SIAM J. NUMER. ANAL.
Vol. 39, No. 6, pp. 2164–2178

SQUARE-CONSERVATIVE SCHEMES FOR A CLASS OF EVOLUTION EQUATIONS USING LIE-GROUP METHODS*

JING-BO CHEN†, HANS MUNTHE-KAAS‡, AND MENG-ZHAO QIN§

Abstract. A new method for constructing square-conservative schemes for a class of evolution equations using Lie-group methods is presented. The basic idea is as follows. First, we discretize the space variable appropriately so that the resulting semidiscrete system of equations can be cast into a system of ordinary differential equations evolving on a sphere. Second, we apply Lie-group methods to the semidiscrete system, and then square-conservative schemes can be constructed since the obtained numerical solution evolves on the same sphere. Both exponential and Cayley coordinates are used. Numerical experiments are also reported.

Key words. square-conservative schemes, Lie-group methods, evolution equations

AMS subject classifications. 65M99, 65M05, 65M20

PII. S0036142901383971

1. Introduction.

We consider a system of evolution equations in the form

$$\frac{\partial \boldsymbol{u}}{\partial t} = F(x, t, \boldsymbol{u}, \boldsymbol{u}^{(n)}) \tag{1.1}$$

with periodic boundary condition $\boldsymbol{u}(0,t) = \boldsymbol{u}(L,t)$. Here $\boldsymbol{u}^{(n)}$ denotes partial derivatives of $\boldsymbol{u}$ with respect to x up to nth order, $\boldsymbol{u} = (u_1(x,t), \ldots, u_m(x,t))^T$, and L is the period. For simplicity, we consider only one space dimension in this paper.

Assume $\boldsymbol{u}(x,t)$ is the solution of (1.1). If $\boldsymbol{u}(x,t)$ satisfies

$$\frac{d}{dt}\int_0^L \boldsymbol{u}^2(x,t)dx = 0, \tag{1.2}$$

we call (1.1) a square-conservative system. Equation (1.2) is called a square-conservative law. For example, the KdV equation and the system of a ferromagnetic chain are both square-conservative systems (see section 2). In this paper, we shall explore the numerical integration of square-conservative systems. Our purpose is to obtain numerical schemes which possess a discrete version of (1.2).

Concretely, we consider a uniform grid of points $(x_i, t_j), \boldsymbol{u}_i^j \approx \boldsymbol{u}(x_i, t_j), i = 0, 1, \ldots, N-1$, $j = 0, 1, \ldots, M-1$, $N\Delta x = L$, $M\Delta t = T$. We consider a one-step scheme of (1.1):

$$\boldsymbol{u}^{j+1} = \mathcal{F}(\boldsymbol{u}^j). \tag{1.3}$$

*Received by the editors January 22, 2001; accepted for publication (in revised form) October 14, 2001; published electronically April 3, 2002. This work is subsidized by State Major Research Program G1999,032800 and State Natural Science Fund (Oil Prospecting 49894190).

http://www.siam.org/journals/sinum/39-6/38397.html

†Institute of Theoretical Physics, Chinese Academy of Sciences, P.O. Box 2735, Beijing 100080, People's Republic of China (chenjb@itp.ac.cn).

‡Department of Informatics, University of Bergen, PB 7800, N-5020 Bergen, Norway (hans@ii.uib.no).

§Institute of Computational Mathematics, AMMS, P.O. Box 2719, Beijing 100080, People's Republic of China (qmz@lsec.cc.ac.cn).

If (1.3) satisfies

$$\sum_{i=0}^{N-1}(\boldsymbol{u}_i^{j+1})^2 = \sum_{i=0}^{N-1}(\boldsymbol{u}_i^{j})^2, \quad j = 0, 1, \ldots, M-1, \tag{1.4}$$

we call (1.3) a square-conservative scheme. Equation (1.4) is called discrete square-conservative law.

Now we recall the definition of stability of numerical schemes [13].

DEFINITION 1.1. *The scheme* (1.3) *for the system* (1.1) *is said to be stable with respect to the norm* $\|\cdot\|$ *if there exist positive constants* Δx_0 *and* Δt_0 *and nonnegative constant* K *depending only on* T *and independent of* Δx *and* Δt *so that*

$$\|\boldsymbol{u}^M\| \le K\|\boldsymbol{u}^0\|, \tag{1.5}$$

for $0 \le T = M\Delta t$, $0 < \Delta x \le \Delta x_0$*, and* $0 < \Delta t \le \Delta t_0$*. Particularly, if* (1.1) *is a nonlinear system, we call* (1.3) *nonlinearly stable. Here we consider only Euclidean norms.*

For numerical schemes of linear systems, we can use the von Neumann method to analyze their stability [12, 13]. For numerical schemes of nonlinear systems, it is very difficult to analyze their nonlinear stability. A usual approach is to analyze their linear stability. However, some numerical schemes of nonlinear systems are nonlinearly instable, although they are linearly stable, i.e., stable for the corresponding linearized system [12]. Therefore, in some cases, it is necessary to discuss nonlinear stability. From Definition 1.1, we can see that square-conservative schemes are stable, and for nonlinear systems they are nonlinearly stable. Thus, square-conservative schemes for nonlinear square-conservative systems not only preserve the square-conservative property of the continuous system but also are nonlinearly stable.

Recently much attention has been paid to geometric integration of ordinary differential equations on manifolds [4, 6, 7, 8, 9]. The main feature of this method is that the numerical solution evolves on the same manifold as the analytical solution. This method is called the Lie-group method. We note that by appropriately discretizing the space variable for some square-conservative systems, the resulting semidiscrete systems of equations can be cast into systems of ordinary differential equations evolving on a sphere. Applying the Lie-group method to the semidiscrete systems, we obtain a numerical solution which evolves on the same sphere. That is, the numerical solution satisfies a discrete square-conservative law. A new method for constructing square-conservative schemes for some square-conservative systems is thus developed.

This paper is organized as follows. In section 2, we present the semidiscretizations of two square-conservative systems. The Lie-group methods for the semidiscrete systems are discussed in section 3. Numerical experiments are reported in section 4. Section 5 contains some comments and conclusions.

2. Space discretizations of two square-conservative systems. In order to obtain square-conservative schemes for (1.1) using Lie-group methods, we first discretize the space variable appropriately so that the resulting semidiscrete system can be cast into a system of ordinary differential equations evolving on a sphere. In general, there is not a universal method to attain this goal. For concrete systems, we need concrete approaches. However, a practical principle exists; that is, we should preserve the symmetric or antisymmetric properties of the differential operators when discretizing. In this section, we shall present space discretizations of two square-conservative systems.

2.1. Space discretizations for the KdV equation. We consider the KdV equation

$$u_t = -uu_x - \delta^2 u_{xxx}, \tag{2.1}$$

with periodic boundary condition $u(0,t) = u(L,t)$. L is the period and δ is a small parameter.

As in [11], we rewrite (2.1) in the form of an operator equation:

$$u_t = A_{\theta,u} u. \tag{2.2}$$

Here $A_{\theta,u}$ is a differential operator and depends on u and a real parameter θ:

$$A_{\theta,u} = -(1-\theta)u\frac{\partial}{\partial x} - \frac{\theta}{2}\frac{\partial u\cdot}{\partial x} - \delta^2\frac{\partial^3}{\partial x^3}. \tag{2.3}$$

The operator $\frac{\partial u\cdot}{\partial x}$ in (2.3) is defined as follows:

$$\frac{\partial u\cdot}{\partial x} f = \frac{\partial}{\partial x}(uf),$$

where f is a differentiable function.

Now we discretize (2.2) in space by using finite difference and Fourier pseudospectral methods, respectively. Our aim is to obtain a semidiscrete system of ordinary differential equations which evolves on a sphere.

For simplicity, we take $L = 2$ and consider the space interval [0, 2]. We will work with a uniform grid of points $x_i = i\Delta x, i = 0, 1, \dots, N-1$, $\Delta x = \frac{L}{N} = \frac{2}{N}$. Let

$$U = (u_0, u_1, \dots, u_{N-1})^T,$$

where $u_i \approx u(i\Delta x, t), i = 0, 1, \dots, N-1$.

We first present the finite difference discretizations. In order to obtain a semidiscrete system of ordinary differential equations which evolves on a sphere, the crucial point is to discretize the operator (2.3).

We approximate the differential operator $A_{\theta,u}$ by the difference operator

$$\mathcal{A}_{\theta,U} = -(1-\theta)U \times.\Delta_0 - \frac{\theta}{2}\Delta_0 U \times. - \delta^2\Delta_+\Delta_0\Delta_-. \tag{2.4}$$

Here the symbol $\times.$ denotes the array multiplication between vectors. For example, suppose that $V = (v_0, v_1, \dots, v_{N-1})$; then we have

$$U \times.V = (u_0v_0, u_1v_1, \dots, u_{N-1}v_{N-1}).$$

Δ_+, Δ_0, and Δ_- are forward, centered, and backward difference operators, respectively, defined by

$$\begin{aligned}
\Delta_+ U &= \frac{1}{\Delta x}(u_1 - u_0, u_2 - u_1, \dots, u_{N-1} - u_{N-2}, u_0 - u_{N-1})^T,\\
\Delta_0 U &= \frac{1}{2\Delta x}(u_1 - u_{N-1}, u_2 - u_0, \dots, u_{N-1} - u_{N-3}, u_0 - u_{N-2})^T,\\
\Delta_- U &= \frac{1}{\Delta x}(u_0 - u_{N-1}, u_1 - u_0, \dots, u_{N-2} - u_{N-3}, u_{N-1} - u_{N-2})^T,
\end{aligned}$$

where we have used the periodic boundary conditions $u_0 = u_N, u_{-1} = u_{N-1}$.

Thus we obtain a semidiscrete system of (2.2):

$$\frac{dU}{dt} = \mathcal{A}_{\theta,U} U. \tag{2.5}$$

The parameter θ can be used to construct a family of difference operators. Taking $\theta = \frac{2}{3}$, (2.5) is equivalent to

$$\begin{aligned} \frac{du_i}{dt} = \; & -\frac{u_{i+1}+u_i+u_{i-1}}{3}\frac{u_{i+1}-u_{i-1}}{2\Delta x} \\ & -\delta^2 \frac{u_{i+2}-2u_{i+1}+2u_{i-1}-u_{i-2}}{2\Delta x^3}, \end{aligned} \tag{2.6}$$

where $i = 0, 1, 2, \ldots, N-1$.

We note that the space discretization in (2.6) is same as that used by Zabusky and Kruskal [14].

Further, we can rewrite (2.6) as

$$\frac{dU}{dt} = f_2(U)U. \tag{2.7}$$

Here $f_2(U)$ is an antisymmetric matrix,

$$f_2(U) = -\frac{1}{6\Delta x} g(U) - \frac{\delta^2}{2\Delta x^3} p, \tag{2.8}$$

where $g(U)$ and p are both antisymmetric matrices:

$$g(U) = \begin{pmatrix} 0 & u_0+u_1 & 0 & 0 & \cdots & 0 & -(u_0+u_{N-1}) \\ -(u_1+u_0) & 0 & u_1+u_2 & 0 & \cdots & 0 & 0 \\ 0 & -(u_2+u_1) & 0 & u_2+u_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ u_{N-1}+u_0 & 0 & 0 & 0 & \cdots & -(u_{N-1}+u_{N-2}) & 0 \end{pmatrix}$$

and

$$p = \begin{pmatrix} 0 & -2 & 1 & 0 & 0 & \cdots & 0 & 0 & -1 & 2 \\ 2 & 0 & -2 & 1 & 0 & \cdots & 0 & 0 & 0 & -1 \\ -1 & 2 & 0 & -2 & 1 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & 0 & \cdots & -1 & 2 & 0 & -2 \\ -2 & 1 & 0 & 0 & 0 & \cdots & 0 & -1 & 2 & 0 \end{pmatrix}. \tag{2.9}$$

Higher order space discretizations can be obtained in a similar way if we preserve the skew-adjoint property of the operators $\frac{\partial}{\partial x}$ and $\frac{\partial^3}{\partial x^3}$ in discretizations.

We denote by $f_q(U)$ the antisymmetric matrix for qth order space discretizations.

Now we consider the Fourier pseudospectral discretization. We approximate the differential operator $A_\theta(u)$ by the operator

$$\tilde{\mathcal{A}}_{\theta,U} = -(1-\theta)U \times .D_1 - \frac{\theta}{2} D_1 U \times . - \delta^2 D_3, \tag{2.10}$$

where D_1 and D_3 are the first order and third order antisymmetric spectral differentiation matrices, respectively [5]:

$$(D_1)_{j,n} = \begin{cases} \frac{1}{2}\mu(-1)^{j+n} \cot\left(\mu \frac{x_j - x_n}{2}\right), & j \neq n, \\ 0, & j = n, \end{cases}$$

$$(D_3)_{j,n} = \begin{cases} \mu^3(-1)^{j+n} \frac{\cos\left(\mu \frac{x_j - x_n}{2}\right)}{\sin^3\left(\mu \frac{x_j - x_n}{2}\right)} + \frac{\mu^3 N^2}{8}(-1)^{j+n+1} \cot\left(\mu \frac{x_j - x_n}{2}\right), & j \neq n, \\ 0, & j = n, \end{cases}$$

where $\mu = \frac{2\pi}{L} = \pi, j = 0, 1, \ldots, N-1, n = 0, 1, \ldots, N-1$.

For the qth order spectral differentiation matrix D_k, we have the following result [3].

THEOREM 2.1. *For the spectral differentiation matrices D_k and $(D_1)^k$, the following equation holds:*

$$(D_k)_{j,n} = (D_1^k)_{j,n} + (-1)^{j+n} \frac{\mu^k}{2N} \left[\left(i \frac{N}{2} \right)^k + \left(-i \frac{N}{2} \right)^k \right]; \tag{2.11}$$

particularly, $D_k = (D_1)^k$ if k is an odd number.

Using the Fourier pseudospectral space discretization, we obtain another semidiscrete system of (2.2):

$$\frac{dU}{dt} = \tilde{\mathcal{A}}_{\theta,U} U. \tag{2.12}$$

Taking $\theta = \frac{2}{3}$, we can rewrite (2.12) as

$$\frac{dU}{dt} = f_{\exp}(U)U, \tag{2.13}$$

where the subscript exp denotes exponential order and $f_{\exp}(U)$ is an antisymmetric matrix,

$$f_{\exp}(U) = -\frac{1}{3}\tilde{g}(U) - \delta^2 D_3, \tag{2.14}$$

where D_3 is the third order antisymmetric spectral differentiation matrix and

$$\tilde{g}(U) = \begin{pmatrix} 0 & (u_0 + u_1)a_{0,1} & (u_0 + u_2)a_{0,2} & \cdots & (u_0 + u_{N-1})a_{0,N-1} \\ (u_1 + u_0)a_{1,0} & 0 & (u_1 + u_2)a_{1,2} & \cdots & (u_1 + u_{N-1})a_{1,N-1} \\ \vdots & \vdots & \vdots & & \vdots \\ (u_{N-1} + u_0)a_{N-1,0} & (u_{N-1} + u_1)a_{N-1,1} & (u_{N-1} + u_2)a_{N-1,2} & \cdots & 0 \end{pmatrix},$$

where $a_{i,j}$, $i = 0, 1, \ldots, N-1$, $j = 0, 1, \ldots, N-1$, are the elements of the first order antisymmetric spectral differentiation matrix D_1.

Now using finite difference and Fourier pseudospectral methods, we have obtained a semidiscrete system of the KdV equation in the form

$$\begin{aligned} \frac{dU}{dt} &= f(U)U, \\ U(0) &= U^0, \end{aligned} \tag{2.15}$$

where $f(U)$ is an antisymmetric matrix, $f(U) \in \mathbf{so}(N)$; $\mathbf{so}(N)$ is the Lie algebra for the orthogonal group $O(N)$ and

$$U^0 = (u_0^0, u_1^0, \ldots, u_{N-1}^0)^T, \quad u_i^0 = u(i\Delta x, 0),\ i = 0, 1, \ldots, N-1.$$

From the above analysis, we can understand the reason why we write the KdV equation (2.1) as in the form of (2.2)–(2.3). It is important to discretize the space by discretizing the operator (2.3) in order to obtain a semidiscrete system in the form of (2.15). In addition, it is necessary to choose $\theta = \frac{2}{3}$. Using other values of θ, we can obtain semidiscrete systems which cannot be cast into the form of (2.15).

The system (2.15) is a system of ordinary differential equations evolving on a sphere with radius $\|U^0\|$. Here $\|\cdot\|$ denotes the Euclidean norm,

$$\|U^0\| = \sqrt{\sum_{i=0}^{N-1} (u_i^0)^2}.$$

2.2. Space discretizations for a system of a ferromagnetic chain. Consider the system of a ferromagnetic chain

$$\boldsymbol{z}_t = \boldsymbol{z} \times \boldsymbol{z}_{xx} + \boldsymbol{z} \times \boldsymbol{h}, \tag{2.16}$$

with periodic boundary condition $\boldsymbol{z}(0,t) = \boldsymbol{z}(L,t)$. Here

$$\boldsymbol{z} = (u(x,t), v(x,t), w(x,t))^T, \qquad \boldsymbol{h} = (h_1(x,t), h_2(x,t), h_3(x,t))^T,$$

and the symbol $\times$ denotes the cross product of vectors [15].

We rewrite (2.16) as

$$\boldsymbol{z}_t = A(\boldsymbol{z}_{xx})\boldsymbol{z} + A(\boldsymbol{h})\boldsymbol{z}, \tag{2.17}$$

where $A(\boldsymbol{z}_{xx})$ and $A(\boldsymbol{h})$ are both antisymmetric matrices:

$$A(\boldsymbol{z}_{xx}) = \begin{pmatrix} 0 & w_{xx} & -v_{xx} \\ -w_{xx} & 0 & u_{xx} \\ v_{xx} & -u_{xx} & 0 \end{pmatrix}, \quad A(\boldsymbol{h}) = \begin{pmatrix} 0 & h_3 & -h_2 \\ -h_3 & 0 & h_1 \\ h_2 & -h_1 & 0 \end{pmatrix}.$$

We will work with a uniform grid of points $x_i = i\Delta x,\ \Delta x = \frac{L}{N},\ i = 0, 1, \ldots, N-1$.

Let

$$U = (u_0, u_1, \ldots, u_{N-1})^T, \quad V = (v_0, v_1, \ldots, v_{N-1})^T,$$
$$W = (w_0, w_1, \ldots, w_{N-1})^T, \quad Z = (U^T, V^T, W^T)^T,$$

where $u_i \approx u(i\Delta x, t),\ v_i \approx v(i\Delta x, t), w_i \approx w(i\Delta x, t),\ i = 0, 1, \ldots, N-1$.

First, we consider the finite difference discretizations. Denote the $2m$th order central difference discretizations of D_{xx} by $\mathcal{D}(2m)$ [10].

$$\mathcal{D}(2m) = -\Delta_+\Delta_- \sum_{j=0}^{m-1} (-1)^j \beta_j \left(\frac{\Delta x^2 \Delta_+ \Delta_-}{4} \right)^j, \tag{2.18}$$

where $\beta_j = [(j!)^2 2^{2j}]/[(2j+1)!(j+1)]$ and Δ_+ and Δ_- are forward and backward difference operators, respectively.

Now we obtain a semidiscrete system of (2.17) with $2m$th order central difference space discretizations

$$\frac{dZ}{dt} = \tilde{f}_{2m}(Z)Z. \tag{2.19}$$

Here $\tilde{f}_{2m}(Z)$ is an antisymmetric matrix given by

$$\tilde{f}_{2m}(Z) = \begin{pmatrix} 0 & D_w & -D_v \\ -D_w & 0 & D_u \\ D_v & -D_u & 0 \end{pmatrix} + \begin{pmatrix} 0 & D_{h_3} & -D_{h_2} \\ -D_{h_3} & 0 & D_{h_1} \\ D_{h_2} & -D_{h_1} & 0 \end{pmatrix},$$

where D_u, D_v, D_w and $D_{h_1}, D_{h_2}, D_{h_3}$ are both $N \times N$ diagonal matrices defined by

$$\begin{aligned} D_u &= \mathrm{diag}\{d_u^i\}, \quad d_u^i = \mathcal{D}(2m)u_i, \quad i = 0, 1, \ldots, N-1, \\ D_v &= \mathrm{diag}\{d_v^i\}, \quad d_v^i = \mathcal{D}(2m)v_i, \quad i = 0, 1, \ldots, N-1, \\ D_w &= \mathrm{diag}\{d_w^i\}, \quad d_w^i = \mathcal{D}(2m)w_i, \quad i = 0, 1, \ldots, N-1, \end{aligned}$$

and

$$\begin{aligned} D_{h_1} &= \mathrm{diag}\{d_{h_1}^i\}, \quad d_{h_1}^i = h_1(i\Delta x, t), \quad i = 0, 1, \ldots, N-1, \\ D_{h_2} &= \mathrm{diag}\{d_{h_2}^i\}, \quad d_{h_2}^i = h_2(i\Delta x, t), \quad i = 0, 1, \ldots, N-1, \\ D_{h_3} &= \mathrm{diag}\{d_{h_3}^i\}, \quad d_{h_3}^i = h_3(i\Delta x, t), \quad i = 0, 1, \ldots, N-1. \end{aligned}$$

Now, consider the Fourier pseudospectral space discretizations. Using the Fourier pseudospectral method, we obtain another semidiscrete system of (2.17) with exponential order space discretizations

$$\frac{dZ}{dt} = \tilde{f}_{\exp}(Z)Z. \tag{2.20}$$

Here $\tilde{f}_{\exp}(Z)$ is an antisymmetric matrix given by

$$\tilde{f}_{\exp}(Z) = \begin{pmatrix} 0 & \bar{D}_w & -\bar{D}_v \\ -\bar{D}_w & 0 & \bar{D}_u \\ \bar{D}_v & -\bar{D}_u & 0 \end{pmatrix} + \begin{pmatrix} 0 & D_{h_3} & -D_{h_2} \\ -D_{h_3} & 0 & D_{h_1} \\ D_{h_2} & -D_{h_1} & 0 \end{pmatrix},$$

where $\bar{D}_u, \bar{D}_v$, and $\bar{D}_w$ are $N \times N$ diagonal matrices defined by

$$\begin{aligned} \bar{D}_u &= \mathrm{diag}\{\bar{d}_u^i\}, \quad \bar{d}_u^i = (D_2 U)_i, \quad i = 0, 1, \ldots, N-1, \\ \bar{D}_v &= \mathrm{diag}\{\bar{d}_v^i\}, \quad \bar{d}_v^i = (D_2 V)_i, \quad i = 0, 1, \ldots, N-1, \\ \bar{D}_w &= \mathrm{diag}\{\bar{d}_w^i\}, \quad \bar{d}_w^i = (D_2 W)_i, \quad i = 0, 1, \ldots, N-1. \end{aligned}$$

Here D_2 is the second order spectral differentiation matrix.

Now using finite difference and Fourier pseudospectral methods, we have obtained a semidiscrete system of (2.16) in the form

$$\begin{aligned} \frac{dZ}{dt} &= \tilde{f}(Z)Z, \\ Z(0) &= Z^0, \end{aligned} \tag{2.21}$$

where $f(Z)$ is an antisymmetric matrix, $\tilde{f}(Z) \in \mathbf{so}(N)$. The system (2.21) is a system of ordinary differential equations evolving on a sphere with radius $\|Z^0\|$:

$$\|Z^0\| = \sqrt{\sum_{i=0}^{N-1} (u^2(i\Delta x, 0) + v^2(i\Delta x, 0) + w^2(i\Delta x, 0))}.$$

Lie-group methods are numerical methods for ordinary differential equations evolving on homogeneous manifolds. The numerical solution obtained by Lie-group methods evolves on the same manifold as the analytical solution. Applying Lie-group methods to (2.15) or (2.21) results in square-conservative schemes for the KdV equation or the system of a ferromagnetic chain.

3. Lie-group methods and square-conservative schemes. We first present Lie-group methods briefly. For details, we refer the reader to [4, 6, 7, 8, 9]. Lie-group methods are numerical methods designed to integrate ordinary differential equations evolving on homogeneous spaces numerically so that the numerical solution evolves on the same homogeneous spaces. Homogeneous spaces are manifolds on which there exists a transitive Lie-group action.

Suppose that $\mathcal{M}$ is a homogeneous space. $\mathbf{g}$ is a Lie algebra and $\lambda : \mathbf{g} \times \mathcal{M} \to \mathcal{M}$ is a Lie algebra action. Using the Lie algebra action, for each element $v \in \mathbf{g}$ we can obtain a vector field on $\mathcal{M}$ such that

$$(\lambda_* v)(y) = \left.\frac{d}{dt}\right|_{t=0} \lambda(tv, y), \quad y \in \mathcal{M}, \tag{3.1}$$

where $\lambda_* : \mathbf{g} \to \mathcal{X}(\mathcal{M})$ denotes the correspondence between $\mathbf{g}$ and $\mathcal{X}(\mathcal{M})$. $\mathcal{X}(\mathcal{M})$ is the set of all vector fields on $\mathcal{M}$.

Let $f : \mathbf{R} \times \mathcal{M} \to \mathbf{g}$ be a smooth function. Using λ_*, we consider the differential equation on $\mathcal{M}$ in the form

$$y' = (\lambda_* f(t, y))(y), \quad y(0) = y_0, \quad y(t) \in \mathcal{M}, \quad t \geq 0. \tag{3.2}$$

There are various Lie-group methods. Here we are concerned only with the most general Runge–Kutta–Munthe–Kaas (RKMK) methods [7, 8, 9]. The basic idea of this method is to solve a differential equation in the Lie algebra instead of (3.2). Using the concept of *ϕ-relatedness* of vector fields, we can prove that the solution of (3.2) is

$$y(t) = \lambda(\sigma(t), y_0) = \exp(\sigma(t))y_0. \tag{3.3}$$

Here exp is the exponential map and $\sigma(t)$ satisfies an equation evolving on the Lie algebra $\mathbf{g}$:

$$\sigma' = dexp_\sigma^{-1}(f(t, \lambda(\sigma, y_0))), \quad \sigma(0) = 0, \quad \sigma(t) \in \mathbf{g}, \quad t \geq 0. \tag{3.4}$$

Here $dexp_\sigma^{-1} : \mathbf{g} \to \mathbf{g}$ is a map in $\mathbf{g}$ and given by

$$dexp_\sigma^{-1}(v) = v - \frac{1}{2} ad_\sigma(v) + \sum_{k=2}^{\infty} \frac{B_k}{k!} ad_\sigma^k(v), \tag{3.5}$$

where B_k is the kth Bernoulli number, $ad_\sigma^0(v) = v, ad_\sigma(v) = [\sigma, v]$, and in general

$$ad_\sigma^k(v) = ad_\sigma^{k-1}(ad_\sigma(v)).$$

The procedure for a qth order RKMK method for (3.2) involves three steps. First, we approximate $dexp_\sigma^{-1}$ by

$$dexpinv(\sigma, v) = v - \frac{1}{2}[\sigma, v] + \sum_{k=2}^{q-1} \frac{B_k}{k!} ad_\sigma^k(v). \tag{3.6}$$

Second, we apply an s-stage qth order Runge–Kutta method to the approximate equation

$$\sigma' = dexpinv(\sigma, f(t, \lambda(\sigma, y_0))), \quad \sigma(0) = 0, \tag{3.7}$$

and obtain

$$\begin{aligned} \Sigma_i &= \Delta t \sum_{j=1}^{s} a_{ij} dexpinv(\Sigma_j, f(c_j \Delta t, \lambda(\Sigma_j, y_0))), \\ \sigma_1 &= \Delta t \sum_{i=1}^{s} b_i dexpinv(\Sigma_i, f(c_i \Delta t, \lambda(\Sigma_i, y_0))). \end{aligned} \tag{3.8}$$

Here a_{ij}, b_i, and c_i are the coefficients of the Runge–Kutta method, Δt is the time steplength, and $\sigma_1 \approx \sigma(\Delta t)$.

In this second step, it is required that $\sigma_1 \in \mathbf{g}$. If an explicit Runge–Kutta method is applied, this requirement is automatically satisfied since in this case all operations involved are the operations in the Lie algebra: sums, scalar, and Lie brackets. If an implicit Runge–Kutta method is applied, we must choose an appropriate iterative method such as fixed point iteration to fulfill this requirement.

Finally, the Lie algebra action is computed approximately (sometimes exactly) and the numerical solution is obtained:

$$y_1 = \lambda(\sigma_1, y_0) = r(\sigma_1) y_0, \quad r(\sigma_1) = \exp(\sigma_1) + \mathcal{O}(\sigma_1^{q+1}). \tag{3.9}$$

Here $r(z)$ is a qth order approximation of $\exp(z)$. In this final step for a qth order RKMK method for (3.2), it is required that $r(\sigma_1) \in G$ (the Lie group corresponding to $\mathbf{g}$). There exist many choices of $r(z)$ to fulfill this requirement. In the end, we obtain a qth order numerical solution $y_1 \in \mathcal{M}$.

Now we come back to the semidiscrete system (2.15) for the KdV equation. The system (2.15) is a system of ordinary differential equations evolving on an $(N-1)$-dimensional sphere. An $(N-1)$-dimensional sphere is a homogeneous space with Lie group $O(N)$ and Lie algebra $\mathbf{so}(N)$.

Therefore, if we apply a qth order RKMK method to the semidiscrete equation (2.15) of the KdV equation, a qth order square-conservative scheme can be obtained:

$$\begin{aligned} \frac{dU}{dt} &= f(U)U, \\ \Sigma_i &= \Delta t \sum_{j=1}^{s} a_{i,j} dexpinv(\Sigma_j, f(\exp(\Sigma_j) U^0)), \\ \sigma_1 &= \Delta t \sum_{i=1}^{s} b_i dexpinv(\Sigma_i, f(\exp(\Sigma_i) U^0)), \\ U^1 &= r(\sigma_1) U^0, \quad r(z) = \exp(z) + \mathcal{O}(z^{q+1}), \end{aligned} \tag{3.10}$$

where $f(U)$ is either $f_q(U)$ for the qth order finite difference space discretization or $f_{\exp}(U)$ for the Fourier pseudospectral space discretization, and $r(z)$ is the qth order diagonal Padé approximation of $\exp(z)$.

We know that $r(v) \in O(N)$ if $v \in \mathbf{so}(N)$. Therefore, (3.10) is indeed a qth order square-conservative scheme of the KdV equation.

Particularly, if we use first order RKMK method in (3.10) where the first order Runge–Kutta method is the explicit Euler method and $r(z)$ is the first order diagonal Padé approximation, (3.10) takes the form

$$\frac{U^1 - U^0}{\Delta t} = f(U^0)\frac{U^1 + U^0}{2}. \tag{3.11}$$

Equation (3.11) is just the first order square-conservative scheme (4.3.5) in [11]. This indicates that our qth order square-conservative scheme is indeed the generalization of the usual square-conservative schemes for the KdV equation.

The drawback of (3.10) is its relatively expensive cost of computations. Fortunately, we can use the Cayley coordinates because $\mathbf{so}(N)$ is a quadratic Lie algebra. If we use the Cayley coordinates, the solution of (3.2) with a quadratic Lie algebra can be written as

$$y(t) = Cay(\sigma(t))y_0 = \frac{1 + \frac{\sigma(t)}{2}}{1 - \frac{\sigma(t)}{2}}y_0. \tag{3.12}$$

Here Cay is the Cayley transformation and σ satisfies

$$\sigma' = dcay_\sigma^{-1}(f(t, \lambda(\sigma, y_0))), \quad \sigma(0) = 0, \quad \sigma(t) \in \mathbf{g}, \quad t \geq 0, \tag{3.13}$$

where $dcay_\sigma^{-1} : \mathbf{g} \to \mathbf{g}$ is a map in $\mathbf{g}$ and given by

$$dcay_\sigma^{-1}(v) = v - \frac{1}{2}[\sigma, v] - \frac{1}{4}\sigma \cdot v \cdot \sigma, \tag{3.14}$$

where $\cdot$ denotes the multiplication of matrix. Using the Cayley coordinates, we need approximation only once rather than three times in the exponential coordinates case for a qth order RKMK method. Therefore, the procedure for a qth order RKMK method for (3.2) using Cayley coordinates involves two steps. First, we apply an s-stage qth order Runge–Kutta method to the equation

$$\sigma' = dcay^{-1}(\sigma, f(t, \lambda(\sigma, y_0))), \quad \sigma(0) = 0, \tag{3.15}$$

and obtain

$$\begin{aligned} \Sigma_i &= \Delta t \sum_{j=1}^{s} a_{ij} dcay^{-1}(\Sigma_j, f(c_j \Delta t, \lambda(\Sigma_j, y_0))), \\ \sigma_1 &= \Delta t \sum_{i=1}^{s} b_i dcay^{-1}(\Sigma_i, f(c_i \Delta t, \lambda(\Sigma_i, y_0))). \end{aligned} \tag{3.16}$$

Here a_{ij}, b_i, and c_i are the coefficients of the Runge–Kutta method, Δt is the time steplength, and $\sigma_1 \approx \sigma(\Delta t)$.

Second, the Lie algebra action is computed exactly and the numerical solution is obtained:

$$y_1 = Cay(\sigma_1)y_0 = \frac{1 + \frac{\sigma_1}{2}}{1 - \frac{\sigma_1}{2}}y_0. \tag{3.17}$$

Using Cayley coordinates, we can obtain a qth order square-conservative scheme for the KdV equation:

$$\begin{aligned}
\frac{dU}{dt} &= f(U)U,\\
\Sigma_i &= \Delta t \sum_{j=1}^{s} a_{i,j} dcay^{-1}(\Sigma_j, f(Cay(\Sigma_j)U^0)),\\
\sigma_1 &= \Delta t \sum_{i=1}^{s} b_i dcay^{-1}(\Sigma_i, f(Cay(\Sigma_i)U^0)),\\
U^1 &= Cay(\sigma_1)U^0,
\end{aligned} \tag{3.18}$$

where $f(U)$ is either $f_q(U)$ for the qth order finite difference space discretization or $f_{\exp}(U)$ for the Fourier pseudospectral space discretization. It should be noted that the Cayley coordinates suffer from a potential problem of mapping matrices with one/several eigenvalues approaching -1.

The scheme (3.18) is more preferable to the scheme (3.10) because of its less expensive computational cost.

For the semidiscrete system (2.21) of a ferromagnetic chain, we can make the same discussions. Applying a qth RKMK method in Cayley coordinates, we can obtain a qth order square-conservative scheme for the system of a ferromagnetic chain.

4. Numerical experiments. In this section, we test our qth order square-conservative scheme (3.18) for the KdV equation

$$u_t = -uu_x - 0.022^2 u_{xxx}, \tag{4.1}$$

with initial condition

$$u(x,0) = \cos(\pi x), \qquad 0 \le x \le 2, \tag{4.2}$$

and periodic boundary condition $u(0,t) = u(2,t)$.

In order to compare (3.18) with the Zabusky–Kruskal scheme which is of second order [14], we apply the second order square-conservative scheme (3.18) in which a second order Runge–Kutta method ($a_{11} = a_{12} = 0, a_{21} = \frac{1}{2}, a_{22} = 0; b_1 = 0, b_2 = 1$) is used.

In Figure 1, waveforms at $\pi t = 1$ and $\pi t = 3.6$ with different spacings are shown. We use the time steplength $\Delta t = \frac{0.004}{\pi}$. We see that waveforms with different spacings are basically the same, which is a result of nonlinear stability of (3.18). If we continue to use larger spacing, say, $\Delta x = 2/100$, small oscillation occurs. In this case, the use of a smaller time steplength cannot eliminate the oscillation (see Figure 2), which indicates an inadequate space resolution with $\Delta x = 2/100$. To further demonstrate the stability of (3.18), we simulate the temporal development of the waveform over long time intervals. In Figure 3, the waveform at $\pi t = 34$ is shown. A train of solitons is clearly observed. In our simulation, we use $\Delta x = \frac{2}{200}$. The discrete square-conservative law is also shown in Figure 3. As is expected, the scheme (3.18) preserves the discrete square-conservative law exactly.

Now we compare (3.18) with the Zabusky–Kruskal scheme

$$\begin{aligned}
u_i^{j+1} = u_i^{j-1} - &\frac{\Delta t}{3\Delta x}(u_{i+1}^j + u_i^j + u_{i-1}^j)(u_{i+1}^j - u_{i-1}^j)\\
&- \frac{0.022^2 \Delta t}{\Delta x^3}(u_{i+2}^j - 2u_{i+1}^j + 2u_{i-1}^j - u_{i-2}^j).
\end{aligned} \tag{4.3}$$

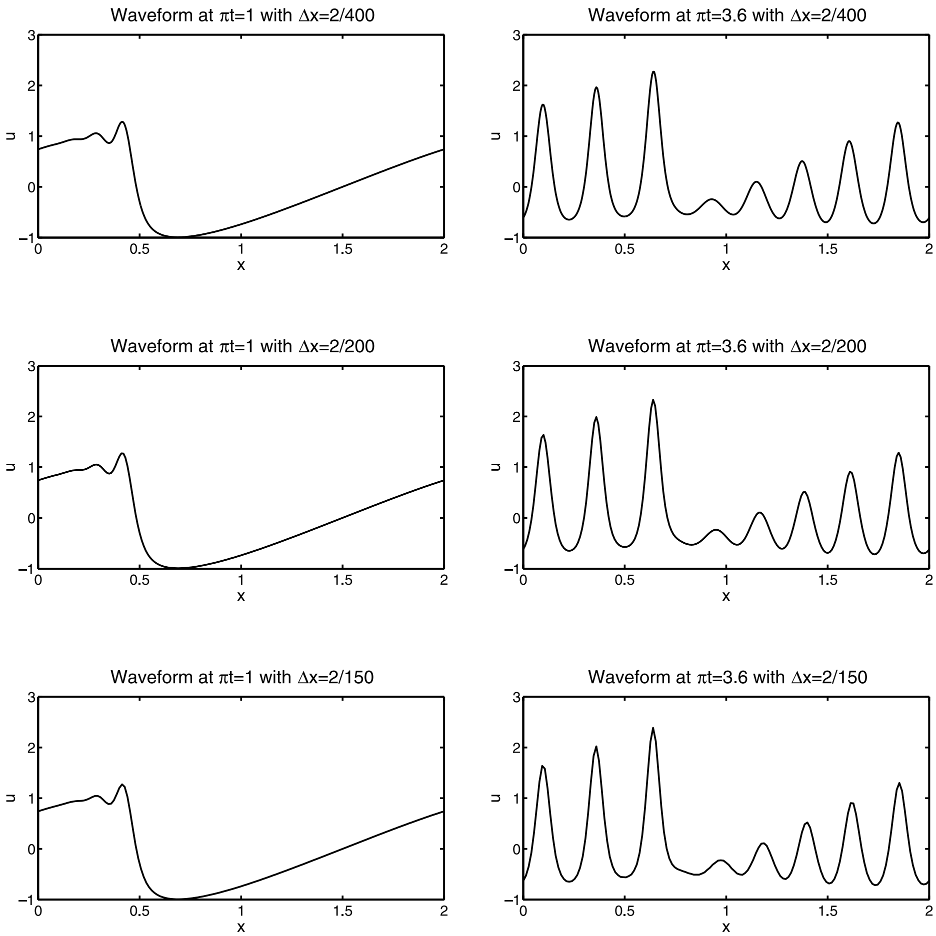

FIG. 1. *Temporal development of waveforms with different spacings.*

The scheme (4.3) satisfies the quasi–square-conservative law

$$\sum_{i=0}^{N-1} u_i^{j+1} u_i^j = \sum_{i=0}^{N-1} u_i^j u_i^{j-1}. \tag{4.4}$$

In Figure 4, the temporal development of waveforms obtained with (3.18) is shown. We use $\Delta x = \frac{2}{300}$ and $\Delta t = \frac{0.0004}{\pi}$. In Figure 5, we show the temporal development of waveforms obtained with (4.3) and use the same space and time steplength. At $\pi t < 16$, the waveforms obtained with the two schemes agree with each other very well. About at $\pi t = 16$, the waveforms by (4.3) begin to exhibit oscillations near $x = 1.4$, and then the oscillations quickly become very large and lead to overflow. In fact, although satisfying (4.4), the scheme (4.3) is instable [1]. The scheme (3.18) is nonlinearly stable and can simulate the temporal development of waveforms for a very long time.

We also compare (3.18) in Cayley coordinates with (3.10) in exponential coordinates. We find that the scheme (3.18) is much more efficient than the scheme (3.10) for

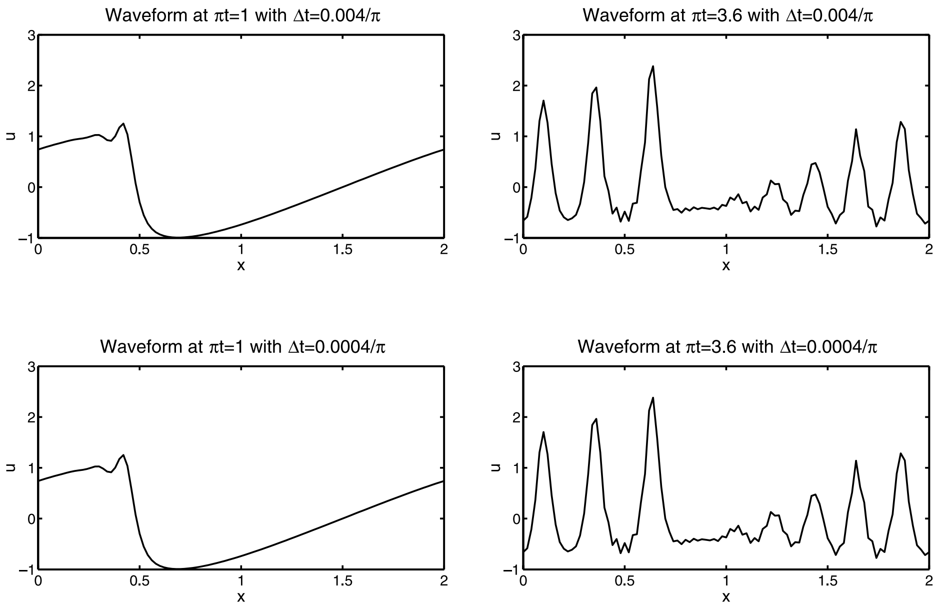

FIG. 2. *Temporal development of waveforms with* $\Delta x = \frac{2}{100}$.

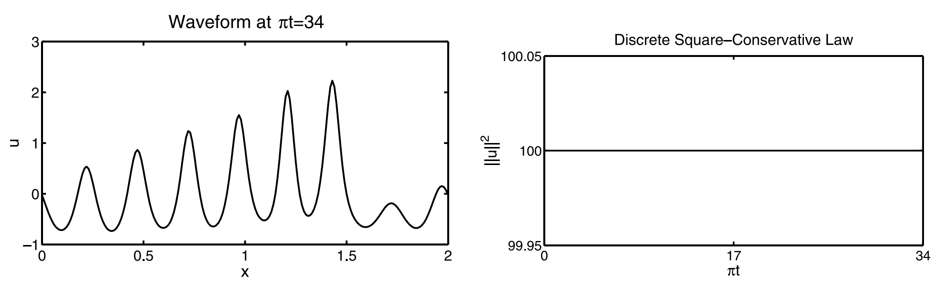

FIG. 3. *The waveform at* $\pi t = 34$ *and the discrete square-conservative law.*

high order methods. This is because for high order methods the approximate equation in Lie algebra in (3.10) becomes very complicated and the high order approximation of the exponential is very expensive, whereas in (3.18) we do not need to approximate the Lie algebra equation, and the Lie algebra action (Cayley transformation) can be computed exactly.

5. Conclusions. In this paper, we present a new method for constructing square-conservative schemes for square-conservative systems. Using the Lie-group method, general qth order square-conservative schemes in both Cayley coordinates and exponential coordinates for the KdV equation and the system of a ferromagnetic chain are constructed. Numerical experiments with the KdV equation show that the scheme has remarkable stability.

The subject of this paper is the application of Lie-group methods to partial differential equations. The basic strategy is to first discretize the space variable appropriately and obtain a semidiscrete system evolving on a desired manifold. In order to construct square-conservative schemes for square-conservative systems, we discretize

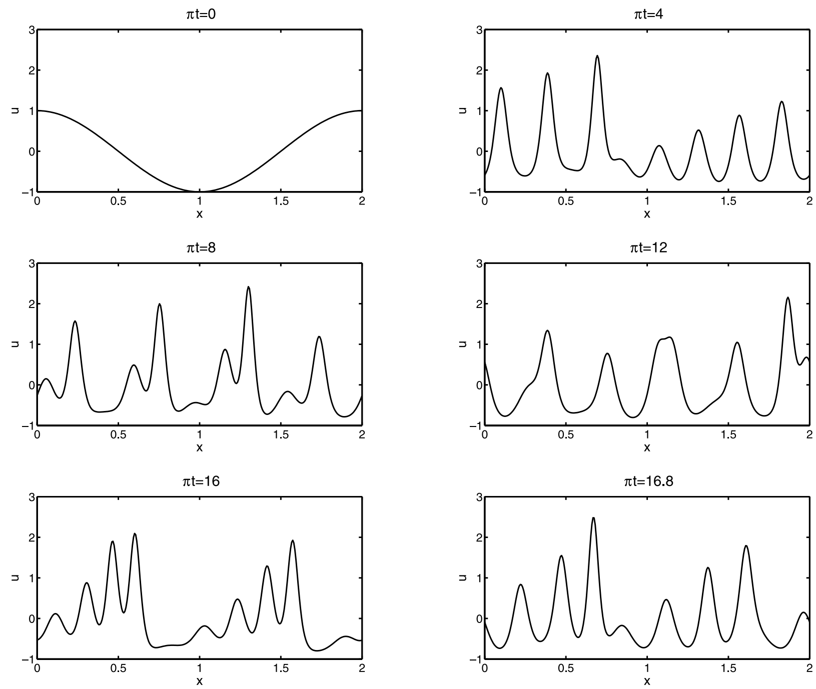

FIG. 4. *Temporal development of waveforms obtained with* (3.18).

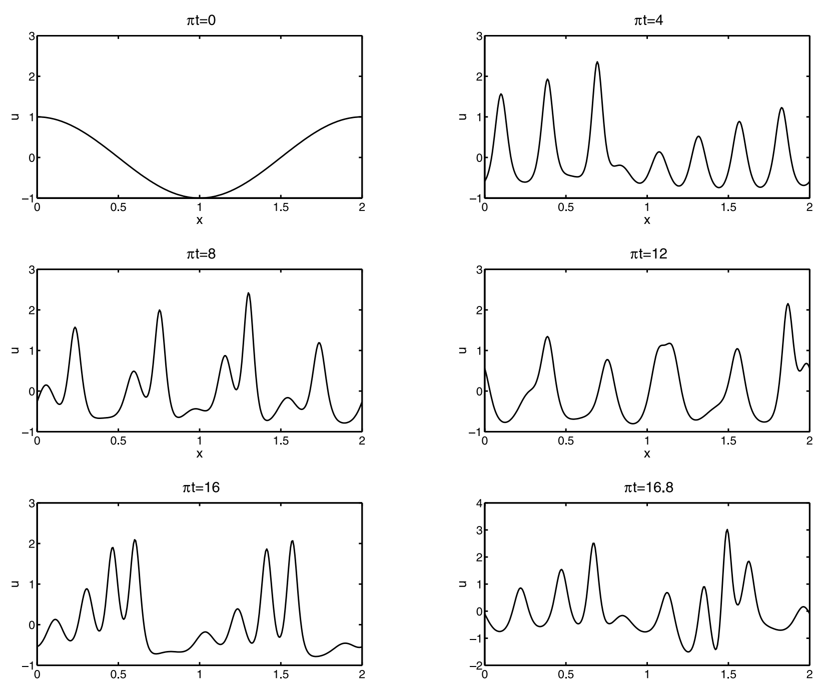

FIG. 5. *Temporal development of waveforms obtained with* (4.3).

the space variable and obtain a semidiscrete system evolving on a sphere. Based on the Lax formulation of the KdV equation, Celledoni obtained a semidiscrete system which evolves on an isospectral manifold and tested the performance of Lie-group integrators as applied to the semidiscrete system [2]. Of course, for concrete systems, we can obtain semidiscrete systems evolving on concrete manifolds and then apply the corresponding Lie-group methods.

Acknowledgments. The authors are very grateful to the referees for valuable suggestions and corrections and referring us to reference [2].

REFERENCES

[1] K. Abe and O. Inoue, *Fourier expansion solution of the Korteweg-de Vries equation*, J. Comput. Phys., 34 (1980), pp. 202–210.

[2] E. Celledoni, *A note on the numerical integration of the KdV equation via isospectral deformations*, J. Phys. A, 34 (2001), pp. 2205–2214.

[3] J. B. Chen and M. Z. Qin, *Multi-symplectic Fourier pseudospectral method for the nonlinear Schrödinger equation*, Electron. Trans. Numer. Anal., 12 (2001), pp. 193–204.

[4] K. Engø, *On the construction of geometric integrators in the RKMK class*, BIT, 40 (2000), pp. 41–61.

[5] D. Gottlieb, M. Y. Hussaini, and S. A. Orszag, *Theory and applications of spectral methods*, in Spectral Methods for Partial Differential Equations, R. G. Voigt, D. Gottlieb, and M. Y. Hussaini, eds., SIAM, Philadelphia, 1984, pp. 1–54.

[6] A. Iserles, H. Z. Munthe-Kaas, S. P. Nørsett, and A. Zanna, *Lie-group methods,* Acta Numer., 9 (2000), pp. 215–365.

[7] H. Z. Munthe-Kaas, *Lie-Butcher theory for Runge-Kutta methods,* BIT, 35 (1995), pp. 572–587.

[8] H. Z. Munthe-Kaas, *Runge-Kutta methods on Lie groups*, BIT, 38 (1998), pp. 92–111.

[9] H. Z. Munthe-Kaas, *High order Runge-Kutta methods on manifolds,* Appl. Numer. Math., 29 (1999), pp. 115–127.

[10] M. Z. Qin and W. J. Zhu, *Construction of symplectic schemes for wave equation via hyperbolic functions sinh(x), cosh(x) and tanh(x)*, Comput. Math. Appl., 26 (1993), pp. 1–11.

[11] M. Z. Qin, *An implicit scheme for nonlinear evolution equations,* J. Comput. Phys., 48 (1982), pp. 57–71.

[12] R. D. Richtmyer and K. W. Morton, *Difference Methods for Initial-Value Problems*, Interscience, New York, 1967.

[13] J. W. Thomas, *Numerical Partial Differential Equation*, Springer-Verlag, New York, 1995.

[14] N. J. Zabusky and M. D. Kruskal, *Interaction of 'solitons' in a collisionless plasma and the recurrence of initial states*, Phys. Rev. Lett., 15 (1965), pp. 240–243.

[15] Y. L. Zhou and B. L. Guo, *Finite difference solution of the boundary problems for the system of ferro-magnetic chain*, J. Comput. Math., 1 (1983), pp. 294–302.