International Journal of Pure and Applied Mathematics

Volume 40 No. 3 2007, 341-366

STRUCTURE PRESERVING SCHEMES FOR BIRKHOFFIAN SYSTEMS

H.L. Su[1], Y.J. Sun[2], M.Z. Qin[3], R. Scherer[4 §]

[1]Department of Mathematics
Remin University
Beijing, 100080, P.R. CHINA

[2,3]Institute of Computational Mathematics and
Scientific/Engineering Computing
Academy of Mathematics and System Sciences
Academic Sinica
B.O. Box 2719, Beijing, 100080, P.R. CHINA
[3]e-mail: qmz@lsec.cc.ac.cn

[4]Institute of Applied and Numerical Mathematics
University of Karlsruhe
Karlsruhe, 76128, GERMANY
e-mail: scherer@math.uni-karlsruhe.de

Abstract: A universal symplectic structure for a Newtonian system including nonconservative cases can be constructed in the framework of Birkhoffian generalization of Hamiltonian mechanics. In this paper the symplectic geometry structure of Birkhoffian system is discussed, then the symplecticity of Birkhoffian phase flow is presented. Based on these properties, a way to construct symplectic schemes for Birkhoffian systems by using the generating function method is explained.

AMS Subject Classification: 65P10
Key Words: Birkhoffian system, method of generating function, symplectic difference schemes, linear and semilinear oscillator equation

1. Introduction

Birkhoffian representation is the generalization of Hamiltonian representation,

Received: August 12, 2007

§Correspondence author

which can be applied to hadron physics, statistical mechanics, space mechanics, engineering, biophysics, etc. (Santilli [13, 14]). All conservative or nonconservative, self-adjoint or non self-adjoint, unconstrained or nonholonomic constrained systems always admit a Birkhoffian representation (Guo [6], Santilli [14]). In last 20 years, many researchers have studied Birkhoffian mechanics and obtained a series of results in integral theory, stability of motion, inverse problem, algebraic and geometric description, etc.

Birkhoff's equations are more complex than Hamilton's equations, and so is the study of their computational methods. In the past, there are not any result on computational methods for Birkhoffian system. The known difference methods are not generally applicable to Birkhoffian system. As a difference scheme to solve Hamiltonian system should be Hamiltonian scheme (Hairer, Lubich and Wanner [7], Sanz-Serna and Calvo [12]), a difference scheme to simulate Birkhoffian system should be a Birkhoffian scheme. However, the conventional difference schemes such as Euler's midpoint scheme, leap-frog scheme etc. are not Birkhoffian schemes. So a way to systematically construct a Birkhoffian scheme is necessary, and this is the main context in this paper.

Both, the Birkhoffian and Hamiltonian systems are usually of finite dimensional (Arnold [1], Marsden and Ratiu [8]), infinite dimension Birkhoffian system has not been proposed before. The algebraic and geometric profiles of finite dimensional Birkhoffian systems are described in local coordinates, and general nonautonomous Hamiltonian systems are considered as autonomous Birkhoffian systems (Santilli [14]). Symplectic schemes are systematically developed for standard Hamiltonian systems and for general Hamiltonian systems on Poisson manifold or those with $K(z)$-symplectic structure, which belong to autonomous and semi-autonomous Birkhoffian systems (Feng and Wang [3], Feng and Qin [5]). So in this paper, we just discuss the nonautonomous Birkhoffian system in detail. Thereby, Einstein's summation convention is used.

In Section 2, Birkhoffian systems are sketched out via variational self-adjointness. It shows the relationship between Birkhoffian and Hamiltonian systems more essentially and directly. Then the basic geometrical properties of Birkhoffian systems are presented. In Section 3, the definition of $\widetilde{K}(\hat{z}, z)$-Lagrangian submanifold is extended to $\widetilde{K}(\hat{z}, z, t, t_0)$-Lagrangian submanifold with parameter t. Then the relationship between $K(z, t)$-symplectic mappings and gradient mappings is discussed. In Section 4, the generating functions for the phase flow of the Birkhoffian systems are constructed and the method to simulate Birkhoffian systems by symplectic schemes of any order is given. Section 5 contains an illustrating example. Schemes of order one, two and four are derived for the linear damped oscillator. In the last section, numerical experiments are given.

2. Birkhoffian Systems

The generalization of Hamilton's equations is given by

$$\left(\frac{\partial F_j}{\partial z_i} - \frac{\partial F_i}{\partial z_j}\right)\frac{\mathrm{d}z_j}{\mathrm{d}t} - \left(\frac{\partial B(z,t)}{\partial z_i} + \frac{\partial F_i(z,t)}{\partial t}\right) = 0, \quad i,j = 1,2,\dots,2n, \tag{2.1}$$

where the following abbreviations

$$K_{ij} = \frac{\partial F_j}{\partial z_i} - \frac{\partial F_i}{\partial z_j}, \quad K = (K_{ij})_{i,j=1,\dots,2n}$$

are further used. Following the terminology suggested by Santilli [14], this is called Birkhoff's equations or Birkhoffian system under some additional assumptions. The function $B(z,t)$ is called the Birkhoffian, because of certain physical difference with Hamiltonian. The F_i, $i = 1,2,\dots,2n$, are Birkhoffian functions. A representation of Newton's equations via Birkhoff's equations is called a Birkhoffian representation.

Definition 2.1. Birkhoff's equations (2.1) are called autonomous when the functions F_i and B are independent of the time variable. In this case the equations are of the simple form

$$K_{ij}(z)\frac{\mathrm{d}z_j}{\mathrm{d}t} - \frac{\partial B(z)}{\partial z_i} = 0. \tag{2.2}$$

They are called semi-autonomous when the functions F_i do not depend explicitly on time. In this case the equations have the more general form

$$K_{ij}(z)\frac{\mathrm{d}z_j}{\mathrm{d}t} - \frac{\partial B(z,t)}{\partial z_i} = 0.$$

They are called nonautonomous when both the functions F_i and B explicitly dependent on time. In this case the equations read

$$K_{ij}(z,t)\frac{\mathrm{d}z_j}{\mathrm{d}t} - \frac{\partial B(z,t)}{\partial z_i} - \frac{\partial F_i(z,t)}{\partial t} = 0. \tag{2.3}$$

They are called regular when the functional determinant is unequal to zero in the region considered, i.e.,

$$\det(K_{ij})(\widetilde{\Re}) \neq 0,$$

otherwise, degenerate.

Given an arbitrary analytic and regular first-order system

$$K_{ij}(z,t)\frac{\mathrm{d}z_j}{\mathrm{d}t} + \mathcal{D}_i(z,t) = 0, \quad i,j = 1,2,\ldots,2n, \tag{2.4}$$

which is self-adjoint if and only if it satisfies the following conditions in a star-shaped region $\widetilde{\Re}^*$ for $i,j = 1,2,\ldots,2n$ (see [2]):

$$\begin{aligned} &K_{ij} + K_{ji} = 0,\\ &\frac{\partial K_{ij}}{\partial z_k} + \frac{\partial K_{jk}}{\partial z_i} + \frac{\partial K_{ki}}{\partial z_j} = 0,\\ &\frac{\partial K_{ij}}{\partial t} = \frac{\partial \mathcal{D}_i}{\partial z_j} - \frac{\partial \mathcal{D}_j}{\partial z_i}. \end{aligned} \tag{2.5}$$

We now simply introduce the geometric significance of the condition of variational self-adjointness (see [10, 15]). Here the region considered is a star-shaped region $\widetilde{\Re}^*$ of points of $R \times T^*M$, T^*M the cotangent space of the M, M a 2n-dimensional manifold. The geometric significance of the condition of self-adjointness (2.5) is the relationship to the integrability condition for a 2-form to be an exact symplectic form.

Consider first the case for which $K_{ij} = K_{ij}(z)$. Given a symplectic structure written as the 2-form in local coordinates

$$\Omega = \sum_{i,j=1}^{2n} K_{ij}(z)\mathrm{d}z_i \wedge \mathrm{d}z_j.$$

One of the fundamental properties of symplectic form is that $\mathrm{d}\Omega = 0$. Because the exact character of two-form implies that

$$\Omega = \mathrm{d}(F_i \mathrm{d}z_i), \tag{2.6}$$

this geometric property is fully characterized by the first two equations of condition (2.5); i.e., the two-form (2.6) describes the geometrical structure of the autonomous case (2.2) of the Birkhoff's equations, it even sketches out the geometric structure of the semi-autonomous case.

For the case $K_{ij} = K_{ij}(z,t)$, the full set of condition (2.5) must be considered. The corresponding geometric structure can be better expressed by transition of the symplectic geometry on the cotangent bundle T^*M with local coordinates z_i to the contact geometry on the manifold $R \times T^*M$ with local coordinates $\widetilde{z}_i$, $i = 0,1,2,\ldots,2n$, $\widetilde{z}_0 = t$ (see [14]). More general formulations of an exact contact 2-form exist, although it is now referred to as a $(2n+1)$-

dimensional space,

$$\widehat{\Omega} = \sum_{i,j=0}^{2n} \widehat{K}_{ij} \mathrm{d}\widetilde{z}_i \wedge \mathrm{d}\widetilde{z}_j = \Omega + 2\mathcal{D}_i \mathrm{d}z_i \wedge \mathrm{d}t,$$

where

$$\widehat{K} = \begin{pmatrix} 0 & -\mathcal{D}^{\mathrm{T}} \\ \mathcal{D} & K \end{pmatrix}, \quad D = (\mathcal{D}_1, \ldots, \mathcal{D}_{2n})^T.$$

If the contact form is also of the exact type

$$\widehat{\Omega} = \mathrm{d}(\widetilde{F}_i \mathrm{d}\widetilde{z}_i), \qquad \widetilde{F}_i = \begin{cases} -B\,, \\ F_i\,, \end{cases} \tag{2.7}$$

the geometric meaning of the condition of the self-adjointness is then the integrability condition for the exact contact structure (2.7). Here B can be calculated from

$$-\frac{\partial B}{\partial z_i} = \mathcal{D}_i + \frac{\partial F_i}{\partial t}$$

for

$$\frac{\partial}{\partial z_j}\left(\mathcal{D}_i + \frac{\partial F_i}{\partial t}\right) = \frac{\partial}{\partial z_i}\left(\mathcal{D}_j + \frac{\partial F_j}{\partial t}\right).$$

All the above discussion can be expressed via the following property.

Theorem 2.1. (Self-Adjointness of Birkhoffian System) *For a general nonautonomous first-order system (2.4) a necessary and sufficient condition for self-adjointness in* $\widetilde{\Re}^*$ *of points of* $R \times T^*R^{2n}$ *is that it is of the Birkhoffian type, i.e., the following representation holds for* $i, j = 1, 2, \ldots, 2n$

$$K_{ij}(z,t)\frac{dz_j}{dt} + \mathcal{D}_i(z,t) = \left(\frac{\partial F_j}{\partial z_i} - \frac{\partial F_i}{\partial z_j}\right)\frac{dz_j}{dt} - \frac{\partial B(z,t)}{\partial z_i} - \frac{\partial F_i(z,t)}{\partial t}. \tag{2.8}$$

Remarks. The functions F_i and B can be calculated according to the rules (see Atherton and Homsy [2])

$$F_i = \int_0^1 \lambda z_j \cdot K_{ji}(\lambda z, t)\mathrm{d}\lambda, \quad B = -\int_0^1 z_i \cdot (\mathcal{D}_i + \frac{\partial F_i}{\partial t})(\lambda z, t)\mathrm{d}\lambda\,,$$

or

$$\widetilde{F}_i = \int_0^1 \lambda \widetilde{z}_j \cdot \widehat{K}_{ji}(\lambda \widetilde{z})\mathrm{d}\lambda.$$

Due to the self-adjointness of Birkhoff's equations, the phase flow of the system

(2.8) conserves the symplecticity

$$\frac{\mathrm{d}}{\mathrm{d}t}\Omega = \frac{\mathrm{d}}{\mathrm{d}t}(K_{ij}\mathrm{d}z_i \wedge \mathrm{d}z_j) = 0.$$

Thereby denoting the phase flow of the equations (2.8) with $(\widehat{z}, t)$ and the initial value (z, t_0) yields

$$K_{ij}(\widehat{z}, t)\mathrm{d}\widehat{z}_i \wedge \mathrm{d}\widehat{z}_j = K_{ij}(z, t_0)\mathrm{d}z_i \wedge \mathrm{d}z_j,$$

respectively the algebraic representation

$$\left(\frac{\partial \widehat{z}}{\partial z}\right)^{\mathrm{T}} K(\widehat{z}, t) \left(\frac{\partial \widehat{z}}{\partial z}\right) = K(z, t_0).$$

In the next sections, the algorithm preserving this geometric property of the phase flow in discrete space will be constructed.

3. Generating Functions for $K(z, t)$-Symplectic Mappings

In this section, general $K(z, t)$-symplectic mappings and their relationship with the gradient mappings and their generating functions are considered (see Feng et al [3, 5]).

Definition 3.1. Let denote

$$J_{2n} = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}, \; J_{4n} = \begin{pmatrix} 0 & I_{2n} \\ -I_{2n} & 0 \end{pmatrix}, \; \widetilde{J}_{4n} = \begin{pmatrix} J_{2n} & 0 \\ 0 & -J_{2n} \end{pmatrix},$$

$$\widetilde{K}(\widehat{z}, z, t, t_0) = \begin{pmatrix} K(\widehat{z}, t) & 0 \\ 0 & -K(z, t_0) \end{pmatrix}.$$

Then a $2n$-dimensional submanifold $L \subset R^{4n}$

$$L = \left\{ \begin{pmatrix} \widehat{z} \\ z \end{pmatrix} \in R^{4n} | z = z(x, t_0), \widehat{z} = \widehat{z}(x, t), x \in U \subset R^{2n}, \text{open set} \right\}$$

is called a J_{4n}-, $\widetilde{J}_{4n}$- or $\widetilde{K}(\widehat{z}, z, t, t_0)$-Lagrangian submanifold if it holds

$$(T_x L)^{\mathrm{T}} J_{4n} (T_x L) = 0, \qquad (T_x L)^{\mathrm{T}} \widetilde{J}_{4n} (T_x L) = 0\,,$$

or

$$(T_x L)^{\mathrm{T}} \widetilde{K}(\widehat{z}, z, t, t_0)(T_x L) = 0,$$

where $T_x L$ is the tangent space to L at x.

Definition 3.2. The mapping with parameters t and t_0 is $z \to \widehat{z} = g(z, t, t_0) : R^{2n} \to R^{2n}$ is called a gradient map or a canonical map or a $K(z, t)$-

symplectic map if its graph

$$\Gamma_g = \left\{ \begin{pmatrix} \widehat{z} \\ z \end{pmatrix} \in R^{4n} | \widehat{z} = g(z, t, t_0), z = z \in R^{2n} \right\}$$

is a J_{4n}- or $\widetilde{J}_{4n}$- or $\widetilde{K}(\widehat{z}, z, t, t_0)$-Lagrangian submanifold.

For differentiable mappings there exists an equivalent definition for the $K(z,t)$-symplecticness, which is also useful for difference schemes.

Definition 3.3. A differentiable mapping $g : M \to M$ is $K(z,t)$-symplectic if

$$\left(\frac{\partial g}{\partial z}\right)^{\mathrm{T}} K(g(z,t,t_0),t) \left(\frac{\partial g}{\partial z}\right) = K(z, t_0).$$

A difference scheme approximating the Birkhoffian system (2.8) with step-size τ

$$z^{k+1} = g^k(z^k, t_k + \tau, t_k), \quad k \geq 0,$$

is called a $K(z,t)$-symplectic scheme, if g^k is $K(z,t)$-symplectic for every k, i.e.,

$$\left(\frac{\partial g^k}{\partial z^k}\right)^{\mathrm{T}} K(z^{k+1}, t_{k+1}) \left(\frac{\partial g^k}{\partial z^k}\right) = K(z^k, t_k).$$

The graph of the phase flow of the Birkhoffian system (2.8) is $g^t(z, t_0) = g(z, t, t_0)$ which is a $\widetilde{K}(\widehat{z}, z, t, t_0)$-Lagrangian submanifold for

$$g_z^t(z, t_0)^{\mathrm{T}} K(g^t(z, t_0), t) g_z^t(z, t_0) = K(z, t_0).$$

Similarly the graph of the phase flow of standard Hamiltonian system is a $\widetilde{J}_{4n}$-Lagrangian submanifold.

Consider the nonlinear transformation with two parameters t and t_0 from R^{4n} to itself,

$$\alpha(t, t_0) : \begin{pmatrix} \widehat{z} \\ z \end{pmatrix} \to \begin{pmatrix} \widehat{w} \\ w \end{pmatrix} = \begin{pmatrix} \alpha_1(\widehat{z}, z, t, t_0) \\ \alpha_2(\widehat{z}, z, t, t_0) \end{pmatrix}, \tag{3.1}$$

$$\alpha^{-1}(t, t_0) : \begin{pmatrix} \widehat{w} \\ w \end{pmatrix} \to \begin{pmatrix} \widehat{z} \\ z \end{pmatrix} = \begin{pmatrix} \alpha^1(\widehat{w}, w, t, t_0) \\ \alpha^2(\widehat{w}, w, t, t_0) \end{pmatrix}.$$

Let denote the Jacobian of α and its inverse by

$$\alpha_*(\widehat{z}, z, t, t_0) = \begin{pmatrix} A_\alpha & B_\alpha \\ C_\alpha & D_\alpha \end{pmatrix}, \qquad \alpha_*^{-1}(\widehat{w}, w, t, t_0) = \begin{pmatrix} A^\alpha & B^\alpha \\ C^\alpha & D^\alpha \end{pmatrix}.$$

Let α be a diffeomorphism from R^{4n} to itself, then it follows that α carries every $\widetilde{K}$-Lagrangian submanifold into a J_{4n}-Lagrangian submanifold, if and only if

$\alpha_*^{\mathrm{T}} J_{4n} \alpha_* = \widetilde{K}$, i.e.,

$$\begin{pmatrix} A_\alpha & B_\alpha \\ C_\alpha & D_\alpha \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} 0 & I_{2n} \\ -I_{2n} & 0 \end{pmatrix} \begin{pmatrix} A_\alpha & B_\alpha \\ C_\alpha & D_\alpha \end{pmatrix} = \begin{pmatrix} K(\widehat{z}, t) & 0 \\ 0 & -K(z, t_0) \end{pmatrix}.$$

Conversely, α^{-1} carries every J_{4n}-Lagrangian submanifold into a $\widetilde{K}$-Lagrangian submanifold.

Theorem 3.1. *Let $\mathcal{M} \subseteq R^{2n\times 2n}$, α given as in (3.1), and define a fractional transformation*

$$\sigma_\alpha : \mathcal{M} \longrightarrow \mathcal{M}, \quad M \longrightarrow N = \sigma_\alpha(M) = (A_\alpha M + B_\alpha)(C_\alpha M + D_\alpha)^{-1}$$

under the transversality condition $|C_\alpha M + D_\alpha| \neq 0$. Then the following four conditions are mutually equivalent:

$$|C_\alpha M + D_\alpha| \neq 0, \qquad |MC^\alpha - A^\alpha| \neq 0,$$
$$|C^\alpha N + D^\alpha| \neq 0, \qquad |NC_\alpha - A_\alpha| \neq 0.$$

The proof is direct and simple, so it is omitted here.

Theorem 3.2. *Let α be defined as above. Let $z \to \widehat{z} = g(z,t,t_0)$ be a $K(z,t)$-symplectic mapping in some neighborhood $\widetilde{\mathcal{R}}$ of R^{2n} with Jacobian $g_z(z,t,t_0) = M(z,t,t_0)$. If M satisfies the transversality condition in $\widetilde{\mathcal{R}}$*

$$|C_\alpha(g(z,t,t_0),z,t,t_0)M(z,t,t_0) + D_\alpha(g(z,t,t_0),z,t,t_0)| \neq 0, \tag{3.2}$$

then there uniquely exists in $\widetilde{\mathcal{R}}$ a gradient mapping $w \to \widehat{w} = f(w,t,t_0)$ with Jacobian $f_w(w,t,t_0) = N(w,t,t_0)$ and a uniquely defined scalar generating function $\phi(w,t,t_0)$ such that

$$f(w,t,t_0) = \phi_w(w,t,t_0),$$

$$\begin{aligned} \alpha_1(g(z,t,t_0),z,t,t_0) &= f(\alpha_2(g(z,t,t_0),z,t,t_0),t,t_0) \\ &= \phi_w(\alpha_2(g(z,t,t_0),z,t,t_0),t,t_0), \end{aligned} \tag{3.3}$$

and

$$N = (A_\alpha M + B_\alpha)(C_\alpha M + D_\alpha)^{-1}, \quad M = (A^\alpha N + B^\alpha)(C^\alpha N + D^\alpha)^{-1}.$$

Proof. Under the transformation α, the image of the graph Γ_g is

$$\alpha(\Gamma_g) = \left\{ \begin{pmatrix} \widehat{w} \\ w \end{pmatrix} \in R^{4n} | \widehat{w} = \alpha_1(g(z,t,t_0),z,t,t_0), \right.$$
$$\left. w = \alpha_2(g(z,t,t_0),z,t,t_0) \right\}.$$

Inequality (3.2) implies

$$|\frac{\partial w}{\partial z}| = |\frac{\partial \alpha_2}{\partial \widehat{z}} \cdot \frac{\partial \widehat{z}}{\partial z} + \frac{\partial \alpha_2}{\partial z}| = \left|C_\alpha M + D_\alpha\right| \neq 0,$$

so $w = \alpha_2(g(z,t,t_0),z,t,t_0)$ is invertible, the inverse function is denoted by $z = z(w,t,t_0)$. Set

$$\widehat{w} = f(w,t,t_0) = \alpha_1(g(z,t,t_0),z,t,t_0)|_{z=z(w,t,t_0)}, \tag{3.4}$$

then

$$N = \frac{\partial f}{\partial w} = \left(\frac{\partial \alpha_1}{\partial \widehat{z}}\frac{\partial g}{\partial z} + \frac{\partial \alpha_1}{\partial z}\right)\left(\frac{\partial z}{\partial w}\right) = \left(A_\alpha M + B_\alpha\right)\left(C_\alpha M + D_\alpha\right)^{-1}.$$

Notice that the tangent space to $\alpha(\Gamma_g)$ at z is

$$T_z(\alpha(\Gamma_g)) = \begin{pmatrix} \frac{\partial \widehat{w}}{\partial z} \\ \frac{\partial w}{\partial z} \end{pmatrix} = \begin{pmatrix} A_\alpha M + B_\alpha \\ C_\alpha M + D_\alpha \end{pmatrix}.$$

It can be concluded that $\alpha\left(\Gamma_g\right)$ is a J_{4n}-Lagrangian submanifold for

$$\begin{aligned}
&T_z\left(\alpha(\Gamma_g)\right)^{\mathrm{T}} J_{4n} T_z\left(\alpha(\Gamma_g)\right) \\
&= \left((A_\alpha M + B_\alpha)^{\mathrm{T}}, (C_\alpha M + D_\alpha)^{\mathrm{T}}\right) J_{4n} \begin{pmatrix} A_\alpha M + B_\alpha \\ C_\alpha M + D_\alpha \end{pmatrix} \\
&= \left(M^{\mathrm{T}}, I\right) \alpha_*^{\mathrm{T}} J_{4n} \alpha_* \begin{pmatrix} M \\ I \end{pmatrix} = \left(M^{\mathrm{T}}, I\right) \widetilde{K} \begin{pmatrix} M \\ I \end{pmatrix} = 0.
\end{aligned}$$

Thus,

$$(A_\alpha M + B_\alpha)^{\mathrm{T}}(C_\alpha M + D_\alpha) - (C_\alpha M + D_\alpha)^{\mathrm{T}}(A_\alpha M + B_\alpha) = 0,$$

i.e., $N = (A_\alpha M + B_\alpha)(C_\alpha M + D_\alpha)^{-1}$ is symmetric. This implies that $\widehat{w} = f(w,t,t_0)$ is a gradient mapping. By the Poincaré Lemma, there is a scalar function $\phi(w,t,t_0)$ such that

$$f(w,t,t_0) = \phi_w(w,t,t_0). \tag{3.5}$$

Consider the construction of $f(w,t,t_0)$ and $z(w,t,t_0)$. Since $z(w,t,t_0) \circ \alpha_2(g(z,t,t_0),z,t,t_0) \equiv z$, substituting $w = \alpha_2(g(z,t,t_0),z,t,t_0)$ in (3.4) and (3.5) yields equation (3.3). □

Theorem 3.3. *$f(w,t,t_0)$ obtained in Theorem 3.2 is also the solution of the following implicit equation*

$$\alpha^1(f(w,t,t_0),w,t,t_0) = g(\alpha^2(f(w,t,t_0),w,t,t_0),t,t_0).$$

Theorem 3.4. *Let α be defined as in Theorem 3.2, let $w \to \widehat{w} = f(w,t,t_0)$ be a gradient mapping in some neighborhood $\widetilde{\mathcal{R}}$ of R^{2n} with Jacobian*

$f_w(w,t,t_0) = N(w,t,t_0)$. *If* N *satisfies in* $\widetilde{\mathcal{R}}$ *the condition*

$$|C^\alpha(f(w,t,t_0),w,t,t_0)N(w,t,t_0) + D^\alpha(f(w,t,t_0),w,t,t_0)| \neq 0,$$

then in $\widetilde{\mathcal{R}}$ *there uniquely exists a K(z,t)-symplectic mapping* $z \to \widehat{z} = g(z,t,t_0)$ *with Jacobian* $g_z(z,t,t_0) = M(z,t,t_0)$ *such that*

$$\alpha^1(f(w,t,t_0),w,t,t_0) = g(\alpha^2(f(w,t,t_0),w,t,t_0),t,t_0),$$
$$M = (A^\alpha N + B^\alpha)(C^\alpha N + D^\alpha)^{-1}, \quad N = (A_\alpha M + B_\alpha)(C_\alpha M + D_\alpha)^{-1}.$$

Remarks. The proofs of Theorems 3.3 and 3.4 are similar to that of Theorem 3.2 and are omitted here. And similar to Theorem 3.3, the function $g(z,t,t_0)$ is the solution of the implicit equation

$$\alpha_1(g(z,t,t_0),z,t,t_0) = f(\alpha_2(g(z,t,t_0),z,t,t_0),t,t_0).$$

4. Symplectic Difference Schemes for Birkhoffian Systems

In Section 2 it is indicated that for general Birkhoffian systems, there exists the common property that their phase flows are $K(z,t)$-symplectic. With the result in the previous sections, $K(z,t)$-symplectic schemes for Birkhoffian systems are constructed by approximating the generating functions.

Birkhoffian phase flow is denoted by $g^t(z,t_0)$ and it is a one-parameter group of $K(z,t)$-symplectic mappings at least local in z and t, i.e., g^{t_0} = identity, $g^{t_1+t_2} = g^{t_1} \circ g^{t_2}$. Here z is taken as an initial value when $t = t_0$, and $\widehat{z}(z,t,t_0) = g^t(z,t_0) = g(t;z,t_0)$ is the solution of the Birkhoffian system (2.8).

Theorem 4.1. *Let* α *be defined as in Theorem* 3.2. *Let* $z \to \widehat{z} = g^t(z,t_0)$ *be the phase flow of the Birkhoffian system* (2.8), $M(t;z,t_0) = g_z(t;z,t_0)$ *is its Jacobian. At some initial point* z, *i.e.,* $t = t_0$, $\widehat{z} = z$, *if*

$$|C_\alpha(z,z,t_0,t_0) + D_\alpha(z,z,t_0,t_0)| \neq 0, \tag{4.1}$$

then for sufficiently small $|t - t_0|$ *and in some neighborhood of* $z \in R^{2n}$ *there exists a gradient mapping* $w \to \widehat{w} = f(w,t,t_0)$ *with symmetric Jacobian* $f_w(w,t,t_0) = N(w,t,t_0)$ *and a uniquely determined scalar generating function* $\phi(w,t,t_0)$ *such that*

$$f(w,t,t_0) = \phi_w(w,t,t_0), \tag{4.2}$$

$$\frac{\partial}{\partial t}\phi_w(w,t,t_0) = \mathcal{A}(\phi_w(w,t,t_0),w,\phi_{ww}(w,t,t_0),t,t_0), \tag{4.3}$$

$$\mathcal{A}(\widehat{w},w,\frac{\partial \widehat{w}}{\partial w},t,t_0) = \bar{\mathcal{A}}(\widehat{z}(\widehat{w},w,t,t_0),z(\widehat{w},w,t,t_0),\frac{\partial \widehat{w}}{\partial w},t,t_0), \tag{4.4}$$

$$\bar{A}(\widehat{z}, z, \frac{\partial \widehat{w}}{\partial w}, t, t_0) = \frac{d}{dt}\widehat{w}(\widehat{z}, z, t, t_0) - \frac{\partial \widehat{w}}{\partial w}\frac{d}{dt}w(\widehat{z}, z, t, t_0)$$
$$= (A_\alpha - \frac{\partial \widehat{w}}{\partial w}C_\alpha)K^{-1}D(\widehat{z}, t) + \frac{\partial \alpha_1}{\partial t} - \frac{\partial \widehat{w}}{\partial w}\frac{\partial \alpha_2}{\partial t}, \tag{4.5}$$

$$\alpha_1(g(t; z, t_0), z, t, t_0) = f(\alpha_2(g(t; z, t_0), z, t, t_0), t, t_0)$$
$$= \phi_w(\alpha_2(g(t; z, t_0), z, t, t_0), t, t_0),$$

and

$$N = \sigma_\alpha(M) = (A_\alpha M + B_\alpha)(C_\alpha M + D_\alpha)^{-1},$$
$$M = \sigma_{\alpha^{-1}}(N) = (A^\alpha N + B^\alpha)(C^\alpha N + D^\alpha)^{-1}.$$

Proof. $M(t; z, t_0)$ is differentiable with respect to z and t. Condition (4.1) guarantees that for sufficiently small $|t - t_0|$ and for $\widehat{z}$ in some neighborhood of $z \in R^{2n}$, there is

$$|C_\alpha(\widehat{z}, z, t, t_0)M(t; z, t_0) + D_\alpha(\widehat{z}, z, t, t_0)| \neq 0.$$

Additionally, the Birkhoffian phase flow is a $K(z, t)$-symplectic mapping, therefore by Theorem 3.2 there exists a time-dependent gradient map $\widehat{w} = f(w, t, t_0)$ and a scalar function $\phi(w, t, t_0)$, such that

$$f(w, t, t_0) = \phi_w(w, t, t_0), \quad \frac{\partial f(w, t, t_0)}{\partial t} = \frac{\partial \phi_w(w, t, t_0)}{\partial t}. \tag{4.6}$$

Notice that $\widehat{z} = g(t; z, t_0)$ is the solution of the following initial-value problem

$$\begin{cases} \frac{\mathrm{d}\widehat{z}}{\mathrm{d}t} = K^{-1}(\widehat{z}, t)(\bigtriangledown B + \frac{\partial F}{\partial t})(\widehat{z}, t)\,, \\ \widehat{z}|_{t=t_0} = z\,. \end{cases}$$

From above equations it follows that

$$\frac{\mathrm{d}\widehat{w}}{\mathrm{d}t} = \frac{\partial \widehat{w}}{\partial \widehat{z}} \cdot \frac{\mathrm{d}\widehat{z}}{\mathrm{d}t} + \frac{\partial}{\partial t}\alpha_1(\widehat{z}, z, t, t_0) = A_\alpha K^{-1}(\bigtriangledown B + \frac{\partial F}{\partial t}) + \frac{\partial \alpha_1}{\partial t},$$
$$\frac{\mathrm{d}w}{\mathrm{d}t} = C_\alpha K^{-1}(\bigtriangledown B + \frac{\partial F}{\partial t}) + \frac{\partial \alpha_2}{\partial t},$$

therefore

$$\frac{\partial \widehat{w}}{\partial t} = \frac{\mathrm{d}\widehat{w}}{\mathrm{d}t} - \frac{\partial \widehat{w}}{\partial w}\frac{\mathrm{d}w}{\mathrm{d}t} = (A_\alpha - \frac{\partial \widehat{w}}{\partial w}C_\alpha)K^{-1}(\bigtriangledown B + \frac{\partial F}{\partial t}) + \frac{\partial \alpha_1}{\partial t} - \frac{\partial \widehat{w}}{\partial w}\frac{\partial \alpha_2}{\partial t}.$$

Since $\frac{\partial \widehat{w}}{\partial w} \neq 0$, so $w = w(\widehat{w}, t)$ exists and is solvable in $(\widehat{w})$, but it cannot be solved explicitly from the transformation α and α^{-1}, we have

$$\bar{A}(\widehat{z}, z, \frac{\partial \widehat{w}}{\partial w}, t, t_0) = \frac{\partial \widehat{w}}{\partial t},$$

and equations (4.4) and (4.5). From (4.6) equation (4.3) follows. $\square$

According to Feng et al [3, 5] we can easily construct symplectic difference schemes of any order for autonomous or semi-autonomous Birkhoffian systems. Because of the simplicity of the ordinary geometry structure, the transformation α in (3.1) needed in these cases is independent of the parameter t, accordingly

$$\frac{\partial \widehat{w}}{\partial t} = \frac{\mathrm{d}\widehat{w}}{\mathrm{d}t} - \frac{\partial \widehat{w}}{\partial w}\frac{\mathrm{d}w}{\mathrm{d}t} = (A_\alpha - \frac{\partial \widehat{w}}{\partial w}C_\alpha)K^{-1} \bigtriangledown B$$
$$= -(B^{\alpha\mathrm{T}} + \left(\frac{\partial \widehat{w}}{\partial w}\right)^{\mathrm{T}} A^{\alpha\mathrm{T}}) \bigtriangledown_z B = -B_w(\widehat{z}(\widehat{w}, w)) \quad (\text{or} = -B_w(\widehat{z}(\widehat{w}, w), t)).$$

Therefore the corresponding Birkhoffian system is completely a Hamiltonian system. The Hamilton-Jacobi equations are

$$\frac{\partial \phi(w,t,t_0)}{\partial t} = -B(\widehat{z}(\phi_w, w)), \ \frac{\partial \phi(w,t,t_0)}{\partial t} = -B(\widehat{z}(\phi_w, w), t) \tag{4.7}$$

in the autonomous and semi-autonomous cases, respectively.

Remarks. Because of the forcing term in (2.1), the Hamilton-Jacobi equation for the generating function $\phi(w, t, t_0)$ cannot directly be derived, but instead of the Hamiltonian-Jacobi equation (4.3) for $\phi_w(w, t, t_0)$ can be easily obtained. Assume the generating function $\phi_w(w, t, t_0)$ can be expanded as a convergent power series in t

$$\phi_w(w,t,t_0) = \sum_{k=0}^{\infty} (t-t_0)^k \phi_w^{(k)}(w, t_0). \tag{4.8}$$

Lemma 4.1. *The k-th order total derivative of $\mathcal{A}$ defined as in Theorem 4.1 with respect to t can be described as*

$$\begin{aligned} D_t^k \mathcal{A} = {} & \partial_{\phi_w}\mathcal{A} \cdot \sum_{i=0}^{\infty}(t-t_0)^i \phi_w^{(k+i)} + \partial_{\phi_{ww}}\mathcal{A} \cdot \sum_{i=0}^{\infty}(t-t_0)^i \phi_{ww}^{(k+i)} \\ & + \partial_t\partial_{\phi_w}\mathcal{A} \cdot \sum_{i=0}^{\infty}(t-t_0)^i \phi_w^{(k-1+i)} + \partial_t\partial_{\phi_{ww}}\mathcal{A} \cdot \sum_{i=0}^{\infty}(t-t_0)^i \phi_{ww}^{(k-1+i)} \\ & + \sum_{m=0}^{k} C_k^m \sum_{n=1}^{k-m} C_{k-m}^n \sum_{l=1}^{k-m-n} \sum_{\substack{h_1+\cdots+h_n+ \\ j_1+\cdots+j_l=k-m}} \partial_{\phi_w}^n \partial_{\phi_{ww}}^l \partial_t^m \mathcal{A} \\ & \cdot (\sum_{i=0}^{\infty}(t-t_0)^i \phi_w^{(h_1+i)}, \cdots, \sum_{i=0}^{\infty}(t-t_0)^i \phi_w^{(h_n+i)}, \\ & \sum_{i=0}^{\infty}(t-t_0)^i \phi_{ww}^{(j_1+i)}, \cdots, \sum_{i=0}^{\infty}(t-t_0)^i \phi_{ww}^{(j_l+i)}), \end{aligned}$$

then at the point of $t = t_0$, *the total derivative of* $\mathcal{A}$ *is as*

$$D_t^k \mathcal{A}_{t_0} = \partial_{\phi_w} \mathcal{A}_{t_0} \cdot \phi_w^{(k)} + \partial_{\phi_{ww}} \mathcal{A}_{t_0} \cdot \phi_{ww}^{(k)} + \partial_t \partial_{\phi_w} \mathcal{A}_{t_0} \cdot \phi_w^{(k-1)} + \partial_t \partial_{\phi_{ww}} \mathcal{A}_{t_0} \cdot \phi_{ww}^{(k-1)} + \sum_{m=0}^{k} C_k^m \sum_{n=1}^{k-m} C_{k-m}^n \sum_{l=1}^{k-m-n} \sum_{\substack{h_1+\cdots+h_n+\\ j_1+\cdots+j_l=k-m}} \partial_{\phi_w}^n \partial_{\phi_{ww}}^l \partial_t^m \mathcal{A}_{t_0} \cdot (\phi_w^{(h_1)}, \cdots, \phi_w^{(h_n)}, \phi_{ww}^{(j_1)}, \cdots, \phi_{ww}^{(j_l)}),$$

$$\mathcal{A}_{t_0} = \mathcal{A}(\phi_w^{(0)}, w, \phi_{ww}^{(0)}, t_0, t_0).$$

By means of the representations of the total derivative of $\mathcal{A}$ the following results are proved.

Theorem 4.2. *Let* $\mathcal{A}$ *and* α *be analytic. Then the generating function* $\phi_{w,\alpha,\mathcal{A}}(w,t,t_0) = \phi_w(w,t,t_0)$ *can be expanded as a convergent power series in* t *for sufficiently small* $|t - t_0|$

$$\phi_w(w,t,t_0) = \sum_{k=0}^{\infty} (t-t_0)^k \phi_w^{(k)}(w,t_0), \tag{4.9}$$

and $\phi_w^{(k)}$, $k \geq 0$, *can be recursively determined by the following equations*

$$\phi_w^{(0)}(w,t_0) = f(w,t_0,t_0), \tag{4.10}$$

$$\phi_w^{(1)}(w,t_0) = \mathcal{A}(\phi_w^{(0)}, w, \phi_{ww}^{(0)}, t_0, t_0), \tag{4.11}$$

$$\phi_w^{(k+1)}(w,t_0) = \frac{1}{(k+1)!} D_t^k \mathcal{A}(\phi_w^{(0)}, w, \phi_{ww}^{(0)}, t_0, t_0). \tag{4.12}$$

Proof. Differentiating equation (4.9) with respect to w and t, we get

$$\phi_{ww}(w,t,t_0) = \sum_{k=0}^{\infty} (t-t_0)^k \phi_{ww}^{(k)}(w,t_0), \tag{4.13}$$

$$\frac{\partial}{\partial t} \phi_w(w,t,t_0) = \sum_{k=0}^{\infty} (k+1)(t-t_0)^k \phi_w^{(k+1)}(w,t_0). \tag{4.14}$$

By equation (4.2),

$$\phi_w^{(0)}(w,t_0) = \phi_w(w,t_0,t_0) = f(w,t_0,t_0).$$

Substituting equations (4.9) and (4.13) in $\mathcal{A}(\widehat{w}, w, \frac{\partial \widehat{w}}{\partial w}, t, t_0)$, and expanding $\mathcal{A}$

in $t = t_0$, we get

$$\mathcal{A}(\phi_w, w, \phi_{ww}, t, t_0) = \mathcal{A}(f(w, t_0, t_0), w, f_w(w, t_0, t_0), t_0, t_0) + \sum_{k=1}^{\infty} \frac{1}{k!}(t - t_0)^k D_t^k \mathcal{A}(\phi_w^{(0)}, w, \phi_{ww}^{(0)}, t_0, t_0). \tag{4.15}$$

Using equation (4.3) and comparing (4.15) with (4.14), we get (4.11) and (4.12). □

In the autonomous and semi-autonomous cases $\mathcal{A}$ are replaced by the Birkhoffian B, which make it much easier to expand the generating functions ϕ. With Theorems 3.2 and 3.4, the relationship between the Birkhoffian phase flow and the generating function $\phi(w, t, t_0)$ is established. With this result, $K(z, t)$-symplectic difference schemes can be directly constructed.

Theorem 4.3. *Let $\mathcal{A}$ and α be analytic. For sufficiently small step-size $\tau > 0$ take*

$$\psi_w^{(m)}(w, t_0 + \tau, t_0) = \sum_{i=0}^{m} \tau^i \phi_w^{(i)}(w, t_0), \qquad m = 1, 2, \dots,$$

where $\phi_w^{(i)}$ are determined by equations (4.10)–(4.12).

Then $\psi_w^{(m)}(w, t_0 + \tau, t_0)$ defines a K(z,t)-symplectic difference scheme $z = z^k \longrightarrow z^{k+1} = \widehat{z}$,

$$\alpha_1(z^{k+1}, z^k, t_{k+1}, t_k) = \psi_w^{(m)}(\alpha_2(z^{k+1}, z^k, t_{k+1}, t_k), t_{k+1}, t_k) \tag{4.16}$$

of m-th order of accuracy.

Proof. Let be $N = \phi_{ww}(w_0, t_0, t_0) = \psi_{ww}^{(m)}(w_0, t_0, t_0)$ and $w_0 = \alpha(z, z, t_0, t_0)$, then Theorem 3.4 yields $|C^\alpha N + D^\alpha|$ because of

$$|C_\alpha(z, z, t_0, t_0) + D_\alpha(z, z, t_0, t_0)| \neq 0.$$

Thus for sufficiently small τ and in some neighborhood of w_0, there exists

$$|C^\alpha N^{(m)}(w, t_0 + \tau, t_0) + D^\alpha| \neq 0,$$

where

$$N^{(m)}(w, t_0 + \tau, t_0) = \psi_{ww}^{(m)}(w, t_0 + \tau, t_0).$$

By Theorem 3.4, $\psi_w^{(m)}(w, t_0 + \tau, t_0)$ defines a $K(z, t)$-symplectic mapping which is expressed in (3.3). Therefore equation (4.16) determines a m-th order $K(z, t)$-symplectic difference scheme for the Birkhoffian system (2.8). □

5. Example

In this section an example illustrates how to obtain schemes preserving the $K(z,t)$-symplectic structure for a nonconservative system expressed in Birkhoffian representation. Consider the linear damped oscillator

$$\ddot{q} + \nu\dot{q} + q = 0. \tag{5.1}$$

We introduce a gradient function p satisfying $p = \dot{q}$, then a Birkhoffian representation of (5.1) is given by

$$\begin{pmatrix} 0 & -\mathrm{e}^{\nu t} \\ \mathrm{e}^{\nu t} & 0 \end{pmatrix}\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} \nu\mathrm{e}^{\nu t}p + \mathrm{e}^{\nu t}q \\ \mathrm{e}^{\nu t}p \end{pmatrix}. \tag{5.2}$$

The structure and the functions are

$$K = \begin{pmatrix} 0 & -\mathrm{e}^{\nu t} \\ \mathrm{e}^{\nu t} & 0 \end{pmatrix}, \qquad K^{-1} = \begin{pmatrix} 0 & \mathrm{e}^{-\nu t} \\ -\mathrm{e}^{-\nu t} & 0 \end{pmatrix},$$

$$F = \begin{pmatrix} \frac{1}{2}\mathrm{e}^{\nu t}p \\ -\frac{1}{2}\mathrm{e}^{\nu t}q \end{pmatrix}, \qquad B = \frac{1}{2}\mathrm{e}^{\nu t}(q^2 + qp + p^2),$$

and the energy function reads

$$H(q,p) = \frac{1}{2}(q^2 + p^2) - \nu p^2. \tag{5.3}$$

The *Euler's Midpoint Scheme* (or one-step Gauss-Runge-Kutta method) for the system (5.2), which can be derived via the discrete Langrange-d'Alembert principle (see Marsden and West [9]), reads

$$\frac{q_{k+1} - q_k}{\tau} = \frac{p_{k+1} + p_k}{2},$$

$$\frac{p_{k+1} - p_k}{\tau} = -\nu\frac{p_{k+1} + p_k}{2} - \frac{q_{k+1} + q_k}{2},$$

and hence,

$$\begin{pmatrix} q_{k+1} \\ p_{k+1} \end{pmatrix} = \frac{1}{\Delta}\begin{pmatrix} -\tau^2 + 2\nu\tau + 4 & 4\tau \\ -4\tau & -\tau^2 - 2\nu\tau + 4 \end{pmatrix}\begin{pmatrix} q_k \\ p_k \end{pmatrix}, \tag{5.4}$$

where $\Delta = \tau^2 + 2\nu\tau + 4$, is not a $K(z,t)$-symplectic scheme.

Now consider the transformation α in (3.1) to be

$$\begin{aligned} \widehat{Q} &= \mathrm{e}^{\nu t}\widehat{p} - \mathrm{e}^{\nu t_0}p, & \widehat{P} &= \widehat{q} - q, \\ Q &= \frac{1}{2}(\widehat{q} + q), & P &= -\frac{1}{2}(\mathrm{e}^{\nu t}\widehat{p} + \mathrm{e}^{\nu t_0}p), \end{aligned} \tag{5.5}$$

where the Jacobian of α is

$$\alpha_* = \begin{pmatrix} 0 & \mathrm{e}^{\nu t} & 0 & -\mathrm{e}^{\nu t_0} \\ 1 & 0 & -1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2}\mathrm{e}^{\nu t} & 0 & -\frac{1}{2}\mathrm{e}^{\nu t_0} \end{pmatrix}.$$

The inverse transformation is

$$\begin{aligned} \widehat{q} &= \frac{1}{2}\widehat{P} + Q, \qquad & \widehat{p} &= \frac{1}{2}\mathrm{e}^{-\nu t}\widehat{Q} - \mathrm{e}^{-\nu t}P, \\ q &= -\frac{1}{2}\widehat{P} + Q, \qquad & p &= -\frac{1}{2}\mathrm{e}^{-\nu t_0}\widehat{Q} - \mathrm{e}^{-\nu t_0}P, \end{aligned} \tag{5.6}$$

and

$$\alpha_*^{-1} = \begin{pmatrix} 0 & \frac{1}{2} & 1 & 0 \\ \frac{1}{2}\mathrm{e}^{-\nu t} & 0 & 0 & -\mathrm{e}^{-\nu t} \\ 0 & -\frac{1}{2} & 1 & 0 \\ -\frac{1}{2}\mathrm{e}^{-\nu t_0} & 0 & 0 & -\mathrm{e}^{-\nu t_0} \end{pmatrix}.$$

Consequently using (5.5), (5.6) and (5.2) we derive

$$\frac{\mathrm{d}\widehat{w}}{\mathrm{d}t} = \begin{pmatrix} \nu\mathrm{e}^{\nu t}\widehat{p} + \mathrm{e}^{\nu t}\dot{\widehat{p}} \\ \dot{\widehat{q}} \end{pmatrix} = \begin{pmatrix} -\mathrm{e}^{\nu t}\widehat{q} \\ \widehat{p} \end{pmatrix} = \begin{pmatrix} -\frac{1}{2}\mathrm{e}^{\nu t}\widehat{P} - \mathrm{e}^{\nu t}Q \\ \frac{1}{2}\mathrm{e}^{-\nu t}\widehat{Q} - \mathrm{e}^{-\nu t}P \end{pmatrix},$$

$$\frac{\mathrm{d}w}{\mathrm{d}t} = \begin{pmatrix} \frac{1}{4}\mathrm{e}^{-\nu t}\widehat{Q} - \frac{1}{2}\mathrm{e}^{-\nu t}P \\ \frac{1}{4}\mathrm{e}^{\nu t}\widehat{P} + \frac{1}{2}\mathrm{e}^{\nu t}Q \end{pmatrix}.$$

Simple calculations yields

$$\phi_w^{(0)} = \begin{pmatrix} \widehat{Q} \\ \widehat{P} \end{pmatrix}\Bigg|_{t=t_0} = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

$$\phi_w^{(1)} = \frac{\mathrm{d}\widehat{w}}{\mathrm{d}t}\bigg|_{t=t_0} - \phi_{ww}^{(0)}\frac{\mathrm{d}w}{\mathrm{d}t}\bigg|_{t=t_0} = \begin{pmatrix} -\mathrm{e}^{\nu t_0}Q \\ -\mathrm{e}^{-\nu t_0}P \end{pmatrix}.$$

Set $\widehat{w} = \phi^{(0)} + \phi^{(1)}\tau$, so the *first order scheme* for the system (5.2) reads

$$\begin{aligned} \frac{q_{k+1} - q_k}{\tau} &= e^{-\nu t_k}\,\frac{e^{\nu t_{k+1}}p_{k+1} + e^{\nu t_k}p_k}{2}, \\ \frac{e^{\nu t_{k+1}}p_{k+1} - e^{\nu t_k}p_k}{\tau} &= -e^{\nu t_k}\,\frac{q_{k+1} + q_k}{2}, \end{aligned}$$

and hence

$$\begin{pmatrix} q_{k+1} \\ p_{k+1} \end{pmatrix} = \frac{1}{\Delta}\begin{pmatrix} 4 - \tau^2 & 4\tau \\ -4\tau\mathrm{e}^{-\nu\tau} & (4 - \tau^2)\mathrm{e}^{-\nu\tau} \end{pmatrix}\begin{pmatrix} q_k \\ p_k \end{pmatrix}, \tag{5.7}$$

where $\Delta = 4+\tau^2$. The transition matrix denoted by A satisfies

$$A^{\mathrm{T}} \begin{pmatrix} 0 & -\mathrm{e}^{\nu t_{k+1}} \\ \mathrm{e}^{\nu t_{k+1}} & 0 \end{pmatrix} A = \begin{pmatrix} 0 & -\mathrm{e}^{\nu t_k} \\ \mathrm{e}^{\nu t_k} & 0 \end{pmatrix}.$$

Next if we take $m=2$,get $\phi^{(2)}$

$$\phi^{(2)} = \begin{pmatrix} -\dfrac{\nu}{2}\mathrm{e}^{\nu t_0} Q \\ \dfrac{\nu}{2}\mathrm{e}^{-\nu t_0} P \end{pmatrix},$$

Direct calculation get Birkhoff symplectic scheme of 2-order.

$$\begin{pmatrix} q_{k+1} \\ p_{k+1} \end{pmatrix} = \begin{pmatrix} \frac{16-ab}{16+ab} & \frac{8a}{16+ab} \\ -\frac{8b}{16+ab}\mathrm{e}^{-\nu\tau} & \frac{16-ab}{16+ab}\mathrm{e}^{-\nu\tau} \end{pmatrix} \begin{pmatrix} q_k \\ p_k \end{pmatrix},$$

where $a = 2\tau - \nu\tau^2$ and $b = 2\tau + \nu\tau^2$.

Then consider the transformation α in (3.1) to be

$$\widehat{Q} = \mathrm{e}^{\nu t/2}\widehat{p} - \mathrm{e}^{\nu t_0/2}p, \qquad \widehat{P} = -\mathrm{e}^{\nu t/2}\widehat{q} + \mathrm{e}^{\nu t_0/2}q,$$
$$Q = \tfrac{1}{2}(\mathrm{e}^{\nu t/2}\widehat{q} + \mathrm{e}^{\nu t_0/2}q), \qquad P = \tfrac{1}{2}(\mathrm{e}^{\nu t/2}\widehat{p} + \mathrm{e}^{\nu t_0/2}p).$$

The Jacobian of α is

$$\alpha_* = \begin{pmatrix} 0 & \mathrm{e}^{\nu t/2} & 0 & -\mathrm{e}^{\nu t_0/2} \\ -\mathrm{e}^{\nu t/2} & 0 & \mathrm{e}^{\nu t_0/2} & 0 \\ \frac{1}{2}\mathrm{e}^{\nu t/2} & 0 & \frac{1}{2}\mathrm{e}^{\nu t_0/2} & 0 \\ 0 & \frac{1}{2}\mathrm{e}^{\nu t/2} & 0 & \frac{1}{2}\mathrm{e}^{\nu t_0/2} \end{pmatrix}$$

and the inverse

$$\alpha_*^{-1} = \begin{pmatrix} 0 & -\frac{1}{2}\mathrm{e}^{-\nu t/2} & \mathrm{e}^{-\nu t/2} & 0 \\ \frac{1}{2}\mathrm{e}^{-\nu t/2} & 0 & 0 & \mathrm{e}^{-\nu t/2} \\ 0 & \frac{1}{2}\mathrm{e}^{-\nu t_0/2} & \mathrm{e}^{-\nu t_0/2} & 0 \\ -\frac{1}{2}\mathrm{e}^{-\nu t_0/2} & 0 & 0 & \mathrm{e}^{-\nu t_0/2} \end{pmatrix}.$$

Take $m=1$

$$\widehat{w} = \phi_w^{(1)}\Delta t$$

we get

$$\phi_\omega^{(1)} = \Big[\frac{\mathrm{d}\widehat{w}}{\mathrm{d}t} - \frac{\partial\widehat{w}}{\partial w}\frac{\mathrm{d}w}{\mathrm{d}t}\Big]\Big|_{t=t_0} = \begin{bmatrix} -\nu/2P - Q \\ -\nu/2Q - P \end{bmatrix}.$$

Direct calculation yields the *scheme of second order*

$$\frac{\mathrm{e}^{\nu t_{k+1}/2}q_{k+1} - \mathrm{e}^{\nu t_k/2}q_k}{\tau}$$

$$= \frac{\mathrm{e}^{\nu t_{k+1}/2}p_{k+1} + e^{\nu t_k/2}p_k}{2} + \nu \frac{e^{\nu t_{k+1}/2}q_{k+1} + \mathrm{e}^{\nu t_k/2}q_k}{4},$$

$$\frac{\mathrm{e}^{\nu t_{k+1}/2}p_{k+1} - \mathrm{e}^{\nu t_k/2}p_k}{\tau}$$
$$= -\frac{\mathrm{e}^{\nu t_{k+1}/2}q_{k+1} + e^{\nu t_k/2}q_k}{2} - \nu \frac{e^{\nu t_{k+1}/2}p_{k+1} + \mathrm{e}^{\nu t_k/2}p_k}{4},$$

and hence,

$$\begin{pmatrix} q_{k+1} \\ p_{k+1} \end{pmatrix} = \frac{\mathrm{e}^{-\nu\tau/2}}{\Delta} \begin{pmatrix} w_1 & -16\tau \\ 16\tau & w_2 \end{pmatrix} \begin{pmatrix} q_k \\ p_k \end{pmatrix}, \tag{5.8}$$

where $\Delta = \nu^2\tau^2 - 4\tau^2 - 16$,

$$w_1 = -16 - 8\nu\tau - \nu^2\tau^2 + 4\tau^2, \quad w_2 = -16 + 8\nu\tau - \nu^2\tau^2 + 4\tau^2.$$

Abbreviating the matrix $\frac{\mathrm{e}^{-\nu\tau/2}}{\Delta}(*)$ in (5.8) by $M(\tau)$, then by composition (see Qin and Zhu [11], Yoshida [16]) we have the *scheme of order four*

$$\begin{pmatrix} q_{k+1} \\ p_{k+1} \end{pmatrix} = M(c_1\tau)M(c_2\tau)M(c_1\tau) \begin{pmatrix} q_k \\ p_k \end{pmatrix}, \tag{5.9}$$

where

$$c_1 = \frac{1}{2 - 2^{1/3}}, \quad c_2 = \frac{-2^{1/3}}{2 - 2^{1/3}}.$$

Take $m = 3$

$$\phi_\omega^{(3)} = \frac{1}{3!}\frac{\partial}{\partial t}\Big\{\frac{\partial}{\partial t}\Big(\frac{\mathrm{d}\widehat{w}}{\mathrm{d}t}\Big) + \frac{\partial}{\partial \widehat{w}}\Big(\frac{\mathrm{d}\widehat{w}}{\mathrm{d}t}\Big)\frac{\partial \widehat{w}}{\partial t} - \frac{\partial \widehat{w}}{\partial w}\frac{\partial}{\partial \widehat{w}}\Big(\frac{\mathrm{d}w}{\mathrm{d}t}\Big)\frac{\partial \widehat{w}}{\partial t}$$
$$- \frac{\partial \widehat{w}}{\partial w}\frac{\partial}{\partial t}\Big(\frac{\mathrm{d}w}{\mathrm{d}t}\Big) - \frac{\partial}{\partial t}\Big(\frac{\partial \widehat{w}}{\partial w}\Big)\frac{\mathrm{d}w}{\mathrm{d}t}\Big\}.$$

For equation $\ddot{q} + \nu\dot{q} + q = 0$, 3-rd derivative of ϕ in time $t = t_0$, only one term to appear, i.e.

$$-\frac{\partial}{\partial t}\Big(\frac{\widehat{w}}{\mathrm{d}w}\Big)\frac{\partial}{\partial \widehat{w}}\Big(\frac{\mathrm{d}\widehat{w}}{\mathrm{d}t}\Big)\frac{\partial \widehat{w}}{\partial t},$$

Simple calculation yields

$$\phi_\omega^{(3)}\big|_{t=t_0} = -\frac{1}{6}\begin{bmatrix} -1 & -\nu/2 \\ -\nu/2 & -1 \end{bmatrix}\begin{bmatrix} 1/8 & -\nu/8 \\ -\nu/8 & 1/4 \end{bmatrix}\begin{bmatrix} -\nu/2P - Q \\ -\nu/2Q - P \end{bmatrix}$$

$$= -\frac{1}{6}\begin{bmatrix} \Big(-\frac{1}{4} + \frac{1}{16}\nu^2\Big)\Big(Q + \frac{\nu P}{2}\Big) \\ \Big(-\frac{1}{4} + \frac{1}{16}\nu^2\Big)\Big(\frac{\nu}{2} + \frac{P}{2}\Big) \end{bmatrix} = \begin{bmatrix} (\nu^2/2 - 2)Q + (\nu^2/2 - 2)\nu/2P \\ (\nu^2/2 - 2)P + (\nu^2/2 - 2)\nu/2Q \end{bmatrix}.$$

We get 4-th order symmetrical symplectic scheme:

$$\begin{aligned}\frac{e^{\nu t_{k+1}/2}q_{k+1}-e^{\nu t_k/2}q_k}{\tau} &= \frac{e^{\nu t_{k+1}/2}p_{k+1}+e^{\nu t_k/2}p_k}{2}+\nu\frac{e^{\nu t_{k+1}/2}q_{k+1}-e^{\nu t_k/2}q_k}{4}\\ &\quad+\frac{1}{24\times 4}\Big[\Big(\frac{\nu^2}{2}-2\Big)\big(e^{\nu t_{k+1}/2}p_{k+1}+e^{\nu t_k/2}p_k\big)\\ &\qquad+\Big(\frac{\nu^2}{2}-2\Big)\frac{\nu}{2}\big(e^{\nu t_{k+1}/2}q_{k+1}+e^{\nu t_k/2}q_k\big)\Big],\end{aligned}$$

$$\begin{aligned}\frac{e^{\nu t_{k+1}/2}p_{k+1}-e^{\nu t_k/2}p_k}{\tau} &= \frac{e^{\nu t_{k+1}/2}q_{k+1}+e^{\nu t_k/2}q_k}{2}-\nu\frac{e^{\nu t_{k+1}/2}p_{k+1}+e^{\nu t_k/2}p_k}{4}\\ &\quad-\frac{1}{24\times 4}\Big[\Big(\frac{\nu^2}{2}-2\Big)\big(e^{\nu t_{k+1}/2}q_{k+1}+e^{\nu t_k/2}q_k\big)\\ &\qquad+\Big(\frac{\nu^2}{2}-2\Big)\frac{\nu}{2}\big(e^{\nu t_{k+1}/2}p_{k+1}+e^{\nu t_k/2}p_k\big)\Big].\end{aligned}$$

Remarks. The derived schemes (5.7), (5.8), and (5.9) are $K(z,t)$-symplectic, i.e., for $\tau > 0$ and $k \geq 0$ they satisfy the Birkhoffian condition

$$e^{\nu t_{k+1}}\ dq_{k+1}\wedge dp_{k+1} = e^{\nu t_k}\ dq_k \wedge dp_k.$$

This method is easily extended to more general ODEs such as

$$\begin{aligned}&\dot{p}+\beta'(t)p+V(r,t)=0\,,\\ &\dot{r}-G(p,t)=0.\end{aligned}$$

The details will be presented elsewhere.

6. Numerical Experiments

In this section we present numerical results for the linear damped oscillator (5.1) respectively (5.2) using the derived $K(z,t)$–symplectic schemes (5.7), (5.8), and (5.9) of order one, two and four, respectively. Further, we use Euler's midpoint scheme (5.4), which is not $K(z,t)$–symplectic but shows satisfactory numerical results (see Marsden and West [9]), and further Euler's explicit scheme for comparison.

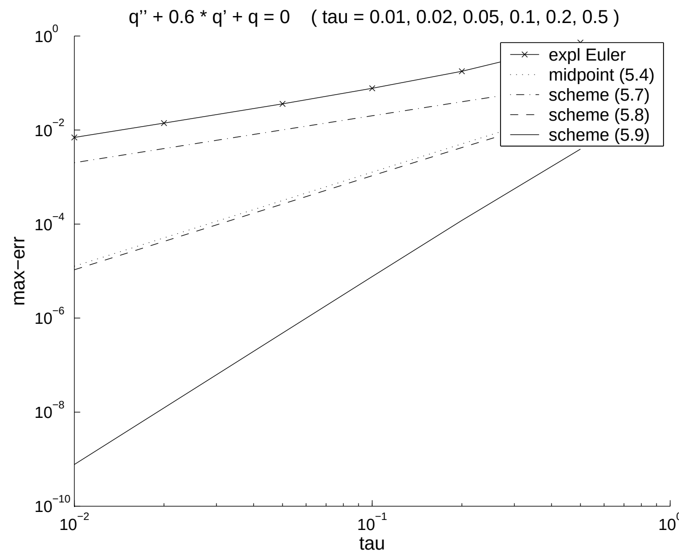

Figure 1: Error comparison between the different schemes for $\nu = 0.6$

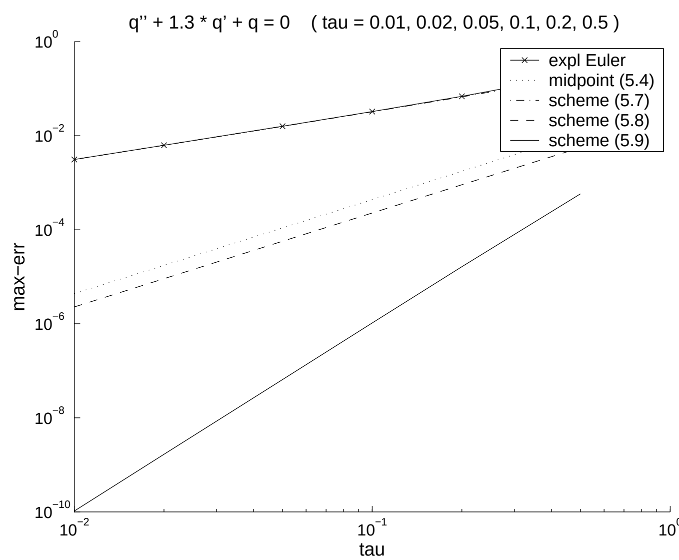

Figure 2: Error comparison between the different schemes for $\nu = 1.3$

In the presented figures the initial values are always chosen as $q(0) = 1,\ p(0) = \dot{q}(0) = -1$, and the time interval is from 0 to 25. In the behaviour

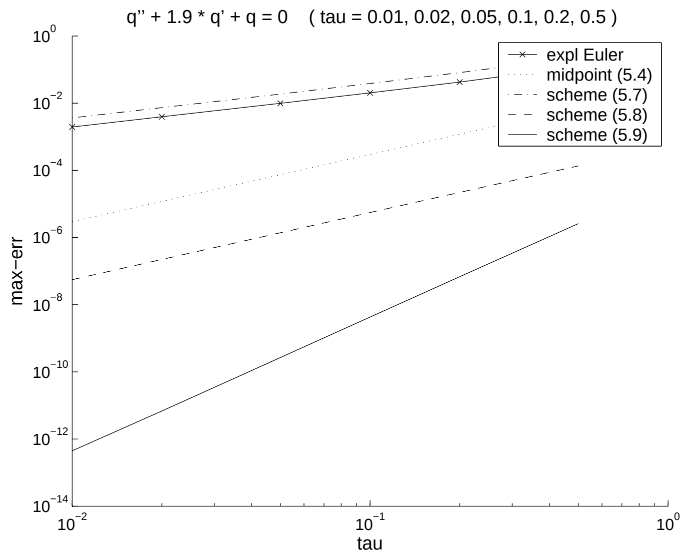

Figure 3: Error comparison between the different schemes for $\nu = 1.9$

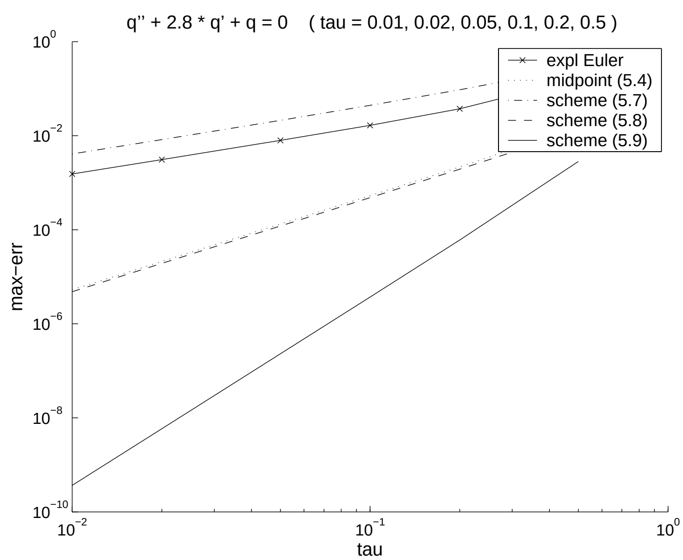

Figure 4: Error comparison between the different schemes for $\nu = 2.8$

of the different schemes there are only small differences choosing other initial values. The damping parameter ν is chosen as 0.6, 1.3, 1.9 and 2.8. The actual

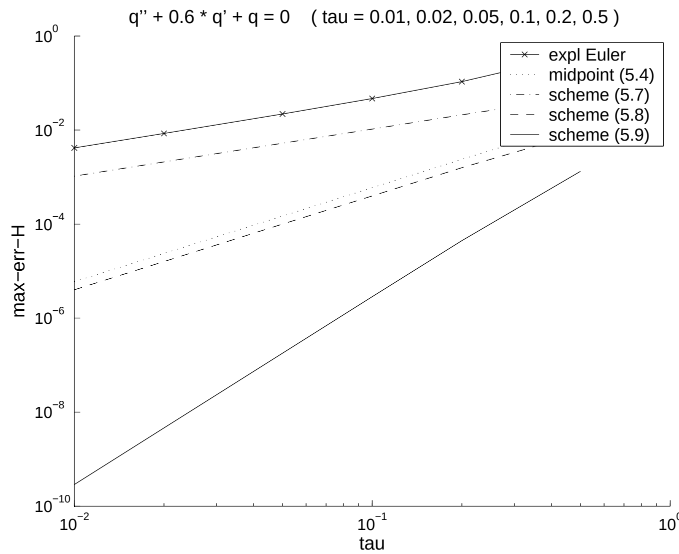

Figure 5: Energy error comparison between the different schemes for $\nu = 0.6$

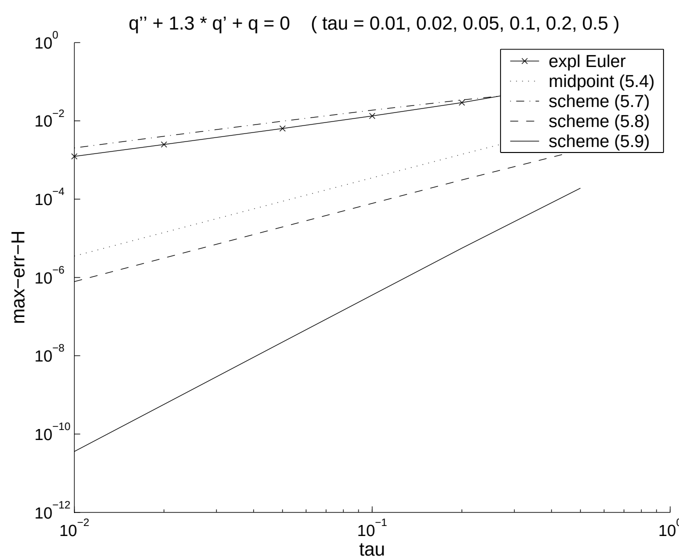

Figure 6: Energy error comparison between the different schemes for $\nu = 1.3$

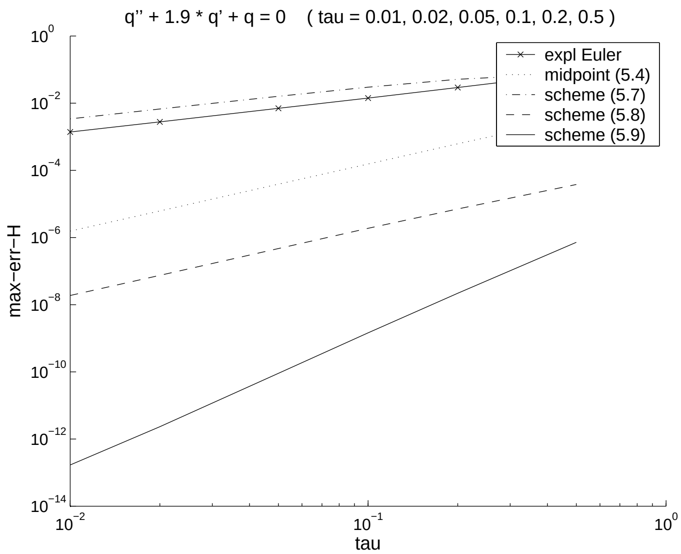

Figure 7: Energy error comparison between the different schemes for $\nu = 1.9$

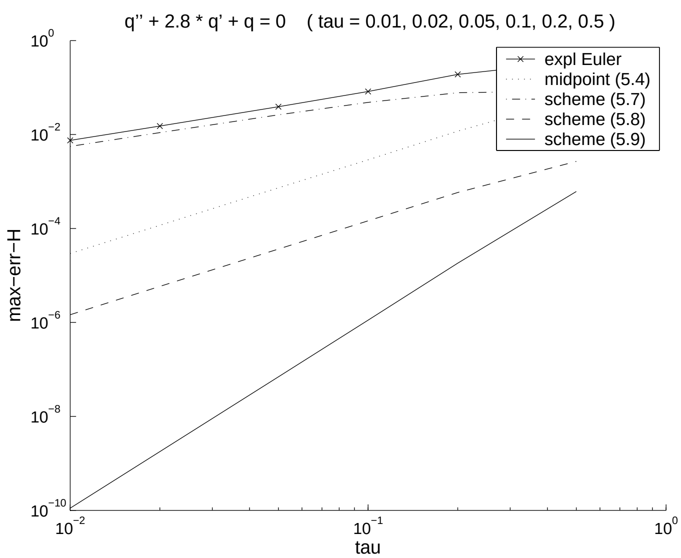

Figure 8: Energy error comparison between the different schemes for $\nu = 2.8$

error, *err* = |approximate solution–true solution|, and its maximal value *max–err* are computed. Using different step–sizes the schemes always show the same quality, which is emphasized by representing the results in a double logarithmic scale using step-sizes tau=0.01, 0.02, 0.05, 0.1, 0.2, 0.5.

The comparison of solution errors between scheme (5.7) and Euler's explicit scheme, both of order one, shows that for smaller ν, i.e., $0 \leq \nu \leq 1.3$ scheme (5.7) is better, and for $\nu > 1.3$ Euler's explicit scheme is better. The comparison of solution errors between scheme (5.8) and Euler's midpoint scheme (5.4), both of order two, shows that for $0 \leq \nu \leq 0.5$ both schemes have the same behaviour, for $0.5 < \nu < 2.8$ scheme (5.8) is better, where the most advantage is around $\nu = 2$, and for $2.8 \geq \nu$ Euler's midpoint scheme is better. The comparison between scheme (5.9) of order four and scheme (5.8) of order two, both having the same structure preserving property, shows that the higher order scheme (5.9) has a clear superiority over the two order scheme. These differences between the discussed schemes are illustrated by the error curves (Figures 1–4).

For the energy function (5.3), the comparisons of the energy error *err–H*, between the different schemes are also done in double logarithmic scales (Figures 5–8). The result shows that the dominance is not clear between scheme (5.7) and Euler's explicit scheme, while scheme (5.8) is always better than Euler's midpoint scheme for growing ν, even for $\nu \geq 2.8$. Scheme (5.9) keeps its superiority in the comparisons.

The comparisons also show that it is possible for different schemes obtained from different transformations α, that different quantities are preserved. This point is proved to be true in the generating function method for Hamiltonian systems (see Feng et al [4, 5]). The extension to application in Birkhoffian systems will also be studied in a prospective paper.

Acknowledgements

This work is supported by the Special Funds for Major State Basic Research Projects, G 1999, 032800, NSFC (No.10401033; 10475082; 10471145) and the Chinese of Sciences with key project of knowledge innovation (KZCXI-SW-18).

M.Z. Qin would like to thank the Karlsruhe University for invitation and support as a visiting professor during one month in 2006. The authors thank Michael Lehn and Tobias Reiling for their help in preparing numerical experi-

ments.

References

[1] V.I. Arnold, *Mathematical Methods of Classical Mechanics*, Springer, New York (1978).

[2] R.W. Atherton, G.M. Homsy, On the existence and formulation of variational principles for nonlinear differential equations, *Studies Appl. Math.*, **54** (1975) 31-60.

[3] K. Feng, D.L. Wang, Symplectic difference schemes for Hamiltonian systems in general symplectic structure, *J. Comput. Math.*, **9** (1991), 86-96.

[4] K. Feng, D.L. Wang, A note on conservation laws of symplectic difference schemes for Hamiltonian systems, *JCM*, **9** (1991), 229-237.

[5] K. Feng, M.Z. Qin, The symplectic methods for the computation of Hamilton's equations, In: *Proc. Conf. on Numerical Methods for PDEs* (Ed-s: Y.L. Guo Ben-Yu), Springer, Berlin (1987), 1-37; Lecture Notes in Math. (1297).

[6] Guo, Y.X., Luo, S.K., M. Shang, F.X. Mei, Birkhoffian formulations of nonholonomic constraint systems, *Rep. Math. Phys.*, **47** (2001), 313-322.

[7] E. Hairer, C. Lubich, G. Wanner, *Geometric Numerical Integration. Structure Preserving Algorithms for Ordinary Differential Equations*, Springer, Berlin (2002).

[8] J.E. Marsden, T.S. Ratiu, *Introduction to Mechanics and Symmetry*, Springer, New York (1994).

[9] J.E. Marsden, M. West, Discrete mechanics and variational integrators, *Acta Numerica*, **10** (2001), 357-514.

[10] E. Massa, E. Pagani, Jet bundle geometry, dynamical connections, and the inverse problem of Lagrangian mechanics, *Ann. Inst. Henri Poincaré, Phys. Théor.*, **61** (1994), 17-62.

[11] M.Z. Qin, W.J. Zhu, Construction of Higher order symplectic schemes by composition, *Computing*, **47** (1993), 309-321.

[12] J.M. Sanz-Serna, M.P. Calvo, *Numerical Hamiltonian Problems*, Chapman and Hall, London (1994).

[13] R.M. Santilli, *Foundations of Theoretical Mechanics I*, Springer, New York (1983).

[14] R.M. Santilli, *Foundations of Theoretical Mechanics II*, Springer, New York (1983).

[15] W. Sarlet, A. Vandecasteele, F. Cantrijn, E. Martinez, Derivation of forms along a map: The framework for time-dependent second-order equations, *Diff. Geom. Appl.*, **5** (1995), 171-203.

[16] H. Yoshida, Construction of higher order symplectic integrators, *Phys. Lett.*, **A 150** (1990), 262-268.