Some Properties of Multi-symplectic Runge-Kutta Methods for Nonlinear Dirac Equations

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Abstract

In this paper, we investigate some properties of the multi-symplectic Runge-Kutta (MSRK) methods for nonlinear Dirac equations in relativistic quantum physics. It is showed that the symplectic Runge-Kutta methods applied to a nonlinear Dirac equation in time and space, respectively, lead to a multi-symplectic integrator which preserves the multi-symplectic structure exactly. With the periodic boundary conditions, we show that the MSRK methods have a discrete charge conservation law, which plays an important role in quantum physics. We also show that MSRK methods preserve the global symplectic structure in time exactly. Under some regularity assumptions, we gives theoretical results on some conservative properties of MSRK methods. With an additional boundary condition, it is showed that MSRK methods preserve the total momentum exactly. In particular, we establish the error analysis theory on energy and momentum conservation laws since MSRK methods, in general, do not preserve energy and momentum exactly. The theory shows that MSRK methods are stable and convergent in the sense of the energy and momentum conservation laws. The theoretical results obtained in this paper can be extended to general multi-symplectic Hamiltonian systems. Numerical examples presented show the match between our analytic results and the corresponding numerical experiments.

Keywords: Multi-symplectic RK methods; Conservation Laws; Nonliear Dirac Equations.

1. Introduction

As well known, the Dirac equation plays an important role in relativistic quantum physics. Some authors have considered numerical methods for solving the equation, such as finite difference methods including conservative type methods[1, 2, 3] and spectral methods[5]. Recently, a new structure-preserving method, the multi-symplectic method, has been proposed and investigated for some important Hamiltonian partial differential equations, such as Schrödinger equations, KdV equations etc. Some interesting and significant results on the method have been presented in [4, 6, 7, 8, 9, 11, 12, 13, 14, 15]. In this paper we discuss properties of multi-symplectic Runge-Kutta methods for $(1+1)$-dimensional nonlinear Dirac equation. This paper is organized as follows, in the rest of this section, we introduce the equation and its basic property, the charge conservation law; we establish the multi-symplecticity and some conservative properties, energy and momentum conservation laws, of the equation in the section

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2; in section 3 we introduce the definition of multi-symplectic discretization, and present the condition of multi-symplecticity of Runge-Kutta discretization for the equation; we discuss the discrete charge conservation law and the total symplecticity in time in the section 4; we give some results on energy analysis and momentum analysis of the MSRK methods in the section 5 and the section 6 respectively, we establish the error analysis theory on energy and momentum conservation laws for MSRK methods; to illustrate our results presented in previous sections, numerical experiments are presented in the section 7. The conclusion of this paper is given in the section 8.

We consider $(1+1)$-dimensional nonlinear Dirac equation

$$\begin{cases} \psi_t = A\psi_x + if(|\psi_1|^2 - |\psi_2|^2)B\psi \\ \psi_1(x,0) = \phi_1(x), \quad \psi_2(x,0) = \phi_2(x), \end{cases} \tag{1.1}$$

where $\psi = (\psi_1, \psi_2)^T$ is a spinorial wave function, which describe a particle with the spin-$\frac{1}{2}$; ψ_1 and ψ_2 are complex functions, which describe the up and down states of the spin-$\frac{1}{2}$ particle respectively, each of them has two components, denoted by the real and imaginary parts of the complex function respectively (for more details, see [1, 2, 3, 5]); $i = \sqrt{-1}$ is the imaginary unit, $f(s)$ is a real function of a real variable s, A and B are matrices

$$A = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \qquad B = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix},$$

the initial function $\phi = (\phi_1, \phi_2)^T$ is sufficiently smooth.

Since a spin-$\frac{1}{2}$ particle has not only the energy and the momentum information, but also the probability information. The concept of probability derives from the quantum theorem. In this context, the charge (the probability information) $\mathcal{Q}$, the linear momentum $\mathcal{P}$ and the energy $\tilde{E}$ are given by

$$\begin{cases} \mathcal{Q}(\psi)(t) = \int_R (|\psi_1(x,t)|^2 + |\psi_2(x,t)|^2)dx, \\ \mathcal{P}(\psi)(t) = \int_R \Im(\bar{\psi_1}\frac{\partial}{\partial x}\psi_1 + \bar{\psi_2}\frac{\partial}{\partial x}\psi_2)dx, \\ \tilde{E}(\psi)(t) = \int_R (\Im(\bar{\psi_1}\frac{\partial}{\partial x}\psi_2 + \bar{\psi_2}\frac{\partial}{\partial x}\psi_1) + \tilde{f}(|\psi_1|^2 - |\psi_2|^2))dx, \end{cases} \tag{1.2}$$

respectively, where $\Im(u)$ and $\bar{u}$ denote the imaginary part and the conjugate of the complex u respectively, $\tilde{f}$ is a primitive function of f, namely

$$\tilde{f}(s) = \int_0^s f(\tau)d\tau.$$

In this paper, we will focus on an important particular case of (1.1)

$$\begin{cases} \frac{\partial\psi_1}{\partial t} + \frac{\partial\psi_2}{\partial x} + im\psi_1 + 2i\lambda(|\psi_2|^2 - |\psi_1|^2)\psi_1 = 0, \\ \frac{\partial\psi_2}{\partial t} + \frac{\partial\psi_1}{\partial x} - im\psi_2 + 2i\lambda(|\psi_1|^2 - |\psi_2|^2)\psi_2 = 0, \end{cases} \tag{1.3}$$

that is,

$$f(s) = m - 2\lambda s$$

in (1.1), where m and λ are real constants. The results obtained can be easily extended to the general case (1.1).

Proposition 1.1 *If the solution ψ of the Dirac equation (1.3) satisfies*

$$\lim_{|x|\to+\infty} |\psi(x,t)| = 0, \qquad \textit{uniformly for} \quad t \in R, \tag{1.4}$$

then

$$\mathcal{Q}(\psi)(t) = \mathcal{Q}(\phi), \tag{1.5}$$

where

$$\mathcal{Q}(\phi)(t) = \int_R (|\phi_1|^2 + |\phi_2|^2)dx, \tag{1.6}$$

Proof. Differentiating the first equation of (1.3) with respect to t, we have

$$\begin{aligned} \frac{d}{dt}\mathcal{Q}(\psi) &= \int_R \frac{\partial}{\partial t}(|\psi_1(x,t)|^2 + |\psi_2(x,t)|^2)dx = \int_R \frac{\partial}{\partial t}(\psi_1\bar{\psi_1} + \psi_2\bar{\psi_2})dx \\ &= \int_R (\bar{\psi_1}\frac{\partial}{\partial_t}\psi_1 + \psi_1\frac{\partial}{\partial t}\bar{\psi_1} + \bar{\psi_2}\frac{\partial}{\partial t}\psi_2 + \psi_2\frac{\partial}{\partial_t}\bar{\psi_2})dx. \end{aligned} \tag{1.7}$$

From the first equation of (1.3), it follows that

$$\begin{aligned} &\bar{\psi_1}\frac{\partial}{\partial t}\psi_1 + \psi_1\frac{\partial}{\partial t}\bar{\psi_1} \\ =&\bar{\psi_1}[-\frac{\partial\psi_2}{\partial x} - im\psi_1 - 2i\lambda(|\psi_2|^2 - |\psi_1|^2)\psi_1] \\ &+ \psi_1[-\frac{\partial\bar{\psi_2}}{\partial x} + im\bar{\psi_1} + 2i\lambda(|\psi_2|^2 - |\psi_1|^2)\bar{\psi_1}] \\ =& - \bar{\psi_1}\frac{\partial\psi_2}{\partial x} - \psi_1\frac{\partial\bar{\psi_2}}{\partial x}. \end{aligned} \tag{1.8}$$

Similarly, by using the second equation of (1.3), we have

$$\bar{\psi_2}\frac{\partial}{\partial t}\psi_2 + \psi_2\frac{\partial}{\partial t}\bar{\psi_2} = -\bar{\psi_2}\frac{\partial\psi_1}{\partial x} - \psi_2\frac{\partial\bar{\psi_1}}{\partial x}. \tag{1.9}$$

Substituting (1.8) and (1.9) into (1.7) leads to

$$\begin{aligned} \frac{d\mathcal{Q}}{dt} &= -\int_R (\bar{\psi_1}\frac{\partial\psi_2}{\partial x} + \psi_1\frac{\partial\bar{\psi_2}}{\partial x} + \bar{\psi_2}\frac{\partial\psi_1}{\partial x} + \psi_2\frac{\partial\bar{\psi_1}}{\partial x})dx \\ &= -\int_R \frac{\partial}{\partial x}(\bar{\psi_1}\psi_2 + \psi_1\bar{\psi_2})dx = -(\bar{\psi_1}\psi_2 + \psi_1\bar{\psi_2})|_{-\infty}^{+\infty} \\ &= 0. \end{aligned} \tag{1.10}$$

The proof is finished. ■

Remark 1.2 *The Dirac equation can be deduced from the time-dependent Schrödinger equation, $|\psi_1|^2$ and $|\psi_2|^2$ represent the probability density of the particle being in the two states respectively, the charge conservation law represents the probability conservation, so it is a important quantity in physics process. Therefore, in latter numerical methods we emphasize on not only* *the discrete geometric structure, the discrete energy and momentum conservation information, but also the discrete charge conservation law.*

We will present proofs of other two conservation laws in the next section.

2. Multi-symplecticity of the Dirac equation

First, we rewrite the complex two-component spinorial wave function as real four-component form, that is, let $\psi_1 = p_1 + iq_1$, $\psi_2 = p_2 + iq_2$, where p_k and q_k be real functions $(k = 1, 2)$ as required above. Now replacing ψ_k in (1.3) by p_k and q_k, leads to

$$\begin{cases} \frac{\partial p_1}{\partial t} + \frac{\partial p_2}{\partial x} - mq_1 - 2\lambda(p_2^2 + q_2^2 - p_1^2 - q_1^2)q_1 = 0 \\ \frac{\partial q_1}{\partial t} + \frac{\partial q_2}{\partial x} + mp_1 + 2\lambda(p_2^2 + q_2^2 - p_1^2 - q_1^2)p_1 = 0 \\ \frac{\partial p_2}{\partial t} + \frac{\partial p_1}{\partial x} + mq_2 + 2\lambda(p_2^2 + q_2^2 - p_1^2 - q_1^2)q_2 = 0 \\ \frac{\partial q_2}{\partial t} + \frac{\partial q_1}{\partial x} - mp_2 - 2\lambda(p_2^2 + q_2^2 - p_1^2 - q_1^2)p_2 = 0. \end{cases} \tag{2.1}$$

We find that (1.3) can be written as

$$Mz_t + Kz_x = \nabla_z S(z) \tag{2.2}$$

with state variable $z = (p_1, q_1, p_2, q_2)^T$, here we use the real vector function z to substitute the complex wave function ψ for latter discussions. M and K are skew-symmetric matrices,

$$M = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}, \qquad K = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

and $S: \ R^4 \ \rightarrow \ R$ is a smooth function,

$$S(z) = \frac{1}{2}(\lambda(p_1^2 + q_1^2 - p_2^2 - q_2^2) - m)(p_1^2 + q_1^2 - p_2^2 - q_2^2).$$

In terms of (1.1), we can get the initial condition

$$z_f(x) = z(x, 0) = (\phi_{11}(x), \phi_{12}(x), \phi_{21}(x), \phi_{22}(x))^T, \tag{2.3}$$

where $\phi_1(x) = \phi_{11}(x) + i\phi_{12}(x), \ \phi_2(x) = \phi_{21}(x) + i\phi_{22}(x)$.

According to [4, 6, 7, 8, 9, 11, 12, 13, 14, 15] and references therein, the above system (2.2) is called multi-symplectic Hamiltonian system, because it has a multi-symplectic conservation law

$$\frac{\partial \omega}{\partial t} + \frac{\partial \kappa}{\partial x} = 0, \tag{2.4}$$

where ω and κ are pre-symplectic forms,

$$\omega = \frac{1}{2} dz \wedge \ Mdz \quad \text{ and } \quad \kappa = \frac{1}{2} dz \wedge \ Kdz. \tag{2.5}$$

The system has an energy conservation law (ECL)

$$\frac{\partial E}{\partial t}+\frac{\partial F}{\partial x}=0 \tag{2.6}$$

with energy density

$$E=S(z)-\frac{1}{2}z^TKz_x$$

and energy flux

$$F=\frac{1}{2}z^TKz_t.$$

Remember the energy formula in (1.2) and compare with the energy density given here, we find that

$$\Im(\bar{\psi_1}\frac{\partial}{\partial x}\psi_2+\bar{\psi_2}\frac{\partial}{\partial x}\psi_1)+\tilde{f}(|\psi_1|^2-|\psi_2|^2)=-2E,$$

that is,

$$\tilde{E}(\psi)(t)=-2\int_R E(z(x,t))dx. \tag{2.7}$$

The system has also a momentum conservation law (MCL)

$$\frac{\partial I}{\partial t}+\frac{\partial G}{\partial x}=0 \tag{2.8}$$

with momentum density

$$I=\frac{1}{2}z^TMz_x$$

and momentum flux

$$G=S(z)-\frac{1}{2}z^TMz_t.$$

Similarly, corresponding to the linear formula given in (1.2), we obtain

$$\Im(\bar{\psi_1}\frac{\partial}{\partial x}\psi_1+\bar{\psi_2}\frac{\partial}{\partial x}\psi_2)=2I,$$

namely

$$\mathcal{P}(\psi)(t)=2\int_R I(z(x,t))dx. \tag{2.9}$$

We must point out that the three conservation laws given above are the local properties which hold for any multi-symplectic system[4], but in general they couldn't provide more information on the global properties of the system. However, under appropriate assumptions, it is possible to obtain the corresponding global conservation laws of the local properties, such as the following proposition.

Proposition 2.1 *Under the assumptions of Proposition 1.1, and if*

$$\lim_{|x|\to+\infty}|\partial_x\psi(x,t)|=0 \ \text{ uniformly for } \ t\in R, \tag{2.10}$$

then the system (1.3) has two conservation laws

$$\mathcal{P}(\psi)(t)=\mathcal{P}(\phi), \tag{2.11}$$

$$\tilde{E}(\psi)(t)=\tilde{E}(\phi) \tag{2.12}$$

on the linear momentum and the energy as mentioned in section 1 respectively, where

$$\mathcal{P}(\phi)(t)=\int_R \Im(\bar{\phi_1}\frac{\partial}{\partial x}\phi_1+\bar{\phi_2}\frac{\partial}{\partial x}\phi_2)dx, \tag{2.13}$$

$$\tilde{E}(\phi)(t)=\int_R \big(\Im(\bar{\phi_1}\frac{\partial}{\partial x}\phi_2+\bar{\phi_2}\frac{\partial}{\partial x}\phi_1)+\tilde{f}(|\phi_1|^2-|\phi_2|^2)\big)dx. \tag{2.14}$$

Proof. We integrate (2.6) over R, then

$$\int_R(\frac{\partial E}{\partial t}+\frac{\partial F}{\partial x})dx=0. \tag{2.15}$$

(2.2) implies that

$$z_t=M^{-1}(\nabla_z S(z)-Kz_x)=-M\nabla_z S(z)+MKz_x, \tag{2.16}$$

since $\nabla_z S(z)$ is a vector function, each of whose entries is a multivariable polynomial with the degree of 3, under the assumptions of this proposition, we can conclude that

$$\lim_{|x|\to+\infty}\nabla_z S(z)=0 \quad \text{and} \quad \lim_{|x|\to+\infty} z_x=0. \tag{2.17}$$

Therefore, (2.16) and (2.17) imply

$$\lim_{|x|\to+\infty} z_t=0. \tag{2.18}$$

The left term of (2.15) can be written as

$$\begin{aligned}&\int_R(\frac{\partial E}{\partial t}+\frac{\partial F}{\partial x})dx=\int_R\frac{\partial E}{\partial t}dx+F|_{-\infty}^{+\infty}\\ =&\frac{d}{dt}\int_R Edx+(\frac{1}{2}z^TKz_t)|_{-\infty}^{+\infty}\\ =&\frac{d}{dt}\int_R Edx.\end{aligned} \tag{2.19}$$

Combining (2.7), we find that

$$\frac{d}{dt}\tilde{E}(\psi)(t)=0, \tag{2.20}$$

which shows that (2.12) holds, namely, we have obtained the energy conservation law. Similarly, combining (2.9) and the local momentum conservation law (2.8), the momentum conservation law can be obtained. This completes the proof. ■

It is significant to find more numerical methods which preserve multi-symplectic conservation law (2.4) for Hamiltonian systems (2.2).

3. Multi-symplectic RK methods

For the numerical discretization, we introduce an uniform grid [10] $(x_j,t_k)\in R^2$ with mesh-length $\triangle t$ in the t-direction and mesh-length $\triangle x$ in the x-direction, and denote the value of the function $\psi(x,t)$ at the mesh point (x_j,t_k) by ψ_j^k. The equation (2.2) and the multi-symplectic conservation law (2.4) can be, respectively, schemed numerically as

$$M\partial_t^{j,k}z_j^k+K\partial_x^{j,k}z_j^k=(\nabla_z S(z))_j^k, \tag{3.1}$$

$$\partial_t^{j,k}\omega_j^k + \partial_x^{j,k}\kappa_j^k = 0, \tag{3.2}$$

where $(\nabla_z S(z))_j^k = (\nabla_z S(z_j^k))$,

$$\omega = \frac{1}{2}(dz)_j^k \wedge\ M(dz)_j^k \quad \text{ and } \quad \kappa = \frac{1}{2}(dz)_j^k \wedge\ K(dz)_j^k,$$

$\partial_t^{j,k}$, $\partial_x^{j,k}$ are discretizations of the partial derivatives ∂_t and ∂_x respectively.

Definition 3.1 *The numerical scheme (3.1) of (2.2) is said to be multi-symplectic if (3.2) is a discrete conservation law of (3.1).*

In [15], Reich showed that the Gauss-Legendre discretization applied to the scalar wave equation (and Schrödinger equation) both in time and space direction, leads to a multi-symplectic integrator (also see [11]). [6] presented the condition of multi-symplecticity of Runge-Kutta methods and Partitioned Runge-Kutta methods for general multi-symplectic Hamiltonian systems with the form (2.2). In this section we characterize the multi-symplectic Runge-Kutta methods for the Dirac equation (1.3). For the convenience of readers, we will give details of proof for the result. To simplify notations, let the starting point $(x_0, t_0) = (0, 0)$. Applying r-stage and s-stage RK methods to the t-direction and x-direction in the multi-symplectic system (2.2) respectively, we will get the following

$$\begin{cases} Z_m^k = z_m^0 + \triangle t \sum\limits_{j=1}^{r} a_{kj}\partial_t Z_m^j, \\ z_m^1 = z_m^0 + \triangle t \sum\limits_{k=1}^{r} b_k \partial_t Z_m^k, \\ Z_m^k = z_0^k + \triangle x \sum\limits_{n=1}^{s} \tilde{a}_{mn}\partial_x Z_n^k, \\ z_1^k = z_0^k + \triangle x \sum\limits_{m=1}^{s} \tilde{b}_m \partial_x Z_m^k, \\ M\partial_t Z_m^k + K\partial_x Z_m^k = \nabla_z S(Z_m^k), \end{cases} \tag{3.3}$$

here we made use of the following notations: $Z_m^k \approx z(c_m\triangle t, d_k\triangle x)$, $z_m^0 \approx z(c_m\triangle x, 0)$, $\partial_t Z_m^k \approx \partial_t z(c_m\triangle x, d_k\triangle t)$, $\partial_x Z_m^k \approx \partial_x z(c_m\triangle x, d_k\triangle t)$, $z_m^1 \approx z(c_m\triangle x, \triangle t)$, $z_0^k \approx z(0, d_k\triangle t)$, $z_m^0 \approx z(c_m\triangle x, 0)$, and

$$c_m = \sum_{n=1}^{s} \tilde{a}_{mn}, \qquad d_k = \sum_{j=1}^{r} a_{kj}.$$

The variational equation corresponding to (3.3) is

$$\begin{cases} dZ_m^k = dz_m^0 + \triangle t \sum\limits_{j=1}^{r} a_{kj} d(\partial_t Z)_m^j, \\ dz_m^1 = dz_m^0 + \triangle t \sum\limits_{k=1}^{r} b_k d(\partial_t Z)_m^k, \\ dZ_m^k = dz_0^k + \triangle x \sum\limits_{n=1}^{s} \tilde{a}_{mn} d(\partial_x Z)_n^k, \\ dz_1^k = dz_0^k + \triangle x \sum\limits_{m=1}^{s} \tilde{b}_m d(\partial_x Z)_m^k, \\ Md(\partial_t Z)_m^k + Kd(\partial_x Z)_m^k = D_{zz}S(Z_m^k)dZ_m^k, \end{cases} \tag{3.4}$$

where we use the abbreviations, dZ_m^k denotes $(dZ)_m^k$, $d(\partial_t Z)_m^k$ denotes $(d(\partial_t Z))_m^k$ and so on.

Theorem 3.2 *If the method (3.3) satisfies the following coefficient conditions*

$$\begin{cases} b_k b_j - b_k a_{kj} - b_j a_{jk} = 0, \\ \tilde{b}_m \tilde{b}_n - \tilde{b}_m \tilde{a}_{mn} - \tilde{b}_n \tilde{a}_{nm} = 0, \end{cases} \tag{3.5}$$

for all $k, j = 1, 2, \cdots, r$, *and* $m, n = 1, \cdots, s$, *then (3.3) is multi-symplectic with the discrete multi-symplectic conservation law*

$$\triangle x \sum_{m=1}^{s} \tilde{b}_m (\omega_m^1 - \omega_m^0) + \triangle t \sum_{k=1}^{r} b_k (\kappa_1^k - \kappa_0^k) = 0, \tag{3.6}$$

where $\omega_m^1 = \frac{1}{2} dz_m^1 \wedge M dz_m^1$, $\kappa_1^k = \frac{1}{2} dz_1^k \wedge K dz_1^k$, $\omega_m^0 = \frac{1}{2} dz_m^0 \wedge M dz_m^0$, $\kappa_0^k = \frac{1}{2} dz_0^k \wedge K dz_0^k$.

Proof. Consider the discrete variational equations (3.4), using the second equation of (3.4), we find

$$\begin{aligned} & dz_m^1 \wedge M dz_m^1 - dz_m^0 \wedge M dz_m^0 \\ =& (dz_m^1 - dz_m^0) \wedge M dz_m^1 + dz_m^0 \wedge M (dz_m^1 - dz_m^0) \\ =& \triangle t \Big[\Big(\sum_{k=1}^{r} b_k d(\partial_t Z)_m^k \Big) \wedge M \Big(dz_m^0 + \triangle t \sum_{j=1}^{r} b_j d(\partial_t Z)_m^j \Big) \\ & + dz_m^0 \wedge M \sum_{k=1}^{r} b_k d(\partial_t Z)_m^k \Big] \\ =& \triangle t \sum_{k=1}^{r} b_k \Big(d(\partial_t Z)_m^k \wedge M dz_m^0 + dz_m^0 \wedge d(\partial_t Z)_m^k \Big) \\ & + \triangle t^2 \sum_{k=1}^{r} \sum_{j=1}^{r} b_k b_j d(\partial_t Z)_m^k \wedge M d(\partial_t Z)_m^j. \end{aligned} \tag{3.7}$$

By using the first equation of (3.4), (3.7) reads

$$\begin{aligned} & \triangle t \sum_{k=1}^{r} b_k \Big[d(\partial_t Z)_m^k \wedge M \Big(dZ_m^k - \triangle t \sum_{j=1}^{r} a_{kj} d(\partial_t Z)_m^j \Big) \\ & + \Big(dZ_m^k - \triangle t \sum_{j=1}^{r} a_{kj} d(\partial_t Z)_m^j \Big) \wedge M d(\partial_t Z)_m^k \Big] \\ & + \triangle t^2 \sum_{k=1}^{r} \sum_{j=1}^{r} b_k b_j d(\partial_t Z)_m^k \wedge M d(\partial_t Z)_m^j \\ =& 2 \triangle t \sum_{k=1}^{r} b_k d(\partial_t Z)_m^k \wedge M dZ_m^k \\ & + \triangle t^2 \sum_{k=1}^{r} \sum_{j=1}^{r} (b_k b_j - b_k a_{kj}) d(\partial_t Z)_m^k \wedge M d(\partial_t Z)_m^j \\ & - \triangle t^2 \sum_{k=1}^{r} \sum_{j=1}^{r} b_k a_{kj} d(\partial_t Z)_m^j \wedge M d(\partial_t Z)_m^k \end{aligned} \tag{3.8}$$

where the constant coefficient 2 derives from the skew-symmetry of the matrix M. When we commute the position of the low index j and k in the last term of the right side of (3.8), noticing that M is skew-symmetric, we can deduce that

$$\begin{aligned}
&2\triangle t\sum_{k=1}^{r}b_k d(\partial_t Z)_m^k\wedge MdZ_m^k\\
&+\triangle t^2\sum_{k=1}^{r}\sum_{j=1}^{r}(b_kb_j-b_ka_{kj}-b_ja_{jk})d(\partial_t Z)_m^k\wedge Md(\partial_t Z)_m^j\\
=&2\triangle t\sum_{k=1}^{r}b_k d(\partial_t Z)_m^k\wedge MdZ_m^k,
\end{aligned}\tag{3.9}$$

where the last equality derives from the multi-symplectic condition (3.5).

According to (3.7)-(3.9), we have

$$\begin{aligned}
&dz_m^1\wedge Mdz_m^1-dz_m^0\wedge Mdz_m^0=2\triangle t\sum_{k=1}^{r}b_k d(\partial_t Z)_m^k\wedge MdZ_m^k\\
=&2\triangle t\sum_{k=1}^{r}b_k dZ_m^k\wedge Md(\partial_t Z)_m^k,
\end{aligned}\tag{3.10}$$

where the last equality derives from the skew-symmetry of M.

By using the third and the fourth equation of (3.4), noticing the skew-symmetry of the matrix K, and with similar calculation, it is deduced that

$$dz_1^k\wedge Kdz_1^k-dz_0^k\wedge Kdz_0^k=2\triangle x\sum_{m=1}^{s}\tilde{b}_m dZ_m^k\wedge Kd(\partial_x Z)_m^k.\tag{3.11}$$

Substituting (3.10) and (3.11) into the left side of (3.6) leads to

$$\begin{aligned}
&\triangle x\sum_{m=1}^{s}\tilde{b}_m(\omega_m^1-\omega_m^0)+\triangle t\sum_{k=1}^{r}b_k(\kappa_1^k-\kappa_0^k)\\
=&2\triangle x\triangle t\sum_{k=1}^{r}\sum_{m=1}^{s}b_k\tilde{b}_m dZ_m^k\wedge\Big(Md(\partial_t Z)_m^k+Kd(\partial_x Z)_m^k\Big).
\end{aligned}\tag{3.12}$$

From the last equation of (3.4), it follows that

$$\begin{aligned}
&\triangle x\sum_{m=1}^{s}\tilde{b}_m(\omega_m^1-\omega_m^0)+\triangle t\sum_{k=1}^{r}b_k(\kappa_1^k-\kappa_0^k)\\
=&2\triangle x\triangle t\sum_{k=1}^{r}\sum_{m=1}^{s}b_k\tilde{b}_m dZ_m^k\wedge D_{zz}S(Z_m^k)dZ_m^k\\
=&0,
\end{aligned}\tag{3.13}$$

where the last equality comes from that the second order derivative matrix $D_{zz}S(Z_m^k)$ is symmetric. The proof is completed. ■

Theorem 3.2 tells us that the symplectic Runge-Kutta discretization applied to the multi-symplectic Hamiltonian system (3.2) both in time and space direction, leads to a multi-symplectic integrator. A great interest is in whether the MSRK methods preserve the physical conservation laws, such as the charge conservation law, momentum conservation law and energy conservation law, etc. We will present some results in the following sections. The discrete conservative properties of some multi-symplectic integrators have been discussed in [4, 9, 6, 11, 12, 13, 14, 15] and some references therein. And for conservative properties of symplectic integrators for Hamiltonian ODEs, see [16].

4. The discrete charge conservation law and the total symplecticity in time

It is recognized that the multi-symplectic conservation law is a local geometric structure of the multi-symplectic equation, which is independent of the initial and boundary conditions. But in numerical methods, the solvability of the origin problem requires some known conditions. The RK methods considered in section 4, 5 and 6 satisfy the condition (3.5) of multi-symplecticity.

First, we replace the whole real spatial region R by the finite interval $[-L/2, L/2]$. The initial condition is given by

$$z(x,0) = z_f(x),$$

where $z_f(x)$ is the same as mentioned in (2.3), but in terms of the discussions of the global conservation properties later, we require that $z_f(x)$ satisfies periodic boundary condition on the interval $[-L/2, L/2]$, namely $z_f(-L/2) = z_f(L/2)$.

Similarly, the consistent periodic boundary condition is given by

$$z(-L/2,t) = z(L/2,t) \quad \text{or} \quad z(-L/2,t) = z(L/2,t) = z_b(t),$$

where $z_b(t)$ is a known real-valued and sufficiently smooth vector function.

Using the conditions given above, we also can obtain the three conservative properties, as mentioned in Proposition 1.1 and 2.1, by replacing the whole real domain R by the finite interval $[-L/2, L/2]$. If setting $z(-L/2,t) = z(L/2,t) = 0$ and let $L \to +\infty$, we will get Proposition 1.1 and 2.1.

Set the spatial points $x_l = -L/2 + lL/N,\ l = 0, 1, \cdots, N$. Let the starting time point $t_0 = 0$, and let $\tau = \triangle t$ and $h = \triangle x = L/N$ be the time step and spatial step respectively, we rewrite the RK method (3.3) over all spatial points as follows

$$\begin{cases} Z_{l,m}^k = z_{l,m}^0 + \tau \sum\limits_{j=1}^{r} a_{kj} \partial_t Z_{l,m}^j, \\ z_{l,m}^1 = z_{l,m}^0 + \tau \sum\limits_{k=1}^{r} b_k \partial_t Z_{l,m}^k, \\ Z_{l,m}^k = z_{l,0}^k + h \sum\limits_{n=1}^{s} \tilde{a}_{mn} \partial_x Z_{l,n}^k, \\ z_{l+1,0}^k = z_{l,0}^k + h \sum\limits_{m=1}^{s} \tilde{b}_m \partial_x Z_{l,m}^k, \\ M \partial_t Z_{l,m}^k + K \partial_x Z_{l,m}^k = \nabla_z S(Z_{l,m}^k), \end{cases} \tag{4.1}$$

where $k = 1, \cdots, r, \quad m = 1, \cdots, s, \quad l = 0, 1, \cdots, N-1, \quad Z_{l,m}^k \approx z((l + c_m)h, d_k\tau)$, $z_{l,m}^0 \approx z((l + c_m)h, 0)$, $z_{l,0}^k \approx z(lh, d_k\tau)$ and so on.

Now we turn to the charge conservation law. For the multi-symplectic Hamiltonian system (2.2), the charge conservation law has the following form

$$\mathcal{Q}(z)(t) = \mathcal{Q}(z_f), \tag{4.2}$$

where $\mathcal{Q}(z)(t) = \int_{-L/2}^{L/2} z(x,t)^T z(x,t)dx$, and $\mathcal{Q}(z_f) = \int_{-L/2}^{L/2} z_f(x)^T z_f(x)dx$.

Theorem 4.1 *The RK method (3.3) satisfying (3.5) has the following discrete charge conservation law*

$$h \sum_{l=0}^{N-1} \sum_{m=1}^{s} \tilde{b}_m \big(Q_e(z_{l,m}^1) - Q_e(z_{l,m}^0)\big) = 0, \tag{4.3}$$

where $Q_e(z) = z^T z$.

Proof. By using the second equation of (4.1), we deduce that

$$\begin{aligned}
&Q_e(z_{l,m}^1) - Q_e(z_{l,m}^0)\\
=& (z_{l,m}^1)^T (z_{l,m}^1 - z_{l,m}^0) + (z_{l,m}^1 - z_{l,m}^0)^T z_{l,m}^0\\
=& (z_{l,m}^1)^T (\tau \sum_{k=1}^{r} b_k \partial_t Z_{l,m}^k) + \tau \sum_{k=1}^{r} b_k (\partial_t Z_{l,m}^k)^T z_{l,m}^0\\
=& \tau (z_{l,m}^0 + \tau \sum_{k=1}^{r} b_k \partial_t Z_{l,m}^k)^T \sum_{k=1}^{r} b_k \partial_t Z_{l,m}^k\\
&+ \tau \sum_{k=1}^{r} b_k (\partial_t Z_{l,m}^k)^T z_{l,m}^0\\
=& \tau \sum_{k=1}^{r} b_k [(z_{l,m}^0)^T \partial_t Z_{l,m}^k + (\partial_t Z_{l,m}^k)^T z_{l,m}^0]\\
&+ \tau^2 \sum_{k=1}^{r} \sum_{j=1}^{r} b_k b_j (\partial_t Z_{l,m}^k)^T \partial_t Z_{l,m}^j.
\end{aligned} \tag{4.4}$$

From the first equation of (4.1), it follows that

$$\begin{aligned}
&\tau \sum_{k=1}^{r} b_k \Big[(Z_{l,m}^k - \tau \sum_{j=1}^{r} a_{kj} \partial_t Z_{l,m}^j)^T \partial_t Z_{l,m}^k\\
&+ (\partial_t Z_{l,m}^k)^T (Z_{l,m}^k - \tau \sum_{j=1}^{r} a_{kj} \partial_t Z_{l,m}^j) \Big] + \tau^2 \sum_{k=1}^{r} \sum_{j=1}^{r} b_k b_j (\partial_t Z_{l,m}^k)^T \partial_t Z_{l,m}^j\\
=& \tau \sum_{k=1}^{r} b_k \Big[(Z_{l,m}^k)^T \partial_t Z_{l,m}^k + (\partial_t Z_{l,m}^k)^T Z_{l,m}^k \Big]\\
&+ \tau^2 \Big[\sum_{k=1}^{r} \sum_{j=1}^{r} (b_k b_j - b_k a_{kj}) (\partial_t Z_{l,m}^k)^T \partial_t Z_{l,m}^j - \sum_{k=1}^{r} \sum_{j=1}^{r} b_k a_{kj} (\partial_t Z_{l,m}^j)^T \partial_t Z_{l,m}^k \Big]\\
=& 2\tau \sum_{k=1}^{r} b_k (Z_{l,m}^k)^T \partial_t Z_{l,m}^k\\
&+ \tau^2 \sum_{k=1}^{r} \sum_{j=1}^{r} (b_k b_j - b_k a_{kj} - b_j a_{jk}) (\partial_t Z_{l,m}^k)^T \partial_t Z_{l,m}^j,
\end{aligned} \tag{4.5}$$

where the last equality is obtained from the commutative technique of low indexes j and k as mentioned in section 3.

Combining (4.4), (4.5) and the multi-symplectic condition (3.5), we get

$$Q_e(z_{l,m}^1) - Q_e(z_{l,m}^0) = 2\tau \sum_{k=1}^{r} b_k (Z_{l,m}^k)^T \partial_t Z_{l,m}^k. \tag{4.6}$$

Here we have introduced some notations, $(P_1)_{l,m}^k \approx p_1((l+c_m)h, d_k\tau)$, $(\partial_t P_1)_{l,m}^k \approx \partial_t p_1((l+c_m)h, d_k\tau)$, $(\partial_x P_1)_{l,m}^k \approx \partial_x p_1((l+c_m)h, d_k\tau)$, $(Q_1)_{l,m}^k \approx q_1((l+c_m)h, d_k\tau)$, and so on.

By using the notations introduced above, the last equation of (4.1) can be written as

$$\begin{cases} (\partial_t P_1)_{l,m}^k + (\partial_x P_2)_{l,m}^k - \underline{\mathrm{m}}(Q_1)_{l,m}^k \\ \qquad - 2\lambda[((P_2)_{l,m}^k)^2 + ((Q_2)_{l,m}^k)^2 - ((P_1)_{l,m}^k)^2 - ((Q_1)_{l,m}^k)^2](Q_1)_{l,m}^k = 0, \\ \\ (\partial_t Q_1)_{l,m}^k + (\partial_x Q_2)_{l,m}^k + \underline{\mathrm{m}}(P_1)_{l,m}^k \\ \qquad + 2\lambda[((P_2)_{l,m}^k)^2 + ((Q_2)_{l,m}^k)^2 - ((P_1)_{l,m}^k)^2 - ((Q_1)_{l,m}^k)^2](P_1)_{l,m}^k = 0, \\ \\ (\partial_t P_2)_{l,m}^k + (\partial_x P_1)_{l,m}^k + \underline{\mathrm{m}}(Q_2)_{l,m}^k \\ \qquad + 2\lambda[((P_2)_{l,m}^k)^2 + ((Q_2)_{l,m}^k)^2 - ((P_1)_{l,m}^k)^2 - ((Q_1)_{l,m}^k)^2](Q_2)_{l,m}^k = 0, \\ \\ (\partial_t Q_2)_{l,m}^k + (\partial_x Q_1)_{l,m}^k - \underline{\mathrm{m}}(P_2)_{l,m}^k \\ \qquad - 2\lambda[((P_2)_{l,m}^k)^2 + ((Q_2)_{l,m}^k)^2 - ((P_1)_{l,m}^k)^2 - ((Q_1)_{l,m}^k)^2](P_2)_{l,m}^k = 0, \end{cases} \tag{4.7}$$

where we use the notation $\underline{\mathrm{m}}$, which distinguishes from the low index m, to denote the constant m in the Dirac equation.

Premultiplying the four equations of (4.7) by $(P_1)_{l,m}^k$, $(Q_1)_{l,m}^k$, $(P_2)_{l,m}^k$ and $(Q_2)_{l,m}^k$, respectively, it follows that

$$\begin{aligned} & (Z_{l,m}^k)^T \partial_t Z_{l,m}^k \\ = \; & (P_1)_{l,m}^k (\partial_t P_1)_{l,m}^k + (P_2)_{l,m}^k (\partial_t P_2)_{l,m}^k + (Q_1)_{l,m}^k (\partial_t Q_1)_{l,m}^k + (Q_2)_{l,m}^k (\partial_t Q_2)_{l,m}^k \\ = \; & (P_1)_{l,m}^k \{ - (\partial_x P_2)_{l,m}^k + \underline{\mathrm{m}}(Q_1)_{l,m}^k + \cdots \} + \cdots \\ = \; & (P_1)_{l,m}^k (\partial_x P_2)_{l,m}^k + (P_2)_{l,m}^k (\partial_x P_1)_{l,m}^k + (Q_1)_{l,m}^k (\partial_x Q_2)_{l,m}^k + (Q_2)_{l,m}^k (\partial_x Q_1)_{l,m}^k, \end{aligned} \tag{4.8}$$

From Theorem 4.4, it follows that

$$\begin{aligned} & \sum_{m=1}^{s} \tilde{b}_m \big[(P_1)_{l,m}^k (\partial_x P_2)_{l,m}^k + (P_2)_{l,m}^k (\partial_x P_1)_{l,m}^k \\ & \quad + (Q_1)_{l,m}^k (\partial_x Q_2)_{l,m}^k + (Q_2)_{l,m}^k (\partial_x Q_1)_{l,m}^k \big] \\ = \; & (p_1 p_2)_{l+1,0}^k + (q_1 q_2)_{l+1,0}^k - (p_1 p_2)_{l,0}^k - (q_1 q_2)_{l,0}^k, \end{aligned} \tag{4.9}$$

where $(p_1)_{l,0}^k = p_1(lh, d_k\tau)$, $(p_1p_2)_{l,0}^k = (p_1)_{l,0}^k(p_2)_{l,0}^k$ and so on. According to (4.8) and (4.9), we have

$$\begin{aligned} & h\sum_{l=0}^{N-1}\sum_{m=1}^{s}\tilde{b}_m(Q_e(z_{l,m}^1) - Q_e(z_{l,m}^0)) \\ = \ & 2h\tau\sum_{k=1}^{r} b_k\sum_{l=0}^{N-1}[(p_1p_2+q_1q_2)_{l+1,0}^k - (p_1p_2+q_1q_2)_{l,0}^k] \\ = \ & 2h\tau\sum_{k=1}^{r} b_k[(p_1p_2+q_1q_2)_{N,0}^k - (p_1p_2+q_1q_2)_{0,0}^k] \\ = \ & 0, \end{aligned} \tag{4.10}$$

where the last equality comes from the periodic boundary condition. This completes the proof. ■

Remark 4.2 *From (4.10), when replacing the periodic boundary conditions by the following weaker one*

$$p_1(-L/2,t)p_2(-L/2,t) + q_1(-L/2,t)q_2(-L/2,t) = p_1(L/2,t)p_2(L/2,t) + q_1(L/2,t)q_2(L/2,t),$$

we also can obtain the discrete charge conservation law.

Remark 4.3 *Quadratic invariants appear in a large number of applications and play an important role in some practical situations, they seem easier than other nonlinear invariants, but even though in the case of Hamiltonian ODEs, symplectic integrators, in general, may not preserve quadratic invariants [16].*

The "continuous" charge conservation law (4.2) shows that $\partial_t\mathcal{Q}(z)(t) = 0$, and the left side of (4.3) is the corresponding discrete approximation of the following local integration

$$\int_0^\tau \partial_t\mathcal{Q}(z)(t) = \mathcal{Q}(z)(\tau) - \mathcal{Q}(z)(0).$$

The following result characterizes the conservative properties of "semi-Runge-Kutta" methods.

Theorem 4.4 *If the following "semi-RK" method is used for two arbitrary functions $p(x)$ and $q(x)$,*

$$\begin{cases} P_{l,m} = p_l + h\sum_{n=1}^{s}\tilde{a}_{mn}\partial_x P_{l,n}, \\ Q_{l,m} = q_l + h\sum_{n=1}^{s}\tilde{a}_{mn}\partial_x Q_{l,n}, \\ p_{l+1} = p_l + h\sum_{m=1}^{s}\tilde{b}_m\partial_x P_{l,m}, \\ q_{l+1} = q_l + h\sum_{m=1}^{s}\tilde{b}_m\partial_x Q_{l,m}, \end{cases} \tag{4.11}$$

where the notations are similar to the above we used. If the coefficients of this RK method satisfies

$$\tilde{b}_m\tilde{b}_n - \tilde{b}_m\tilde{a}_{mn} - \tilde{b}_n\tilde{a}_{nm} = 0, \tag{4.12}$$

for any $m, n = 1, \cdots, s$, then we have

$$(pq)_{l+1} - (pq)_l - h\sum_{m=1}^{s}\tilde{b}_m(P_{l,m}\partial_x Q_{l,m} + Q_{l,m}\partial_x P_{l,m}) = 0. \tag{4.13}$$

Proof. By using the last two equations of (4.11), one has

$$\begin{aligned}
&(pq)_{l+1}-(pq)_l=(p_{l+1}-p_l)q_{l+1}+p_l(q_{l+1}-q_l)\\
=\;& h\sum_{m=1}^{s}\tilde{b}_m\partial_x P_{l,m}\;q_{l+1}+h\sum_{m=1}^{s}\tilde{b}_m p_l\partial_x Q_{l,m}\\
=\;& h\sum_{m=1}^{s}\tilde{b}_m(\partial_x P_{l,m}\;q_l+p_l\partial_x Q_{l,m})+h^2\sum_{m=1}^{s}\sum_{n=1}^{s}\tilde{b}_m\tilde{b}_n\partial_x P_{l,m}\partial_x Q_{l,n}.
\end{aligned}\tag{4.14}$$

Simultaneously, by using the first two equations of (4.11), we can deduce that

$$\begin{aligned}
& h\sum_{m=1}^{s}\tilde{b}_m(P_{l,m}\partial_x Q_{l,m}+Q_{l,m}\partial_x P_{l,m})\\
=\;& h\sum_{m=1}^{s}\tilde{b}_m[(p_l+h\sum_{n=1}^{s}\tilde{a}_{mn}\partial_x P_{l,n})\partial_x Q_{l,m}+(q_l+h\sum_{n=1}^{s}\tilde{a}_{mn}\partial_x Q_{l,n})\partial_x P_{l,m}].
\end{aligned}\tag{4.15}$$

Substituting (4.14) and (4.15) into the left side of (4.13), we have

$$\begin{aligned}
& (pq)_{l+1}-(pq)_l-h\sum_{m=1}^{s}\tilde{b}_m(P_{l,m}\partial_x Q_{l,m}+Q_{l,m}\partial_x P_{l,m})\\
=\;& h^2\sum_{m=1}^{s}\sum_{n=1}^{s}(\tilde{b}_m\tilde{b}_n-\tilde{b}_m\tilde{a}_{mn})\partial_x P_{l,m}\partial_x Q_{l,n}\\
& -h^2\sum_{m=1}^{s}\sum_{n=1}^{s}\tilde{b}_m\tilde{a}_{mn}\partial_x P_{l,n}\partial_x Q_{l,m}\\
=\;& h^2\sum_{m=1}^{s}\sum_{n=1}^{s}(\tilde{b}_m\tilde{b}_n-\tilde{b}_m\tilde{a}_{mn}-\tilde{b}_n\tilde{a}_{nm})\partial_x P_{l,m}\partial_x Q_{l,n}\\
=\;& 0.
\end{aligned}\tag{4.16}$$

The proof is finished. ■

As mentioned in Remark 1.2, the charge conservation law means the probability conservation, it is the basic conservative quantity in quantum physics. As well known, the energy and momentum information of the particle with the spin are also important, we will discuss the discrete energy and momentum conservation laws in section 5 and 6 respectively.

Discrete conservation of multi-symplecticity as discussed in section 3 is a local property of the multi-symplectic Hamiltonian system. *Locality is the natural setting for discretizations such as finite difference discretizations. On the other hand, a nature question is whether the corresponding global properties can be reflected by a numerical method*(see [4]). Here, the global symplecticity we will consider is in time, that is, when we integrate the local multi-symplectic conservation law on the spatial domain and with some additional boundary conditions, we can get the global symplectic conservation in time. In the discrete situation, a corresponding problem is that whether it has the discrete conservation when summed over all spatial grid points.

When we integrate the multi-symplectic conservation law (2.4) over the spatial interval

$[-L/2, L/2]$, which yields the following identity

$$\begin{aligned} 0 &= \int_{-L/2}^{L/2} (\frac{\partial}{\partial t}\omega + \frac{\partial}{\partial x}\kappa) dx \\ &= \int_{-L/2}^{L/2} \frac{\partial}{\partial t}\omega dx + \kappa(L/2, t) - \kappa(-L/2, t) \\ &= \frac{d}{dt}\int_{-L/2}^{L/2} \omega dx, \end{aligned} \tag{4.17}$$

namely,

$$\int_{-L/2}^{L/2} \omega(x,t) dx = \int_{-L/2}^{L/2} \omega(x,0) dx, \tag{4.18}$$

which shows the global symplecticity is conserved in time in the continuous case. When we sum the discrete symplectic conservation law over all spatial grid points, we have

$$\begin{aligned} 0 &= h \sum_{l=0}^{N-1} \sum_{m=1}^{s} \tilde{b}_m (\omega_{l,m}^1 - \omega_{l,m}^0) + \tau \sum_{l=0}^{N-1} \sum_{k=1}^{r} b_k (\kappa_{l+1,0}^k - \kappa_{l,0}^k) \\ &= h \sum_{l=0}^{N-1} \sum_{m=1}^{s} \tilde{b}_m (\omega_{l,m}^1 - \omega_{l,m}^0) + \tau \sum_{k=1}^{r} b_k (\kappa_{N,0}^k - \kappa_{0,0}^k) \\ &= h \sum_{l=0}^{N-1} \sum_{m=1}^{s} \tilde{b}_m (\omega_{l,m}^1 - \omega_{l,m}^0), \end{aligned} \tag{4.19}$$

where the last equality comes from the periodic boundary condition on the spatial domain. This implies the following discrete global symplectic conservation law in time

$$h \sum_{l=0}^{N-1} \sum_{m=1}^{s} \tilde{b}_m \omega_{l,m}^1 = h \sum_{l=0}^{N-1} \sum_{m=1}^{s} \tilde{b}_m \omega_{l,m}^0, \tag{4.20}$$

comparing (4.20) with (4.18), we find that (4.20) is the discrete approximation of (4.18) and we draw a conclusion that multi-symplectic RK methods have the discrete global symplectic conservation law in time. Indeed we have shown that — with appropriate boundary conditions, here we use periodic boundary conditions, the local symplectic property implies the global property. In following two sections we will discuss the local energy and momentum conservation laws when applying the MSRK methods to the multi-symplectic Hamiltonian system. And under assumptions of the periodic boundary condition, we also discuss some global properties.

5. Energy analysis for the multi-symplectic RK methods

Since symplectic RK methods conserve quadratic invariants of ODEs exactly [16], it is concluded that multi-symplectic RK methods can preserve the energy and momentum conservation laws precisely if the multi-symplectic Hamiltonian $S(z)$ is quadratic or linear(see [4]). But in Dirac equations, the Hamiltonian $S(z)$ in the multi-symplectic form (2.2) is not quadratic or linear, so the scheme (3.3) in general hasn't the discrete energy and momentum conservation laws. We investigate the local error estimation of ECL and MCL in section 5 and section 6 respectively.

Due to (2.7) and (2.9), we can omit the integral coefficients -2 and 2 in (2.7) and (2.9) respectively, which will not affect the discussions of the following discrete conservation properties, in other words, we denote the total energy by

$$\mathcal{E}_L(t) = \int_{-L/2}^{L/2} E(z(x,t))dx \tag{5.1}$$

and the total momentum by

$$\mathcal{I}_L(t) = \int_{-L/2}^{L/2} I(z(x,t))dx. \tag{5.2}$$

When we integrate the energy conservation law over the local domain, namely

$$\int_0^h \int_0^\tau (\frac{\partial E}{\partial t} + \frac{\partial F}{\partial x})dtdx = 0, \tag{5.3}$$

then (5.3) has the following form without the derivative symbols in the integrand,

$$\int_0^h [E(z(x,\tau)) - E(z(x,0))]dx + \int_0^\tau [F(z(h,t)) - F(z(0,t))]dt = 0. \tag{5.4}$$

Corresponding to RK method (3.3), we use a discrete form

$$E_{le} \triangleq h\sum_{m=1}^{s} \tilde{b}_m(E(z_m^1) - E(z_m^0)) + \tau\sum_{k=1}^{r} b_k(F(z_1^k) - F(z_0^k)) \tag{5.5}$$

to approximate the left side of (5.4).

An important question is: how is (5.4) preserved by MSRK method (3.3)? Under given conditions, there exists a constant $C > 0$, such that for sufficient small τ and h, $|E_{le}| \leq C\tau h$. To answer the above question, it suffice to find out a modification of the above estimation when applying MSRK (3.3) to (2.2).

Now, the derivative symbols in the left side of ECL (2.6) are eliminated by the local integration, but we also face another similar problem—that the energy, momentum densities, and the fluxes are not the algebraic functions—they depend on derivatives, and the derivatives are contained in the nonlinear terms, which can not be eliminated by using the local integration. In the numerical methods, we have a question that how to transform the derivatives into the algebraic equations. To deal with this, we introduce the following auxiliary system

$$\begin{cases} \partial_x Z_m^k = (\partial_x z)_m^0 + \tau \sum\limits_{j=1}^{r} a_{kj}(\partial_t\partial_x Z)_m^j, \\ (\partial_x z)_m^1 = (\partial_x z)_m^0 + \tau \sum\limits_{k=1}^{r} b_k(\partial_t\partial_x Z)_m^k, \\ \partial_t Z_m^k = (\partial_t z)_0^k + h \sum\limits_{n=1}^{s} \tilde{a}_{mn}(\partial_x\partial_t Z)_{nk}, \\ (\partial_t z)_1^k = (\partial_t z)_0^k + h \sum\limits_{m=1}^{s} \tilde{b}_m(\partial_x\partial_t Z)_m^k, \end{cases} \tag{5.6}$$

where $(\partial_x z)_m^0$ and $(\partial_t z)_0^k$ satisfy

$$z_m^0 = z_0^0 + h\sum_{n=1}^{s} \tilde{a}_{mn}(\partial_x z)_n^0, \tag{5.7}$$

$$z_0^k = z_0^0 + \tau \sum_{j=1}^{r} a_{kj} (\partial_t z)_0^k, \tag{5.8}$$

respectively, and

$$(\partial_t \partial_x Z)_m^k \approx \partial_{tx} z(c_m h, d_k \tau),$$
$$(\partial_x \partial_t Z)_m^k \approx \partial_{xt} z(c_m h, d_k \tau).$$

Assume that matrices $A = (a_{kj})_{r\times r}$ and $\tilde{A} = (\tilde{a}_{mn})_{s\times s}$ are invertible, we have

$$(\partial_t \partial_x Z)_m^k = (\partial_x \partial_t Z)_m^k. \tag{5.9}$$

In fact, the first equation of (3.3), the third equation of (5.6) and (5.8) imply that

$$Z_m^k = z_m^0 + z_0^k - z_0^0 + \tau h \sum_{j=1}^{r} \sum_{n=1}^{s} a_{kj} \tilde{a}_{mn} (\partial_x \partial_t Z)_n^j. \tag{5.10}$$

Similarly, the third equation of (3.3), the first equation of (5.6) and (5.7) imply that

$$Z_m^k = z_0^k + z_m^0 - z_0^0 + h\tau \sum_{j=1}^{r} \sum_{n=1}^{s} a_{kj} \tilde{a}_{mn} (\partial_t \partial_x Z)_n^j. \tag{5.11}$$

From (5.10) and (5.11), we conclude that (5.9) holds for $m = 1, \cdots, s$ and $k = 1, \cdots, r$.

Now we don't distinguish the notations $(\partial_t \partial_x Z)_m^k$ and $(\partial_x \partial_t Z)_m^k$, and use only one notation Y_m^k to denote them. In what follows, we assume that in considering (x, t)-domain, the variables determined by (3.3) and (5.6) all are bounded.

Theorem 5.1 *If the matrices of RK methods in (3.3) satisfying (3.5) are invertible, then for the method (3.3), the error of discrete energy conservation law satisfies*

$$|E_{le}| \leq C\tau^3 h \tag{5.12}$$

for sufficiently small τ and h, where the constant C is independent of τ and h.

Proof. Because

$$E(z_m^1) - E(z_m^0) = S(z_m^1) - S(z_m^0) - \frac{1}{2}[(z_m^1)^T K \partial_x z_m^1 - (z_m^0)^T K \partial_x z_m^0], \tag{5.13}$$

$$F(z_1^k) - F(z_0^k) = \frac{1}{2}[(z_1^k)^T K \partial_t z_1^k - (z_0^k)^T K \partial_t z_0^k], \tag{5.14}$$

by using the second equation of (3.3) and the second equation of (5.6), we have

$$\begin{aligned}
& (z_m^1)^T K \partial_x z_m^1 - (z_m^0)^T K \partial_x z_m^0 \\
= \ & (z_m^1 - z_m^0)^T K \partial_x z_m^1 + (z_m^0)^T K (\partial_x z_m^1 - \partial_x z_m^0) \\
= \ & (\tau \sum_{k=1}^{r} b_k \partial_t Z_m^k)^T K (\partial_x z_m^0 + \tau \sum_{k=1}^{r} b_k Y_m^k) + \tau (z_m^0)^T \sum_{k=0}^{r} K Y_m^k,
\end{aligned} \tag{5.15}$$

from the first equation of (3.3) and the first equation of (5.6), (5.15) reads

$$
\begin{aligned}
& \tau \sum_{k=1}^{r} b_k[(\partial_t Z_m^k)^T K \partial_x Z_m^k + (Z_m^k)^T K Y_m^k] \\
& +\tau^2 \sum_{k=1}^{r}\sum_{j=1}^{r} (b_k b_j - b_k a_{kj} - b_j a_{jk})(\partial_t Z_m^k)^T K Y_m^j \\
= & \ \tau \sum_{k=1}^{r} b_k[(\partial_t Z_m^k)^T K \partial_x Z_m^k + (Z_m^k)^T K Y_m^k].
\end{aligned} \tag{5.16}
$$

Similarly, it follows that

$$
\begin{aligned}
& (z_1^k)^T K \partial_t z_1^k - (z_0^k)^T K \partial_t z_0^k \\
= & \ h \sum_{m=1}^{s} \tilde{b}_m[(\partial_x Z_m^k)^T K \partial_t Z_m^k + (Z_m^k)^T K Y_m^k] \\
& +h^2 \sum_{m=1}^{s}\sum_{n=1}^{s} (\tilde{b}_m \tilde{b}_n - \tilde{b}_m \tilde{a}_{mn} - \tilde{b}_n \tilde{a}_{nm})(\partial_x Z_m^k)^T K Y_n^k \\
= & \ h \sum_{m=1}^{s} \tilde{b}_m[(\partial_x Z_m^k)^T K \partial_t Z_m^k + (Z_m^k)^T K Y_m^k].
\end{aligned} \tag{5.17}
$$

Premultiply the last equation of (3.3) by $(\partial_t Z_m^k)^T$, and notice that M is skew-symmetric, we find that

$$(\partial_t Z_m^k)^T K \partial_x Z_m^k = (\partial_t Z_m^k)^T \nabla_z S(Z_m^k). \tag{5.18}$$

And (5.13)-(5.18) imply that

$$
\begin{aligned}
E_{le} = & \ h \sum_{m=1}^{s} \tilde{b}_m[S(z_m^1) - S(z_m^0)] \\
& +\tfrac{h\tau}{2} \sum_{m=1}^{s}\sum_{k=1}^{r} \tilde{b}_m b_k[(\partial_x Z_m^k)^T K \partial_t Z_m^k - (\partial_t Z_m^k)^T K \partial_x Z_m^k] \\
= & \ h \sum_{m=1}^{s} \tilde{b}_m[S(z_m^1) - S(z_m^0) - \tau \sum_{k=1}^{r} b_k (\partial_t Z_m^k)^T \nabla_z S(Z_m^k)] \\
& +h\tau \sum_{m=1}^{s}\sum_{k=1}^{r} \tilde{b}_m b_k \Big[(\partial_t Z_m^k)^T \nabla_z S(Z_m^k) + \tfrac{1}{2}(\partial_x Z_m^k)^T K \partial_t Z_m^k \\
& -\tfrac{1}{2}(\partial_t Z_m^k)^T K \partial_x Z_m^k\Big] \\
= & \ h \sum_{m=1}^{s} \tilde{b}_m[S(z_m^1) - S(z_m^0) - \tau \sum_{k=1}^{r} b_k (\partial_t Z_m^k)^T \nabla_z S(Z_m^k)].
\end{aligned} \tag{5.19}
$$

Well, we present the following identity

$$
\begin{aligned}
& S(z_m^1) - S(z_m^0) - \tau \sum_{k=1}^{r} b_k (\partial_t Z_m^k)^T \nabla_z S(Z_m^k) \\
= & \ h \sum_{m=1}^{s} \tilde{b}_m[S(z_m^0 + \tau \sum_{k=1}^{r} b_k \partial_t Z_m^k) - S(z_m^0) - \tau \sum_{k=1}^{r} b_k (\partial_t Z_m^k)^T \nabla_z S(Z_m^k)].
\end{aligned} \tag{5.20}
$$

Notice that $S(z)$ is a multi-variable polynomial function with the degree of 4, then the expansion of $S(z+\tau y)$ is

$$
\begin{aligned}
S(z+\tau y) = S(z) + \tau S^{(1)}(z)(y) + \frac{\tau^2}{2} S^{(2)}(z)(y,y) \\
+ \frac{\tau^3}{6} S^{(3)}(z)(y,y,y) + \frac{\tau^4}{24} S^{(4)}(z)(y,y,y,y),
\end{aligned} \tag{5.21}
$$

where the notation $S^{(1)}(z)$ is the first order derivative with respect to z as a linear map (the gradient $\nabla_z S(z)$), $S^{(2)}(z)$ the second order derivative as a bilinear map (the second order derivative matrix $D_{zz}S(z)$) and similarly for higher order derivatives. Since the degree of the polynomial is 4, $S^{(k)}(z)=0$ for $k\geq 5$.

Now we introduce two new notations

$$\hat{z}_m=\sum_{k=1}^{r} b_k\partial_t Z_m^k \quad\text{and}\quad \breve{z}_m^k=-\sum_{j=1}^{r} a_{kj}\partial_t Z_m^j.$$

By using the expansion (5.21), (5.20) can be written as

$$\begin{aligned} & S(z_m^0+\tau\hat{z}_m)-S(z_m^0)-\tau\sum_{k=1}^{r} b_k(\partial_t Z_m^k)^T\nabla_z S(Z_m^k)\\ = \;& \tau S^{(1)}(z_m^0)(\hat{z}_m)-\tau\sum_{k=1}^{r} b_k(\partial_t Z_m^k)^T\nabla_z S(Z_m^k)+\tfrac{\tau^2}{2}S^{(2)}(z_m^0)(\hat{z}_m,\hat{z}_m)\\ & +\hat{C}_m\tau^3+\hat{D}_m\tau^4, \end{aligned}\tag{5.22}$$

where $\hat{C}_m=\frac{1}{6}S^{(3)}(z_m^0)(\hat{z}_m,\hat{z}_m,\hat{z}_m)$, $\hat{D}_m=\frac{1}{24}S^{(4)}(z_m^0)(\hat{z}_m,\hat{z}_m,\hat{z}_m,\hat{z}_m)$, and

$$\begin{cases} S^{(1)}(z_m^0)(\hat{z}_m)=[\nabla_z S(z_m^0)]^T\hat{z}_m=(\hat{z}_m)^T\nabla_z S(z_m^0),\\ S^{(2)}(z_m^0)(\hat{z}_m,\hat{z}_m)=(\hat{z}_m)^T(D_{zz}S(z_m^0))\hat{z}_m. \end{cases}\tag{5.23}$$

From (5.22) and (5.23), it follows that

$$\begin{aligned} & \tau\sum_{k=1}^{r} b_k(\partial_t Z_m^k)^T(\nabla_z S(z_m^0)-\nabla_z S(Z_m^k))\\ & +\frac{\tau^2}{2}\sum_{k=1}^{r}\sum_{j=1}^{r} b_kb_j(\partial_t Z_m^k)^T(D_{zz}S(z_m^0))\partial_t Z_{mj}\\ & +\hat{C}_m\tau^3+\hat{D}_m\tau^4\\ =&\tau\sum_{k=1}^{r} b_k(\partial_t Z_m^k)^T(\nabla_z S(Z_m^k-\tau\sum_{j=1}^{r} a_{kj}\partial_t Z_m^j)-\nabla_z S(Z_m^k))\\ & +\frac{\tau^2}{2}\sum_{k=1}^{r}\sum_{j=1}^{r} b_kb_j(\partial_t Z_m^k)^T(D_{zz}S(Z_m^k-\tau\sum_{j=1}^{r} a_{kj}\partial_t Z_m^j))\partial_t Z_m^j\\ & +\hat{C}_m\tau^3+\hat{D}_m\tau^4\\ =&\frac{\tau^2}{2}\sum_{k=1}^{r}\sum_{j=1}^{r}(b_kb_j-b_ka_{kj}-b_ja_{jk})(\partial_t Z_m^k)^T(D_{zz}S(Z_m^k))\partial_t Z_m^j\\ & +\hat{C}_m\tau^3+\hat{D}_m\tau^4+\breve{C}_m\tau^3+\breve{D}_m\tau^4\\ =&(\hat{C}_m+\breve{C}_m)\tau^3+(\hat{D}_m+\breve{D}_m)\tau^4, \end{aligned}\tag{5.24}$$

where

$$\breve{C}_m=\frac{1}{2}\Big[\sum_{k=1}^{r} b_kS^{(3)}(Z_m^k)\big(\partial_t Z_m^k,\breve{z}_m^k,\breve{z}_m^k\big)+\sum_{k=1}^{r}\sum_{j=1}^{r} b_kb_jS^{(3)}(Z_m^k)\big(\partial_t Z_m^k,\partial_t Z_m^j,\breve{z}_m^k\big)\Big]$$

and

$$\breve{D}_m = \frac{1}{6}\sum_{k=1}^{r} b_k S^{(4)}(Z_m^k)\big(\partial_t Z_m^k, \breve{z}_m^k, \breve{z}_m^k, \breve{z}_m^k\big) + \frac{1}{4}\sum_{k=1}^{r}\sum_{j=1}^{r} b_k b_j S^{(4)}(Z_m^k)\big(\partial_t Z_m^k, \partial_t Z_m^j, \breve{z}_m^k, \breve{z}_m^k\big).$$

By the assumption, z, $\partial_t z$, $\partial_x z$ are bounded in the considering (x,t)-domain, namely, there is an $M^* > 0$, s.t.

$$|z| \le M^*, \quad |\partial_t z| \le M^*, \quad |\partial_x z| \le M^*$$

for all (x,t) in the domain.

Since $S(z)$ is a polynomial function, and the degree of the polynomial is 4, then $S(z)$ and its derivatives with respect to z are all bounded.

With the assumptions and the brief analysis above, combing (5.19) and (5.24), we have

$$|E_{le}| \le Ch\tau^3, \tag{5.25}$$

for sufficiently small τ and h, where the constant C is independent of τ, h. ■

From the expansion (5.21) and the calculation (5.24), we can see that for any multi-symplectic Hamiltonian $S(z)$, the local error E_{le} of ECL can be written as follows

$$E_{le} = f_3\tau^3 + f_4\tau^4 + \cdots\ ,$$

where f_i has the following form

$$f_i = \sum_j f_{i,j} S^{(i)}((Z_p)_j),$$

where $(Z_p)_j$ is a parameter just like the parameter z in (5.21).

Hence, if

$$S(z) = \frac{1}{2} z^T H z + b^T z, \tag{5.26}$$

where H is an arbitrary matrix with the size in terms of z, and b is any vector with the same size of z, we can get

$$S^{(k)}(z) \equiv 0 \text{ for } k \ge 3.$$

In other words, we find that

$$E_{le} \equiv 0, \tag{5.27}$$

and in this situation, we can get that

Corollary 5.2 *For the multi-symplectic system $Mz_t + Kz_x = \nabla_z S(z)$, if the multi-symplectic Hamiltonian $S(z)$ has the form $S(z) = \frac{1}{2}z^T Hz + b^T z$, then MSRK methods have the discrete ECL.*

Remark 5.3 *E_{le} is a discrete approximation of the local integration (5.4) of the energy conservation law, similarly, we can use*

$$E_{le}^* = \sum_{m=1}^{s} \tilde{b}_m \frac{(E(z_m^1) - E(z_m^0))}{\tau} + \sum_{k=1}^{r} b_k \frac{(F(z_1^k) - F(z_0^k))}{h} \tag{5.28}$$

to approximate the energy conservation law (2.6), under the assumptions of Theorem 3.5, we have

$$|E_{le}^*| \le C\tau^2. \tag{5.29}$$

Remark 5.4 *The calculation of the estimate (5.25) or (5.29) can be extended to the general multi-symplectic system, if the system satisfies the regularity conditions as mentioned in above theorem.*

Integrating the local energy conservation law (2.6) over the whole considering spatial interval $[-L/2, L/2]$ leads to

$$\begin{aligned} 0 &= \int_{-L/2}^{L/2} \left(\frac{\partial E}{\partial t} + \frac{\partial F}{\partial x} \right) dx \\ &= \int_{-L/2}^{L/2} \frac{\partial E}{\partial t} \, dx + F(L/2, t) - F(-L/2, t) \\ &= \frac{d}{dt} \int_{-L/2}^{L/2} E dx, \end{aligned} \tag{5.30}$$

where the last equality derives from the periodic boundary condition.

The calculation above implies the total energy conservation law

$$\frac{d}{dt} \mathcal{E}_L(t) = 0. \tag{5.31}$$

Now from the former discussion on the discrete approximation of the local energy conservation law, we can define the discrete total energy at time t_i as

$$\left(\mathcal{E}_L^d\right)^i = h \sum_{l=0}^{N-1} \sum_{m=1}^{s} \tilde{b}_m E(z_{l,m}^i), \tag{5.32}$$

where $z_{l,m}^i \approx z(lh + c_m h, i\tau)$ and i is a non-negative integer.

Theorem 5.5 *Under the assumptions of Theorem 5.1, and assume that z, $S(z)$ and their derivatives satisfy the regularity conditions, then the local error of the discrete total energy conservation law satisfies*

$$|E_{te}| \triangleq |\left(\mathcal{E}_L^d\right)^1 - \left(\mathcal{E}_L^d\right)^0| \leq C\tau^3, \tag{5.33}$$

for sufficiently small τ and h, where the constant C is independent of τ and h.

Proof. From (5.13) and (5.15), we can get

$$\begin{aligned} &(\mathcal{E}_L^d)^1 - (\mathcal{E}_L^d)^0 \\ =& h \sum_{l=0}^{N-1} \sum_{m=1}^{s} \tilde{b}_m \left\{ S(z_{l,m}^1) - S(z_{l,m}^0) - \frac{1}{2} \left[(z_{l,m}^1)^T K \partial_x z_{l,m}^1 - (z_{l,m}^0)^T K \partial_x z_{l,m}^0 \right] \right\} \\ =& h \sum_{l=0}^{N-1} \sum_{m=1}^{s} \tilde{b}_m \left[S(z_{l,m}^1) - S(z_{l,m}^0) \right] \\ &- \frac{h\tau}{2} \sum_{l=0}^{N-1} \sum_{m=1}^{s} \sum_{k=1}^{r} \tilde{b}_m b_k \left[(\partial_t Z_{l,m}^k)^T K \partial_x Z_{l,m}^k + (Z_{l,m}^k)^T K Y_{l,m}^k \right], \end{aligned} \tag{5.34}$$

On the other hand, we have

$$
\begin{aligned}
& h\sum_{l=0}^{N-1}\sum_{m=1}^{s}\tilde{b}_m\Big[(\partial_x Z_{l,m}^k)^T K\partial_t Z_{l,m}^k+(Z_{l,m}^k)^T KY_{l,m}^k\Big]\\
=&\sum_{l=0}^{N-1}\Big[(z_{l+1}^k)^T K\partial_t z_{l+1}^k-(z_l^k)^T K\partial_t z_l^k\Big]\\
=&(z_N^k)^T K\partial_t z_N^k-(z_0^k)^T K\partial_t z_0^k\\
=&0,
\end{aligned}
\tag{5.35}
$$

where the last equality comes from the periodic boundary conditions.

Combining (5.34) and (5.35), and noticing the skew-symmetry of the matrix K and the calculation (5.13)-(5.19), we can get

$$
\big(\mathcal{E}_L^d\big)^1-\big(\mathcal{E}_L^d\big)^0=h\sum_{l=0}^{N-1}\sum_{m=1}^{s}\tilde{b}_m\Big[S(z_{l,m}^1)-S(z_{l,m}^0)-\tau\sum_{k=1}^{r}b_k(\partial_t Z_{l,m}^k)^T K\partial_x Z_{l,m}^k\Big]. \tag{5.36}
$$

The global regular assumptions and the calculation (5.20)-(5.25) imply that

$$
\begin{aligned}
&\Big|\big(\mathcal{E}_L^d\big)^1-\big(\mathcal{E}_L^d\big)^0\Big|\\
=&\Big|h\sum_{l=0}^{N-1}\sum_{m=1}^{s}\tilde{b}_m\Big[S(z_{l,m}^1)-S(z_{l,m}^0)-\tau\sum_{k=1}^{r}b_k(\partial_t Z_{l,m}^k)^T K\partial_x Z_{l,m}^k\Big]\Big|\\
\le&\sum_{l=0}^{N-1}\Big|h\sum_{m=1}^{s}\tilde{b}_m\Big[S(z_{l,m}^1)-S(z_{l,m}^0)-\tau\sum_{k=1}^{r}b_k(\partial_t Z_{l,m}^k)^T K\partial_x Z_{l,m}^k\Big]\Big|\\
\le&\sum_{l=0}^{N-1}Ch\tau^3=CNh\tau^3=LC\tau^3\\
=&\tilde{C}\tau^3,
\end{aligned}
\tag{5.37}
$$

where $\tilde{C}$ is a constant as said above. ■

When multi-symplectic numerical methods are applied to multi-symplectic systems, in general, it doesn't have the discrete total energy conservation law. However, the numerical experiments [9] show that the discrete total energy oscillates near its initial value with the evolution of long-time. Hence, one says that multi-symplectic numerical methods give rise to a good total energy conservation, with essentially no accumulation of errors in quite long time. Here we give a theoretical result.

Corollary 5.6 *Under the assumptions of Corollary 5.2, then the MSRK methods have the the discrete total energy conservation law*

$$
(\mathcal{E}_L^d)^1-(\mathcal{E}_L^d)^0=0. \tag{5.38}
$$

Theorem 5.7 *Under the assumptions of Theorem 5.4, for $T>0$, there exists a $\tau_0>0$, such that for $\tau<\tau_0$,*

$$
|\big(\mathcal{E}_L^d\big)^n-\big(\mathcal{E}_L^d\big)^0|\le C\tau^2,\quad\text{uniformly for}\quad n\tau\le T, \tag{5.39}
$$

where the constant C is independent of τ and T.

Proof.

$$\begin{aligned}
&\Big|(\mathcal{E}_L^d)^n - (\mathcal{E}_L^d)^0\Big| \\
=&\Big|\Big((\mathcal{E}_L^d)^n - (\mathcal{E}_L^d)^{n-1}\Big) + \cdots \Big((\mathcal{E}_L^d)^1 - (\mathcal{E}_L^d)^0\Big)\Big| \\
\leq&\Big|\Big((\mathcal{E}_L^d)^n - (\mathcal{E}_L^d)^{n-1}\Big)\Big| + \cdots + \Big|\Big((\mathcal{E}_L^d)^1 - (\mathcal{E}_L^d)^0\Big)\Big| \\
\leq&\sum_{i=1}^{n} C\tau^3 = n\tau C\tau^2 \leq TC\tau^2 \\
=&\tilde{C}\tau^2,
\end{aligned} \tag{5.40}$$

where $\tilde{C}$ is a constant as said in (5.39). ■

Remark 5.8 *For the general multi-symplectic systems, if the regularity conditions as mentioned in Remark 5.3 hold, then the estimates (5.30) and (5.32) can be obtained too. This result shows that MSRK methods are stable in the sense of energy conservation law.*

6. Momentum analysis for the multi-symplectic RK methods

As discussed in energy analysis, we use the integral form of the local momentum conservation law (2.8)

$$\int_0^h \int_0^\tau \Big(\frac{\partial I}{\partial t} + \frac{\partial G}{\partial x}\Big) dt dx = 0, \tag{6.1}$$

namely

$$\int_0^h [I(z(x,\tau)) - I(z(x,0))]dx + \int_0^\tau [G(z(h,t)) - G(z(0,t))]dt = 0. \tag{6.2}$$

We define

$$M_{le} = h\sum_{m=1}^{s} \tilde{b}_m (I(z_m^1) - I(z_m^0)) + \tau \sum_{k=1}^{r} b_k (G(z_1^k) - G(z_0^k)) \tag{6.3}$$

as the discrete form of the left side of (6.2), namely the local momentum conservation law. Since the Dirac equations we consider are nonlinear, it doesn't have the discrete local momentum conservation law, but we also can get the local error estimate of discrete form of the conservation law.

Our interest is in how (6.2) is preserved by MSRK methods (3.3). The following theorem gives an estimation of M_{le} when applying (3.3) to (2.2).

Theorem 6.1 *Under the assumptions of Theorem 5.1, the following estimation*

$$|M_{le}| \leq C\tau h^3 \tag{6.4}$$

holds for sufficiently small τ and h, where the positive constant C is independent of z, $\partial_t z$, $\partial_x z$, and S.

Proof. From (5.6)-(5.18), similarly, it can be deduced that

$$\begin{aligned} M_{le} &= h\sum_{m=1}^{s}\tilde{b}_m(I(z_m^1)-I(z_m^0))+\tau\sum_{k=1}^{r}b_k(G(z_1^k)-G(z_0^k)) \\ &= \tau\sum_{k=1}^{r}b_k\Big[S(z_1^k)-S(z_0^k)-h\sum_{m=1}^{s}\tilde{b}_m\big(\partial_x Z_m^k\big)^T\nabla_z S\big(Z_m^k\big)\Big]. \end{aligned} \tag{6.5}$$

Following the second half of the proof of Theorem 5.1 leads to

$$|S(z_1^k)-S(z_0^k)-h\sum_{m=1}^{s}\tilde{b}_m\big(\partial_x Z_m^k\big)^T\nabla_z S\big(Z_m^k\big)|\leq Ch^3. \tag{6.6}$$

According to (6.5) and (6.6), we have

$$|M_{le}|\leq C\tau h^3, \tag{6.7}$$

where C is a constant as said above. ■

Corollary 6.2 *Under the assumptions of Corollary 5.2, we can get* $M_{le}=0$*, namely, the system has a discrete momentum conservation law.*

Remark 6.3 *As similar as what said in Remark 5.3,* M_{le} *is the discrete approximation of the integration (6.2) of the local momentum conservation law, similarly, we make use of*

$$M_{le}^*=\sum_{m=1}^{s}\tilde{b}_m\frac{(I(z_m^1)-I(z_m^0))}{\tau}+\sum_{k=1}^{r}b_k\frac{(G(z_1^k)-G(z_0^k))}{h} \tag{6.8}$$

to approximate the momentum conservation law (2.8), under the assumptions of Theorem 6.1, we have

$$|M_{le}^*|\leq Ch^2, \tag{6.9}$$

where C *is a constant as the same as mentioned in (6.4) or (6.7).*

Remark 6.4 *As similarly as said in Remark 5.4, the local error estimates (6.4) and (6.9) can be extended to any multi-symplectic system with the regularity conditions as required in Remark 5.4. The result gives the stability of MSRK methods in the sense of momentum conservation law.*

Now we turn to the discussion of the total momentum. First, integrating the local momentum conservation law (2.8) over the spatial interval $[-L/2, L/2]$, gives

$$\begin{aligned} 0 &= \int_{-L/2}^{L/2}\Big(\frac{\partial I}{\partial t}+\frac{\partial G}{\partial x}\Big)dx \\ &= \int_{-L/2}^{L/2}\frac{\partial I}{\partial t}\,dx+G(L/2,t)-G(-L/2,t) \\ &= \frac{d}{dt}\int_{-L/2}^{L/2}Idx=\frac{d}{dt}\mathcal{I}_L(t), \end{aligned} \tag{6.10}$$

in the above calculation we make use of the periodic boundary conditions. It implies that the total momentum is conserved in the continuous case. In our RK methods, we define the total momentum at time t_i as

$$\left(\mathcal{I}_L^d\right)^i = h \sum_{l=0}^{N-1} \sum_{m=1}^{s} \tilde{b}_m I(z_{l,m}^i), \tag{6.11}$$

where $z_{l,m}^i$ and i have the same meaning as before.

Theorem 6.5 *Under the assumptions of Theorem 6.1, with the periodic boundary condition given in section 3, if $\partial_x z$ is a periodic function on the spatial interval $[-L/2, L/2]$, namely $\partial_x z(-L/2, t) = \partial_x z(L/2, t)$ for all t, then we have the following discrete total momentum conservation law*

$$\left(\mathcal{I}_L^d\right)^1 = \left(\mathcal{I}_L^d\right)^0. \tag{6.12}$$

Proof. From (5.6)-(5.11), with the similar calculation of (5.13)-(5.18), we get

$$\begin{aligned} I(z_{l,m}^1) - I(z_{l,m}^0) &= \frac{1}{2}\left[(z_{l,m}^1)^T M \partial_x z_{l,m}^1 - (z_{l,m}^0)^T M \partial_x z_{l,m}^0\right. \\ &= \frac{\tau}{2} \sum_{k=1}^{r} b_k \Big[\big(\partial_t Z_{l,m}^k\big)^T M \partial_x Z_{l,m}^k + \big(Z_{l,m}^k\big)^T M Y_{l,m}^k\Big], \end{aligned} \tag{6.13}$$

where $Y_{l,m}^k$ denotes $\big(\partial_t \partial_x Z\big)_{l,m}^k$ or $\big(\partial_x \partial_t Z\big)_{l,m}^k$.

From (6.13), it follows that

$$\begin{aligned} &\left(\mathcal{I}_L^d\right)^1 - \left(\mathcal{I}_L^d\right)^0 \\ =&\frac{\tau h}{2} \sum_{k=1}^{r} b_k \Big\{ \sum_{l=0}^{N-1} \sum_{m=1}^{s} \tilde{b}_m \Big[\big(\partial_t Z_{l,m}^k\big)^T M \partial_x Z_{l,m}^k + \big(Z_{l,m}^k\big)^T M Y_{l,m}^k\Big] \Big\}. \end{aligned} \tag{6.14}$$

On the other hand, it is deduced that

$$\begin{aligned} &(z_{l+1}^k)^T M \partial_x z_{l+1}^k - (z_l^k)^T M \partial_x z_l^k \\ =&h \sum_{m=1}^{s} \tilde{b}_m \Big[\big(\partial_t Z_{l,m}^k\big)^T M \partial_x Z_{l,m}^k + \big(Z_{l,m}^k\big)^T M Y_{l,m}^k\Big]. \end{aligned} \tag{6.15}$$

Combing (6.14) and (6.15), we have

$$\begin{aligned} &\left(\mathcal{I}_L^d\right)^1 - \left(\mathcal{I}_L^d\right)^0 \\ =&\frac{\tau}{2} \sum_{k=1}^{r} b_k \Big\{ \sum_{l=0}^{N-1} \Big[(z_{l+1}^k)^T M \partial_x z_{l+1}^k - (z_l^k)^T M \partial_x z_l^k\Big] \Big\} \\ =&\frac{\tau}{2} \sum_{k=1}^{r} b_k \Big[(z_N^k)^T M \partial_x z_N^k - (z_0^k)^T M \partial_x z_0^k\Big] \\ =&0, \end{aligned} \tag{6.16}$$

where the last equality comes from the periodic boundary conditions of z and $\partial_x z$. ■

Remark 6.6 *From the calculation (6.16), just as said in Remark 4.2, when we use*

$$z^T(-L/2,t)M\partial_x z(-L/2,t) = z^T(L/2,t)M\partial_x z(L/2,t) \quad \text{for all} \quad t$$

to substitute the periodic boundary conditions as mentioned in the theorem, we can obtain the total momentum conservation law when applying MSRK methods to a general multi-symplectic system.

Remark 6.7 *For any multi-symplectic system, if the phase variable z and the first order derivatives of z with respect to spatial variables are periodic in the spatial domain, then, applying the multi-symplectic RK methods to this system, we can get the discrete total momentum conservation law with the same form of (6.12).*

7. Numerical experiments

In this section, the implementation of MSRK method for the Dirac equation verifies and illustrate how energy, momentum and charge conservation laws are preserved and whether the energy and momentum analysis theories in the section 5 and 6, respectively, have practical validity.

Without loss of generality, we take the constants $m = 1$ and $\lambda = \frac{1}{2}$ in (1.3). In this situation, the nonlinear Dirac equation (1.3) has the following theoretical solitary wave solution

$$\psi_s(x,t) = (M(x),\ iN(x))^T e^{-i\Lambda t}, \tag{7.1}$$

where

$$\begin{cases} M(x) = (2(1-\Lambda^2))^{1/2}(1+\Lambda)^{1/2}\frac{\cosh((1-\Lambda^2)^{1/2}x)}{1+\Lambda\cosh((1-\Lambda^2)^{1/2}x)}, \\ \\ N(x) = (2(1-\Lambda^2))^{1/2}(1-\Lambda)^{1/2}\frac{\sinh((1-\Lambda^2)^{1/2}x)}{1+\Lambda\cosh((1-\Lambda^2)^{1/2}x)} \end{cases}$$

with the frequency $\Lambda = 0.75$.

We discretize the nonlinear Dirac equation (1.3) by the simplest multi-symplectic RK method with $r = 1$ (midpoint in time) and $s = 1$ (midpoint in space). Since $\psi_s(x,t)$ is exponentially small away from $x = 0$, we implement periodic boundary conditions $\psi(-L,t) = \psi(L,t)$ with $L = 24$, and we use the exact initial conditions

$$\begin{cases} \phi_1(x) = M(x), \\ \\ \phi_2(x) = iN(x). \end{cases} \tag{7.2}$$

We let the spatial step $h = 0.3$, the time step $\tau = 0.05$, and the time interval $t \in [0, 100]$. In our experiments, we use the fixed point iteration method to solve the nonlinear systems generated by the scheme, each iteration will stop when the maximum absolute error of the two next iterative values less than 10^{-15}.

The numerical simulation of the four solitary waves, namely the four spinor components are pictured in Figure 1, Figure 2, Figure 3, and Figure 4 respectively.

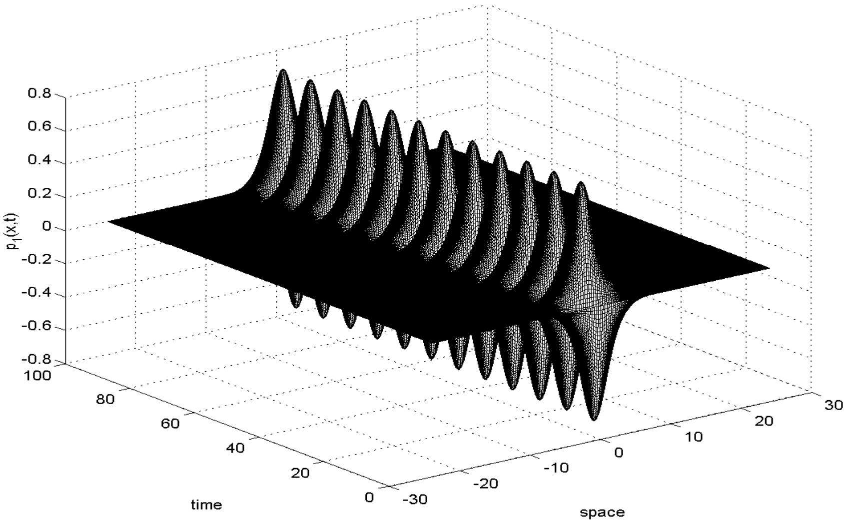

Figure 1: The first component $p_1(x, t)$ of the solitary wave function.

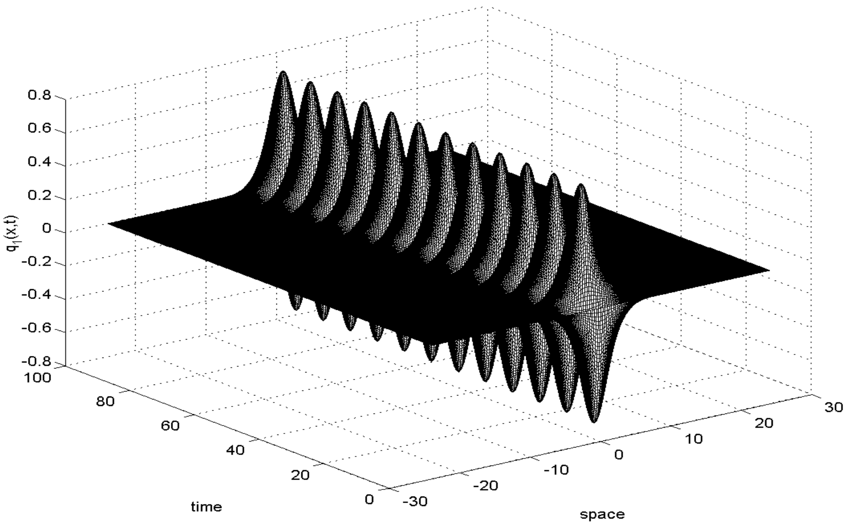

Figure 2: The second component $q_1(x, t)$ of the solitary wave function.

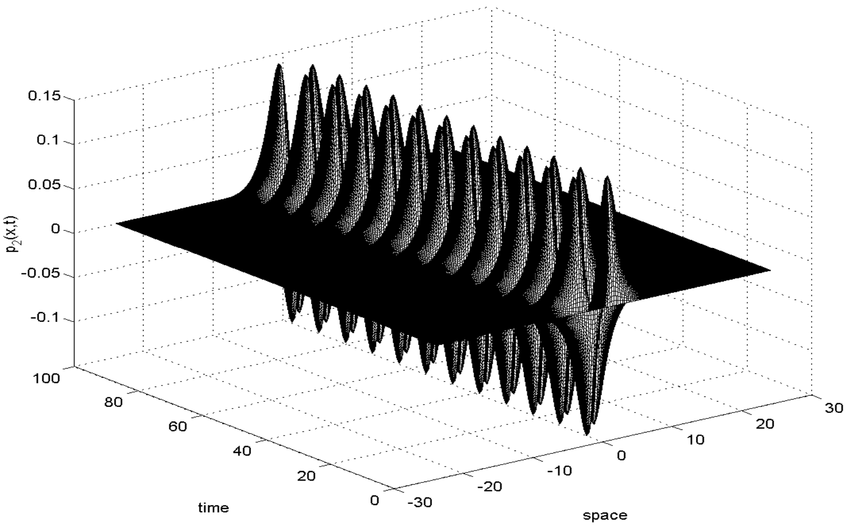

Figure 3: The third component $p_2(x,t)$ of the solitary wave function.

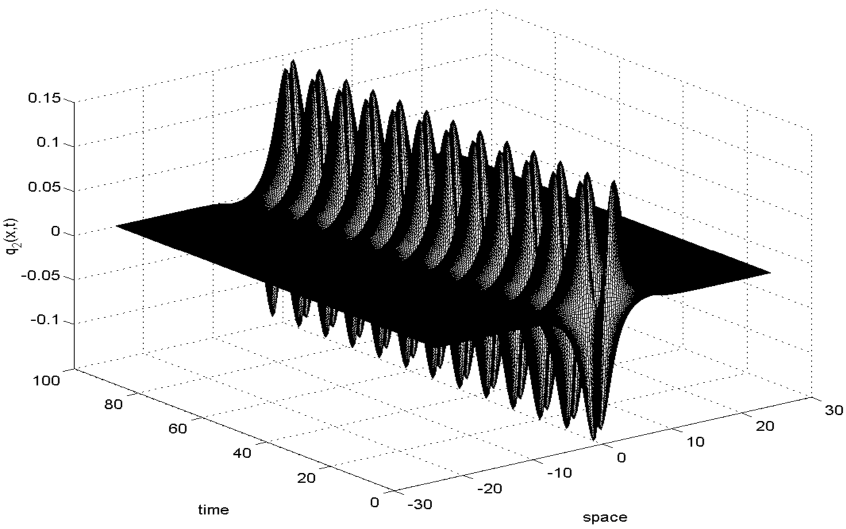

Figure 4: The fourth component $q_2(x,t)$ of the solitary wave function.

Figure 5 shows the global error of the discrete total energy, here we use $\left(\mathcal{E}_L^d\right)^i - \left(\mathcal{E}_L^d\right)^0$ to denote the global error of the discrete total energy. Similarly, we use $\left(\mathcal{I}_L^d\right)^i - \left(\mathcal{I}_L^d\right)^0$ to denote the global error of the discrete total momentum, and which are pictured in Figure 6.

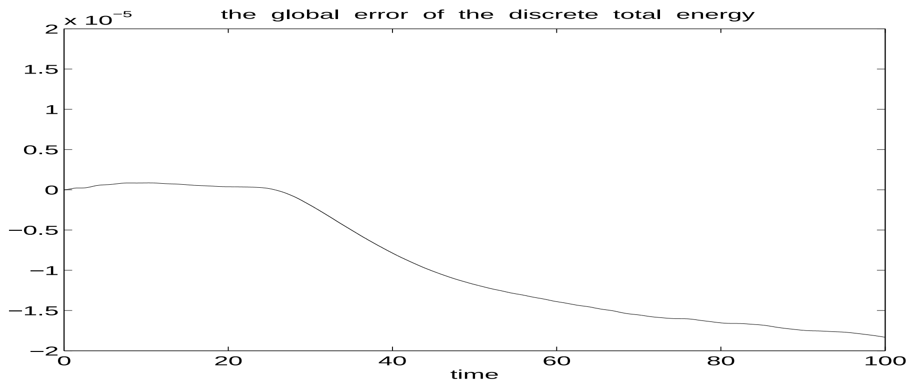

Figure 5: The global error of the discrete total energy conservation law.

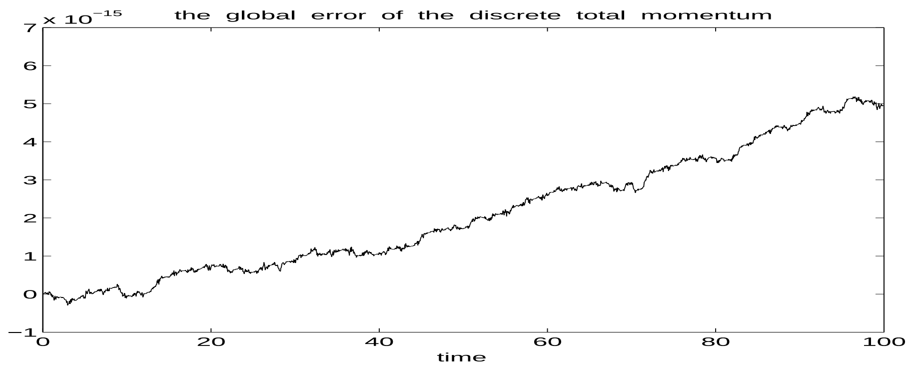

Figure 6: The global error of the discrete total momentum conservation law.

Figure 7 gives that the error in the energy conservation law, here we use

$$(E_{le}^*)_l^i = \sum_{m=1}^{s} \tilde{b}_m \frac{(E(z_{l,m}^{i+1}) - E(z_{l,m}^i))}{\tau} + \sum_{k=1}^{r} b_k \frac{(F(z_{l+1}^{i,k}) - F(z_l^{i,k}))}{h}$$

to denote the error of the ECL, which is the general form of (5.25) at the mesh point (x_l, t_i), we use $\max_{0 \le l < N} |(E_{le}^*)_l^i|$ to denote the the maximum error for all spatial grid points at the time t_i.

Similarly, we use $\max_{0 \le l < N} |(M_{le}^*)_l^i|$ to denote the maximum error of the momentum conservation law, the development of maximum error with time evolution can be seen in Figure 8.

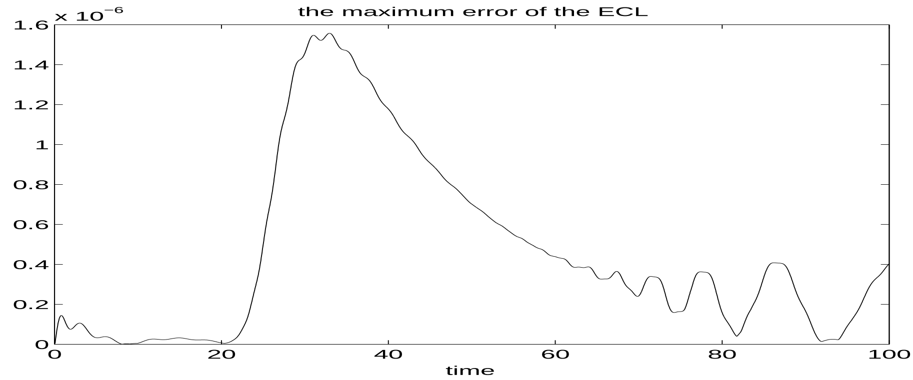

Figure 7: The maximum error of the discrete local ECL.

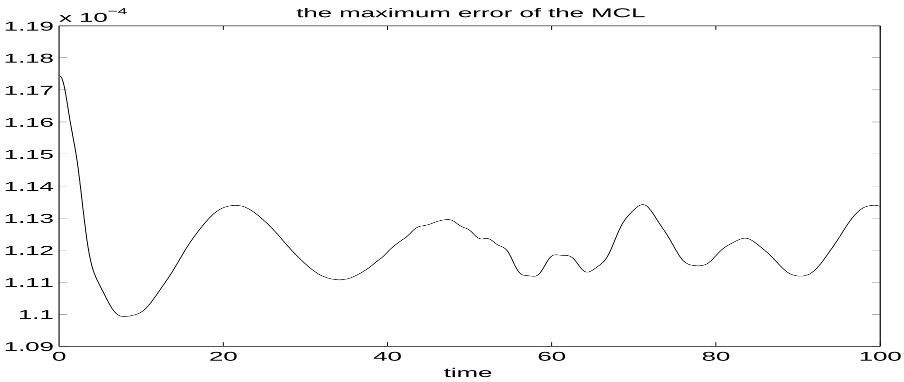

Figure 8: The maximum error of the discrete local MCL.

We use $\mathcal{Q}^i - \mathcal{Q}^0$ to denote the global error of the charge conservation law (CCL). The following figure shows the global error of CCL in the time interval $[0, 25]$.

The above figures show the match between our theoretical results and numerical experiments.

8. Conclusions

For the Runge-Kutta discretization of the nonlinear Dirac equation, the symplecticity both in time and space directions implies the multi-symplecticity of the integrator. The preservation of charge, energy and momentum conservation laws is very important under the struture-preserving discretization. A known result that the multi-symplectic integrator preserves the local energy and momentum exactly if the multi-symplectic Hamiltonian is of quadratic is contained in our energy and momentum analysis. In particular, from the theorem 5.1 and 6.1, it follows that, under given conditions, there exists a constant $C > 0$ such that for sufficient small τ and h, we have

$$|E_{le} + M_{le}| \le C\tau h(\tau^2 + h^2),$$

which shows the local symmetry of energy and momentum under the discretization of MSRK

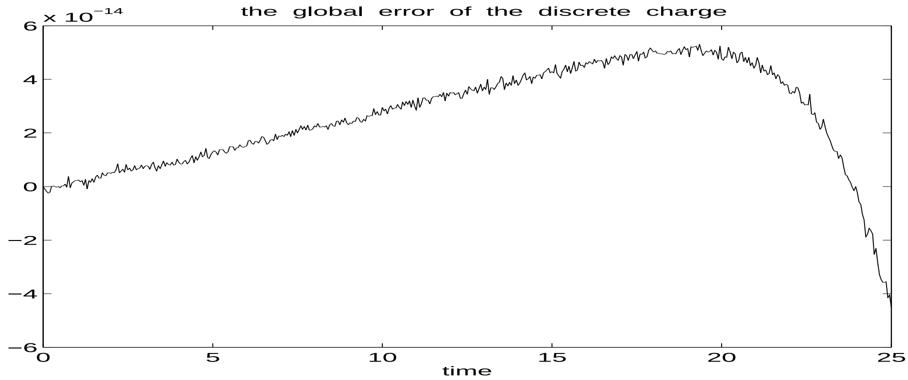

Figure 9: The global error of the discrete charge conservation law.

(3.3). Theorem 5.7 and theorem 6.5 tell us that MSRK methods are stable and convergent in the sense of energy and momentum conservation laws. Our numerical experiments explain the theoretical result intuitively, we need point out that in our experiments the global error of the discrete charge conservation law given in the figure is over the interval $[0, 25]$, but with accumulation of errors in time, it becomes a little worse than the result in $[0, 25]$, even over the interval $[0, 100]$, it still be controlled less than 10^{-7}, we think that this is relative with not only the scheme we choose, the algebraic methods we use in our program, but also the solution itself. The other results in the experiments obey our theoretical analysis. Our work shows that the traditional methods in numerical analysis can be brought in the geometric numerical methods, but we must give a new development for the the traditional methods, in this sense, our work is important and just in the beginning.

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