entire collision process is presented in a space–time plot. Fig. 3 illustrates the kink–antikink collision in the Sine–Gordon equation. As time evolves, the two solitary waves approach each other, interact non-linearly, and then emerge unchanged in shape. Fig. 4 shows the collision of two solitary waves for the Φ^4 equation where two waves bounce backward after colliding. It should be pointed out that all the pictures are generated in larger time frames, and the stability of the results is striking.

5. Conclusion

We have presented the symplectic integration scheme for Sine–Gordon type systems that can be effectively used for the numerical study of the solutions to general Sine–Gordon systems. We also conduct several numerical tests for these schemes. Our numerical results show that these schemes have very good resolution and preservation of structure for the numerical solution.

References

[1] D.K. Campbell, J.F. Schonfeld, C.A. Wingate, Resonance windows in kink-antikink interactions in Φ^4 theory, Physica D 9 (1983) 1–32.

[2] D.K. Campbell, M. Peyrard, P. Sodano, Kink-antikink interactions in the double Sine–Gordon equation, Physica D 19 (1986) 165–205.

[3] P. Chernoff, J. Marsden, Properties of infinite dimensional Hamilton system, in: Lecture Notes in Mathematics, vol. 425, Springer, New York.
[4] K. Feng, Difference schemes for Hamiltonian formalism and symplectic geometry, J. Comput. Math. 4 (1986) 279–289.
[5] K. Feng, M. Qin, The symplectic methods for the computation of Hamiltonian equation, in: Z. You-lan, G. Ben-Yu (Eds.), Proceedings of the First Chinese Conference on Numerical Methods of PDE's, Lecture Notes in Mathematics, vol. 1297, Springer, New York, 1987, pp. 1–37.
[6] K. Feng, H. Wu, M. Qin, D. Wang, Construction of canonical difference schemes for Hamiltonian formalism via generating functions, J. Comput. Math. 7 (1989) 71–96.
[7] C. Li, M. Qin, A symplectic difference scheme for the infinite dimensional Hamilton system, J. Comput. Math. 6 (1988) 164–174.
[8] X. Lu, R. Schmid, A symplectic algorithm for wave equations, Mathematics and Computers in Simulation 43 (1997) 29–38.
[9] P. Marcati, R. Natalini, Global weak entropy solutions to quasilinear wave equations of Klein–Gordon and Sine–Gordon type, IEEE Trans. Comput. 38 (1989) 1526–1538.
[10] M. Qin, M. Zang, Multi-stage symplectic schemes of two kinds of Hamiltonian systems for wave equations, Comput. Math. Appl. 19 (1990) 51–62.
[11] M. Qin, D. Wang, M. Zhang, Explicit symplectic difference scheme for separatable Hamiltonian system, J. Comput. Math. 9 (1991) 211–221.
[12] J.M. Sanz-Serna, M.P. Calvo, Numerical Hamiltonian Problems, Chapman & Hall, London, 1994.