Journal of Computational Physics 418 (2020) 109599

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Energy and quadratic invariants preserving (EQUIP) multi-symplectic methods for Hamiltonian wave equations

Chuchu Chen[a,b,*], Jialin Hong[a,b], Chol Sim[c], Kwang Sonwu[c]

[a] LSEC, ICMSEC, Academy of Mathematics and Systems Science, CAS, Beijing 100190, China
[b] School of Mathematical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China
[c] Institute of Mathematics, Academy of Sciences, Pyongyang, Democratic People's Republic of Korea

A R T I C L E   I N F O

Article history:
Received 5 May 2019
Received in revised form 16 April 2020
Accepted 23 May 2020
Available online 29 May 2020

Keywords:
Hamiltonian wave equations
Energy preservation
EQUIP multi-symplectic methods

A B S T R A C T

It is well-known that a numerical method which is at the same time geometric structure-preserving and physical property-preserving cannot exist in general for Hamiltonian partial differential equations. Motivated by EQUIP methods proposed in Brugnano et al. (2012) [13], in this paper, we present a novel class of parametric multi-symplectic Runge-Kutta methods, called EQUIP multi-symplectic methods, for Hamiltonian wave equations, which can also conserve energy simultaneously in a weaker sense with a suitable parameter. The existence of such a parameter, which enforces the energy-preserving property, is proved under certain assumptions on the fixed step sizes and the fixed initial condition. We compare the proposed method with the classical multi-symplectic Runge-Kutta method in numerical experiments, which shows the remarkable energy-preserving property of the proposed method and illustrates the validity of theoretical results. These theoretical and numerical results show that EQUIP methods can be well adapted to handle Hamiltonian partial differential equations.

1. Introduction

The Hamiltonian wave equation is an important mathematical model in some scientific fields like quantum mechanics, plasma physics, etc. This equation is a typical example of a Hamiltonian partial differential equation (PDE) of the form:

$$M\partial_t z + K\partial_x z = \nabla_z S(z), \qquad (x,t) \in \mathbb{R}^d \times \mathbb{R}_+, \tag{1}$$

where $z \in \mathbb{R}^n$, $M, K \in \mathbb{R}^{n\times n}$ are two skew-symmetric matrices, $S: \mathbb{R}^n \to \mathbb{R}$ is a given smooth function (at least twice continuously differentiable), $\nabla_z S(z)$ is the classical gradient on $\mathbb{R}^n$, and x, t denote the spatial and temporal directions, respectively.

For the Hamiltonian PDE (1), the two most prominent characteristics are multi-symplecticity, i.e.,

$$\partial_t \omega + \partial_x \kappa = 0 \tag{2}$$

with $\omega = dz \wedge Mdz$, $\kappa = dz \wedge Kdz$, and conservativeness, for example, the energy conservation law (ECL):

* Corresponding author.
E-mail addresses: chenchuchu@lsec.cc.ac.cn (C. Chen), hjl@lsec.cc.ac.cn (J. Hong), simchol@star-co.net.kp (C. Sim).

https://doi.org/10.1016/j.jcp.2020.109599
0021-9991/

$$\partial_t E(z) + \partial_x F(z) = 0 \tag{3}$$

with the energy density and the energy flux being $E(z) = S(z) - \frac{1}{2}z^\top K\partial_x z$ and $F(z) = \frac{1}{2}z^\top K\partial_t z$, respectively, and the momentum conservation law (MCL):

$$\partial_t I(z) + \partial_x G(z) = 0, \tag{4}$$

with the momentum density and the momentum flux being $I(z) = \frac{1}{2}z^\top M\partial_x z$, and $G(z) = S(z) - \frac{1}{2}z^\top M\partial_t z$, respectively.

A well-known principle to design numerical methods is that numerical methods should preserve as much as possible the intrinsic properties of the underlying system. Generally, the numerical approximations of Hamiltonian systems fall into two categories: geometric structure-preserving numerical methods and physical property-preserving numerical methods. We start from the numerical study for Hamiltonian ordinary differential equations (ODEs), which has formed a well-developed subject through several decades of efforts (see e.g. the monographs [1,2]). On the construction of symplectic numerical methods, there are several approaches, e.g., symplectic Runge-Kutta (RK) type methods ([3]), methods based on generating functions ([4]), variational integrators ([5]), etc., while on the construction of physical property-preserving numerical methods, different approaches, e.g., methods with projection-type techniques ([6]), discrete gradient methods ([7]), Hamiltonian boundary value methods ([8,9]), etc., are proposed. Except for the symplecticity-preservation, another important feature of symplectic numerical methods is that they can preserve exactly quadratic invariants (specially, quadratic Hamiltonian functions); see [3] for instance. Generally, the famous Ge-Marsden theorem ([10]) shows the nonexistence of a constant time stepping algorithm which is at the same time symplectic and energy conserving. The efforts towards this purpose on methods inheriting both features are made in a weaker sense. For example, [11] proposes the adaptive time stepping symplectic-energy-momentum integrators with the symplecticity being viewed in the space-time sense. The constructive idea by introducing a parameter in each step which can be suitably tuned in a way to enforce the energy conservation, is introduced in [12], and is developed refinedly and called the EQUIP method in [13–15]. More precisely, they introduce a family of one-step methods $y_1(\alpha) = \Phi_h(y_0, \alpha)$ depending on a real parameter α such that this family of methods are symplectic for any fixed choice of α, and that a special value of the parameter can be chosen depending on y_0 and h with the conservation of energy at the same time. For a Hamiltonian PDE, the multi-symplecticity and the ECL/MCL are the most relevant features characterizing its intrinsic properties. A natural question arises: can one find a numerical method which combines the multi-symplectic structure and the ECL/MCL at the same time in certain sense? It is believed that the difficulties in such a problem not only come from the balance of geometric structure and physical property, but also result from the numerical analysis of PDEs such as the interaction of time and space, etc.

For the numerical study of Hamiltonian PDEs, the multi-symplectic structure is investigated and then a lot of reliable numerical methods (e.g. [16–23]) preserving the multi-symplectic structure, for instance, muti-symplectic RK/Partitioned RK methods, collocation methods, splitting methods, spectral methods, etc., have been developed. Especially, we refer to [19,24–26] and references therein for the multi-symplectic methods of the Hamiltonian wave equation. On the physical property-preserving aspect, as we mentioned that classical conservation laws such as the ECL (3) and the MCL (4) play an important role in Hamiltonian PDEs. Though they locally character the conservativeness, they are equivalent to the global conservation laws when an appropriate boundary condition is endowed. The conservation of quadratic ECL and MCL under multi-symplectic methods is proved in [19,24]. The accuracy of conservation laws of energy and momentum for Hamiltonian PDEs under RK discretizations is investigated in [24]. The approximate preservation of the global energy, momentum, and all harmonic actions over long time under temporal symplectic methods and spatial spectral methods applied to semilinear wave equation is rigorously proved in [27]. There have been several works on numerically preserving the local ECL and MCL of Hamiltonian PDEs, e.g., see [16] for a systematic framework. However, as far as we know, there are no known results about numerical methods which preserve the multi-symplectic structure and the ECL/MCL simultaneously for Hamiltonian PDEs.

The main aim of this paper is to propose a class of multi-symplectic discretizations by applying the EQUIP method to the Hamiltonian wave equation to share the property of energy conservation at the same time. The EQUIP method is proposed and analyzed in [13,15,28] for Hamiltonian ODEs to preserve symplecticity and energy simultaneously. We apply the parametric symplectic RK methods to Hamiltonian PDEs in space and time, respectively, with the same real parameter α, which is proved to be a concatenated α-RK method preserving the multi-symplectic structure for all real parameters. This class of methods is also called EQUIP multi-symplectic methods in this paper. The preservation of the ECL under the EQUIP multi-symplectic method is obtained by suitably tuning the parameter, that is, we can show that the parameter α^* exists at each element domain composed by spatial and temporal step sizes, which leads to the preservation of multi-symplecticity and ECL. That is a weaker version of the standard conservativeness, since the existence of this parameter depends on the step sizes Δx, Δt, and on the initial data.

This paper is organized as follows. In section 2, we present the Hamiltonian wave equation and its multi-symplectic form. Then a family of RK methods concatenated in the spatial and temporal directions is introduced. In section 3, we propose a concatenated parametric RK method (also called an EQUIP multi-symplectic method) by using the W-transformation, which is multi-symplectic for all parameters. The preservation of the ECL of the EQUIP multi-symplectic method is investigated in section 4, by selecting a suitable parameter. We prove the existence of such parameter with the aid of the Lyapunov-Schmidt decomposition method, the homotopy continuation method and the implicit function theorem under some assumptions on

RK matrices, the spatial and temporal step sizes, etc. In section 5, we present some numerical experiments to show the effectiveness in energy-preserving of the proposed method. A short conclusion is given in section 6.

2. Multi-symplectic Runge-Kutta methods

Consider the scalar wave equation

$$\partial_{tt}u = \partial_{xx}u - V'(u), \qquad (x,t) \in \mathbb{R} \times \mathbb{R}_+, \tag{5}$$

where $V : \mathbb{R} \to \mathbb{R}$ is a smooth function, which is a typical example of a Hamiltonian PDE (1). By introducing canonical momenta $v := \partial_t u$, $w := \partial_x u$ and defining the state variable $z = (u, v, w)^\top \in \mathbb{R}^3$, we rewrite the wave equation (5) as

$$\begin{aligned} \partial_t u &= v, \\ \partial_x u &= w, \\ \partial_t v - \partial_x w &= -V'(u). \end{aligned} \tag{6}$$

Using this variable, we obtain

$$M = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad K = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}$$

as well as the Hamiltonian $S(z) = \frac{1}{2}(v^2 - w^2) + V(u)$.

The multi-symplectic conservation law (2), for the wave equation (5), is equivalent to $\partial_t[du \wedge dv] - \partial_x[du \wedge dw] = 0$. We also obtain the ECL (3) with

$$E(z) = \frac{1}{2}(w^2 + v^2) + V(u) \quad \text{and} \quad F(z) = -vw \tag{7}$$

and the MCL (4) with $I(z) = -vw$ and $G(z) = \frac{1}{2}(w^2 + v^2) - V(u)$, respectively.

Now, we start our study with a multi-symplectic RK method for the Hamiltonian wave equation (5). First, we recall the definition of multi-symplectic integrators for Hamiltonian PDEs. For the purpose of numerical approximation, following [20], we introduce a uniform grid $(x_j, t_k) \in \mathbb{R} \times \mathbb{R}_+$, in the plan of (x,t), with a spatial step size Δx and a temporal step size Δt. The approximated value of $z(x,t)$ at the mesh point (x_j, t_k) is denoted by $z_{j,k}$. A numerical discretization of (1) and (2), can be written, respectively, as

$$M\partial_t^{j,k} z_{j,k} + K\partial_x^{j,k} z_{j,k} = (\nabla_z S_{j,k})_{j,k}, \tag{8}$$

$$\partial_t^{j,k}\omega_{j,k} + \partial_x^{j,k}\kappa_{j,k} = 0, \tag{9}$$

where $S_{j,k} := S(z_{j,k}, x_j, t_k)$, $\partial_t^{j,k}$, $\partial_x^{j,k}$ are discretizations of the derivatives ∂_t and ∂_x, respectively. The numerical method (8) is called a multi-symplectic integrator of the system (1) if (9) is a discrete conservation law of (8) (see [20]).

Next, we consider multi-symplectic RK methods to solve the Hamiltonian wave equation. It is proved in [19] that Gauss-Legendre discretizations applied to the scalar wave equation (and Schrödinger equation) in both space and time directions lead to multi-symplectic methods, and further in [17] that symplectic RK methods applied to the general Hamiltonian PDEs in both space and time directions lead to the multi-symplecticity. Applying s- and r-stage symplectic RK methods (c, A, b) and $(\tilde{c}, \tilde{A}, \tilde{b})$ to the multi-symplectic formulation (6) of the nonlinear wave equation (5) in space and time, respectively, the resulting discretization is as follows:

$$U_{i,m} = u_0^{[m]} + \Delta x \sum_{j=1}^{s} a_{ij}\partial_x U_{j,m},$$

$$W_{i,m} = w_0^{[m]} + \Delta x \sum_{j=1}^{s} a_{ij}\partial_x W_{j,m},$$

$$u_1^{[m]} = u_0^{[m]} + \Delta x \sum_{i=1}^{s} b_i \partial_x U_{i,m},$$

$$w_1^{[m]} = w_0^{[m]} + \Delta x \sum_{i=1}^{s} b_i \partial_x W_{i,m},$$

$$\begin{aligned}
U_{i,m} &= u_{[i]}^0 + \Delta t \sum_{n=1}^{r} \tilde{a}_{mn} \partial_t U_{i,n}, \\
V_{i,m} &= v_{[i]}^0 + \Delta t \sum_{n=1}^{r} \tilde{a}_{mn} \partial_t V_{i,n}, \\
u_{[i]}^1 &= u_{[i]}^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t U_{i,m}, \\
v_{[i]}^1 &= v_{[i]}^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t V_{i,m}, \\
\partial_t U_{i,m} &= V_{i,m}, \\
\partial_x U_{i,m} &= W_{i,m}, \\
\partial_t V_{i,m} - \partial_x W_{i,m} &= -V'(U_{i,m}),
\end{aligned} \tag{10}$$

where $A = (a_{ij})_{i,j=1}^s$, $b = (b_1, \ldots, b_s)^\top$, and $\tilde{A} = (\tilde{a}_{i,j})_{i,j=1}^r$, $\tilde{b} = (\tilde{b}_1, \ldots, \tilde{b}_r)^\top$ are coefficients associated to the RK methods in space and time directions, respectively. Here we introduce the notations $U_{i,m} \approx u(c_i \Delta x, d_m \Delta t)$, $u_{[i]}^1 \approx u(c_i \Delta x, \Delta t)$, $u_1^{[m]} \approx u(\Delta x, d_m \Delta t)$, etc., with $c_i = \sum_{j=1}^s a_{ij}$, $d_m = \sum_{n=1}^r \tilde{a}_{mn}$, for $i = 1, \ldots, s$, $m = 1, \ldots, r$.

Remark 2.1. Recall that the conditions of multi-symplecticity of the method (10) are as follows:

$$\begin{cases} b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, & \forall\, i, j = 1, 2, \ldots, s, \\ \tilde{b}_m \tilde{a}_{mn} + \tilde{b}_n \tilde{a}_{nm} - \tilde{b}_m \tilde{b}_n = 0, & \forall\, m, n = 1, 2, \ldots, r, \end{cases} \tag{11}$$

or equivalently,

$$\begin{cases} M \equiv BA + A^\top B - bb^\top = 0, \\ \tilde{M} \equiv \tilde{B}\tilde{A} + \tilde{A}^\top \tilde{B} - \tilde{b}\tilde{b}^\top = 0, \end{cases} \tag{11$'$}$$

where $B = \mathrm{diag}(b)$ and $\tilde{B} = \mathrm{diag}(\tilde{b})$. We also refer interested readers to [3] for symplectic RK methods for Hamiltonian ODEs.

We give some examples of the multi-symplectic RK methods by using the Butcher tableau.

Example 2.1. If $r = s = 1$ with the following Butcher tableaux, we obtain a multi-symplectic Gauss collocation method with midpoint in time and space respectively, i.e., the centered Preissman scheme.

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array} \qquad \begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array} \quad .$$

If $r = 1$, $s = 2$ with the following Butcher tableaux, we obtain a multi-symplectic Gauss collocation method with midpoint in time and fourth order Gauss collocation method in space.

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array} \qquad \begin{array}{c|cc} \frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \quad .$$

For the numerical method (10), the discrete ECL corresponding to (3) with (7) is

$$\sum_{i=1}^{s} b_i [E_i^1 - E_i^0] \Delta x + \sum_{m=1}^{r} \tilde{b}_m [F_1^m - F_0^m] \Delta t = 0, \tag{12}$$

with

$$E_i^\ell = \frac{1}{2}((w_{[i]}^\ell)^2 + (v_{[i]}^\ell)^2) + V(u_{[i]}^\ell), \qquad F_\ell^m = -v_\ell^{[m]} w_\ell^{[m]}, \qquad \ell = 0, 1, \tag{13}$$

and the discrete MCL can be given in the same manner. It is well-known that if the method (10) is multi-symplectic, then this method preserves the discrete ECL (12) for a general quadratic V. The motivation of this paper is to construct a new numerical method which can preserve the multi-symplectic structure and the discrete ECL for the general V simultaneously.

3. EQUIP multi-symplectic methods

This section proposes a class of parametric multi-symplectic RK methods, called EQUIP multi-symplectic methods, by applying the EQUIP method to the Hamiltonian wave equation. This class of methods is multi-symplectic for all the real parameters, and can conserve the ECL simultaneously in a weak sense with a suitable parameter. The existence of such a parameter is presented in section 4.

The W-transformation is very useful in the characterization and construction of A-stable RK methods and is also practicable to construct high-order symplectic RK type methods. Now we give some definitions and results on the W-transformation.

Consider the shifted and normalized Legendre polynomials $P_k(x) = \frac{\sqrt{2k+1}}{k!}\frac{d^k}{dx^k}(x^k(x-1)^k)$ in $[0,1]$. These polynomials satisfy the integration formulas:

$$\int_0^x P_0(t)dt = \xi_1 P_1(x) + \frac{1}{2}P_0(x),$$

$$\int_0^x P_k(t)dt = \xi_{k+1}P_{k+1}(x) - \xi_k P_{k-1}(x), \qquad k = 1, 2, \ldots$$

with $\xi_k = \frac{1}{2\sqrt{4k^2-1}}$.

The definition of W-transformation relies on a generalized Vandermonde matrix $W = (w_{ij})_{i,j=1}^s$ whose elements are the shifted and normalized Legendre polynomials of degree j for $j = 0, 1, \ldots, s-1$, evaluated at c_i $(i = 1, 2, \ldots, s)$, i.e., $w_{ij} = P_{j-1}(c_i)$.

Definition 3.1. [29, p.81]. Let η, ξ be given integers between 0 and $s-1$. We say that an $s \times s$-matrix W satisfies $T(\eta, \xi)$ for the quadrature formula $(b_i, c_i)_{i=1}^s$ if

(1) W is nonsingular;
(2) $w_{i,j} = P_{j-i}(c_i)$, $i = 1, 2, \ldots, s$, $j = 1, 2, \ldots, \max(\eta, \xi) + 1$;
(3) $W^\top BW = \begin{pmatrix} I & 0 \\ 0 & R \end{pmatrix}$, where I is the $(\xi+1) \times (\xi+1)$ identity matrix and R is an arbitrary $(s-\xi-1) \times (s-\xi-1)$ matrix.

If W satisfies $T(\eta, \xi)$ for the quadrature formula $(b_i, c_i)_{i=1}^s$, then the W-transformation for an s-stage RK method is defined by

$$X = W^\top BAW. \tag{14}$$

Further, if A is the coefficient matrix for the Gauss method of order $2s$, then

$$X = W^\top BAW = W^{-1}AW = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & & \\ \xi_1 & 0 & -\xi_2 & & \\ & \xi_2 & \ddots & \ddots & \\ & & \ddots & 0 & -\xi_{s-1} \\ & & & \xi_{s-1} & 0 \end{pmatrix},$$

where $\xi_k = \frac{1}{2\sqrt{4k^2-1}}$ (see Theorem 5.6 and Theorem 5.9 in [29]). Note that the multi-symplectic condition $(11)'$ can be written in the form:

$$\begin{cases} W^\top MW = X + X^\top - e_1 e_1^\top = 0, \\ \tilde{W}^\top \tilde{M}\tilde{W} = \tilde{X} + \tilde{X}^\top - \tilde{e}_1\tilde{e}_1^\top = 0, \end{cases} \tag{15}$$

where $e_1 = (1, 0, \ldots, 0)^\top \in \mathbb{R}^s$ and $\tilde{e}_1 = (1, 0, \ldots, 0)^\top \in \mathbb{R}^r$.

For two given RK methods (c, A, b) and $(\tilde{c}, \tilde{A}, \tilde{b})$ with the transformation matrices X and $\tilde{X}$ defined by (14), we follow the idea of EQUIP methods in [13] to define the perturbed matrices $X(\alpha)$ and $\tilde{X}(\alpha)$ as

$$X(\alpha) = X + \alpha V, \quad \tilde{X}(\alpha) = \tilde{X} + \alpha\tilde{V}, \tag{16}$$

where α is a real parameter and

$$V = \begin{pmatrix} 0 & \cdots & 0 & & & & \\ \vdots & \ddots & & \ddots & & & \\ 0 & & \ddots & & -1 & & \\ & \ddots & & \ddots & & \ddots & \\ & & 1 & & \ddots & & 0 \\ & & & \ddots & & \ddots & \vdots \\ & & & & 0 & \cdots & 0 \end{pmatrix}.$$

Nonzero elements 1 and -1 in the matrix V should be arranged such that the matrix keeps being skew-symmetric. The matrix $\tilde{V}$ is defined similarly as V.

With the above preliminaries, we give the definition of EQUIP multi-symplectic methods.

Definition 3.2. Given a multi-symplectic RK method (10) with s- and r-stage symplectic RK methods (c, A, b) and $(\tilde{c}, \tilde{A}, \tilde{b})$ in space and time, respectively, for the Hamiltonian wave equation. The corresponding EQUIP multi-symplectic method is defined by using $(c, A(\alpha), b)$, $(\tilde{c}, \tilde{A}(\alpha), \tilde{b})$ instead, where

$$A(\alpha) = (W^\top B)^{-1} X(\alpha) W^{-1} = A + \alpha (W^\top B)^{-1} V W^{-1}, \tag{17}$$
$$\tilde{A}(\alpha) = (\tilde{W}^\top \tilde{B})^{-1} \tilde{X}(\alpha) \tilde{W}^{-1} = \tilde{A} + \alpha (\tilde{W}^\top \tilde{B})^{-1} \tilde{V} \tilde{W}^{-1}. \tag{18}$$

If the quadrature (b, c) has order $\geq 2s-1$ and $(\tilde{b}, \tilde{c})$ has order $\geq 2r-1$, (17) and (18) are reduced, respectively, to

$$A(\alpha) = W X(\alpha) W^{-1} = A + \alpha W V W^{-1}, \tag{19}$$
$$\tilde{A}(\alpha) = \tilde{W} \tilde{X}(\alpha) \tilde{W}^{-1} = \tilde{A} + \alpha \tilde{W} \tilde{V} \tilde{W}^{-1}. \tag{20}$$

The multi-symplecticity of the method (17)-(18) is stated in the following theorem.

Theorem 3.1. *Given a multi-symplectic RK method, if W (resp. $\tilde{W}$) satisfies $T(\eta, \xi)$ for $(b_i, c_i)_{i=1}^s$ (resp. $(\tilde{b}_i, \tilde{c}_i)_{i=1}^r$), then for any parameter α, the corresponding parametric method in (17)-(18) is also multi-symplectic.*

Proof. By utilizing (15), the proof follows from the anti-symmetricity of V and $\tilde{V}$. $\square$

Example 3.1. Based on (19)-(20), we give an example of the EQUIP multi-symplectic method with $r = 1$ and $s = 2$, whose Butcher tableaux are as follows:

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array} \qquad \begin{array}{c|cc} \frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} - \alpha \\ \frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} + \alpha & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}.$$

Consequently, if $\alpha = 0$, we retrieve the multi-symplectic Gauss collocation method with $r = 1$, $s = 2$. Note that in this example the method in space is exactly the EQUIP method (2.14) in [13, Example 1].

Remark 3.1. Since matrix V must be skew-symmetric, it vanishes in the case of $r = 1$. As is shown in the above example, it is sufficient to introduce the parameter α only in the spatial direction for the preservation of energy.

Similarly to the case of $\alpha = 0$, by concatenating any two parametric Gauss collocation methods in spatial and temporal directions respectively, we can construct a EQUIP multi-symplectic method.

Remark 3.2. If the periodic boundary condition $u(0, t) = u(L, t)$ is endowed, (3) yields the preservation of the "global" energy:

$$\mathcal{E}(t) := \int_0^L E(z(x, t)) dx = \int_0^L E(z(x, 0)) dx =: \mathcal{E}(0). \tag{21}$$

One can also have the conservation of the "global" momentum if $u(0, t) = u(L, t)$, i.e.,

$$\mathcal{I}(t) := \int_0^L I(z(x,t))dx = \int_0^L I(z(x,0))dx =: \mathcal{I}(0). \tag{22}$$

We will show through numerical experiments that the method proposed in this paper conserves well the local and "global" energies in section 5.

4. Energy-preserving of EQUIP multi-symplectic RK methods

In this section, we give an existence result of the parameter α^* which ensures the energy-preserving property of the proposed EQUIP multi-symplectic methods. The existence of such a parameter is in a weaker sense, which means that this parameter depends on the step sizes Δx, Δt, and on the initial data.

To find such a parameter α^*, we need to solve a nonlinear system with $4rs+1$ unknowns:

$$\begin{cases} U_{i,m} = u_0^{[m]} + \Delta x \sum_{j=1}^s a_{ij}(\alpha) W_{j,m}, \\ W_{i,m} = w_0^{[m]} + \Delta x \sum_{j=1}^s a_{ij}(\alpha) \partial_x W_{j,m}, \\ U_{i,m} = u_{[i]}^0 + \Delta t \sum_{n=1}^r \tilde{a}_{mn}(\alpha) V_{i,n}, \\ V_{i,m} = v_{[i]}^0 + \Delta t \sum_{n=1}^r \tilde{a}_{mn}(\alpha) \partial_t V_{i,n}, \\ \partial_t V_{i,m} - \partial_x W_{i,m} = -V'(U_{i,m}), \\ \sum_{i=1}^s b_i [E_i^1 - E_i^0] \Delta x + \sum_{m=1}^r \tilde{b}_m [F_1^m - F_0^m] \Delta t = 0. \end{cases} \tag{23}$$

Denoting

$$U = (U_1, U_2, \dots, U_r)^\top, \quad V = (V_1, V_2, \dots, V_r)^\top, \quad W = (W_1, W_2, \dots, W_r)^\top,$$
$$\partial_t V = (\partial_t V_1, \partial_t V_2, \dots, \partial_t V_r)^\top, \qquad \partial_x W = (\partial_x W_1, \partial_x W_2, \dots, \partial_x W_r)^\top$$

with $U_m = (U_{1,m}, U_{2,m}, \dots, U_{s,m}) \in \mathbb{R}^s$ and $V_m, W_m, \partial_t V_m, \partial_x W_m \in \mathbb{R}^s$, $m = 1, 2, \dots, r$ being defined similarly, the nonlinear system (23) can be rewritten in a compact form:

$$\begin{cases} U = u_0 \otimes e_s + \Delta x [I_r \otimes A(\alpha)] W, \\ W = w_0 \otimes e_s + \Delta x [I_r \otimes A(\alpha)][\partial_t V + R(U)], \\ U = e_r \otimes u^0 + \Delta t [\tilde{A}(\alpha) \otimes I_s] V, \\ V = e_r \otimes v^0 + \Delta t [\tilde{A}(\alpha) \otimes I_s] \partial_t V, \\ b^\top (E^1 - E^0) \Delta x + \tilde{b}^\top (F_1 - F_0) \Delta t = 0, \end{cases} \tag{24}$$

where $\otimes$ denotes the Kronecker product, $u^0 = (u_{[1]}^0, u_{[2]}^0, \dots, u_{[s]}^0)^\top$, $u^1 = (u_{[1]}^1, u_{[2]}^1, \dots, u_{[s]}^1)^\top$, $u_0 = (u_0^{[1]}, u_0^{[2]}, \dots, u_0^{[r]})^\top$, $u_1 = (u_1^{[1]}, u_1^{[2]}, \dots, u_1^{[r]})^\top$, and $v^0, v^1, v_0, v_1, w^0, w^1, w_0, w_1$ have the similar definitions. In addition,

$$e_s = (1, 1, \dots, 1)^\top \in \mathbb{R}^s, \qquad e_r = (1, 1, \dots, 1)^\top \in \mathbb{R}^r,$$
$$R(U) = (\tilde{V}_1^\top, \tilde{V}_2^\top, \dots, \tilde{V}_r^\top)^\top, \qquad \tilde{V}_m = (V'(U_{1,m}), \dots, V'(U_{s,m}))^\top,$$
$$A(\alpha) = (a_{ij}(\alpha))_{i,j=1}^s, \qquad \tilde{A}(\alpha) = (\tilde{a}_{mn}(\alpha))_{m,n=1}^r,$$
$$E^1 = (E_1^1, E_2^1, \dots, E_s^1)^\top, \quad E^0 = (E_1^0, E_2^0, \dots, E_s^0)^\top,$$
$$F_1 = (F_1^1, F_1^2, \dots, F_1^r)^\top, \quad F_0 = (F_0^1, F_0^2, \dots, F_0^r)^\top.$$

Using the above notations and the definitions of E_i^ℓ, F_ℓ^m, $\ell = 0, 1$, $i = 1, \dots, s$, $m = 1, \dots, r$ in (13), we rewrite the last equation in (24) using notations u^1, v^1, w^1, v_1, w_1 and u^0, v^0, w^0, v_0, w_0 directly, which is summarized in the following proposition.

Proposition 4.1. *The ECL, i.e., the last equation in (24), can be rewritten as*

$$\begin{aligned} &\Big[\frac{1}{2} b^\top \mathrm{diag}(w^1) w^1 + \frac{1}{2} b^\top \mathrm{diag}(v^1) v^1 + b^\top V(u^1) - \frac{1}{2} b^\top \mathrm{diag}(w^0) w^0 \\ &\quad - \frac{1}{2} b^\top \mathrm{diag}(v^0) v^0 - b^\top V(u^0)\Big] \Delta x + \Big[\tilde{b}^\top \mathrm{diag}(v_0) w_0 - \tilde{b}^\top \mathrm{diag}(v_1) w_1\Big] \Delta t = 0, \end{aligned} \tag{25}$$

where $V(u^0) = \left(V(u_{[1]}^0), V(u_{[2]}^0), \dots, V(u_{[s]}^0)\right)^\top$ *and* $V(u^1) = \left(V(u_{[1]}^1), V(u_{[2]}^1), \dots, V(u_{[s]}^1)\right)^\top$.

Therefore, we rewrite (24) as

$$\begin{cases} L(\Delta x, \Delta t, \alpha)Y - \Delta x F(Y, \alpha) = Y_0, \\ T(u^1, v^1, w^1, v_1, w_1) - T(u^0, v^0, w^0, v_0, w_0) = 0, \end{cases} \tag{26}$$

where $Y = (U^\top, V^\top, W^\top, \partial_t V^\top)^\top$, $Y_0 = ((u_0 \otimes e_s)^\top, (w_0 \otimes e_s)^\top, (e_r \otimes u^0)^\top, (e_r \otimes v^0)^\top)^\top$, $T(x, y, z, p, q) = \left[\frac{1}{2}b^\top \mathrm{diag}(z)z + \frac{1}{2}b^\top \mathrm{diag}(y)y + b^\top V(x)\right]\Delta x - \tilde{b}^\top \mathrm{diag}(p)q\Delta t$, and

$$L(\Delta x, \Delta t, \alpha) = \begin{pmatrix} I_{rs} & -\Delta x(I_r \otimes A(\alpha)) & O_{rs} & O_{rs} \\ O_{rs} & O_{rs} & I_{rs} & -\Delta x(I_r \otimes A(\alpha)) \\ I_{rs} & -\Delta t(\tilde{A}(\alpha) \otimes I_s) & O_{rs} & O_{rs} \\ O_{rs} & I_{rs} & O_{rs} & -\Delta t(\tilde{A}(\alpha) \otimes I_s) \end{pmatrix},$$

$$F(Y, \alpha) = \begin{pmatrix} 0_{rs} \\ (I_r \otimes A(\alpha))R(U) \\ 0_{rs} \\ 0_{rs} \end{pmatrix},$$

with O_{rs} being an $(rs \times rs)$-zero matrix and 0_{rs} being an rs-zero vector.

From (10), we have

$$w_1^{[m]} = w_0^{[m]} + \Delta x \sum_{i=1}^{s} b_i(\partial_t V_{i,m} + V'(U_{i,m})),$$

$$u_{[i]}^1 = u_{[i]}^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m V_{i,m},$$

$$v_{[i]}^1 = v_{[i]}^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t V_{i,m}.$$

Meanwhile, we introduce two auxiliary systems:

$$V_{i,m} = v_0^{[m]} + \Delta x \sum_{j=1}^{s} a_{ij}(\alpha)\partial_x V_{j,m},$$

$$v_1^{[m]} = v_0^{[m]} + \Delta x \sum_{i=1}^{s} b_i \partial_x V_{i,m},$$

$$W_{i,m} = w_{[i]}^0 + \Delta t \sum_{n=1}^{r} \tilde{a}_{mn}(\alpha)\partial_t W_{i,n},$$

$$w_{[i]}^1 = w_{[i]}^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t W_{i,m} = w_{[i]}^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_x V_{i,m},$$

where we use $\partial_x V_{i,m} = \partial_t W_{i,m}$ in the last equation. Thus the equations for u^1, v^1, w^1, v_1, w_1 can be written as

$$\begin{aligned} u^1 &= u^0 + \Delta t \tilde{B}_* V, \\ v^1 &= v^0 + \Delta t \tilde{B}_* \partial_t V, \\ w^1 &= w^0 + \Delta t \tilde{B}_* \partial_x V \\ v_1 &= v_0 + \Delta x B_* \partial_x V, \\ w_1 &= w_0 + \Delta x B_* (\partial_t V + R(U)), \end{aligned} \tag{27}$$

where $\tilde{B}_* = \tilde{b}^\top \otimes I_s$ and $B_* = I_r \otimes b^\top$.

Now we are in a position to show the existence of a proper parameter α^* such that the EQUIP multi-symplectic method (see Definition 3.2) preserves the ECL, following the idea in [13, Section 3]. Let $y_1 = (u^1, v^1, w^1, v_1, w_1)^\top$, $y_0 = (u^0, v^0, w^0, v_0, w_0)^\top$. Define the error function in the discrete ECL as $G(\alpha) = T(y_1) - T(y_0)$. When needed, $G(\alpha)$ may be written as $G(\alpha, \Delta x, \Delta t)$ to emphasize the dependence on step sizes Δx and Δt. The numerical solution of the EQUIP multi-symplectic method (17)-(18) defines a corresponding mapping of the form $y_1 = \Phi_{\Delta x, \Delta t}(y_0, \alpha)$. The nonlinear system (24), in which $4rs+1$ unknowns $U, V, W, \partial_t V$ and α need to be solved in every rectangular domain composed of length Δx and width Δt, reads

$$\begin{cases} L(\Delta x, \Delta t, \alpha)Y = Y_0 + \Delta x F(Y, \alpha), \\ G(\alpha) = 0. \end{cases} \tag{28}$$

The solvability of this system yields the existence of the energy-preserving method. For convenience, we denote $h := \Delta x$, $\tau := \Delta t$, and define the vector function

$$\varphi(h, \tau, y_1, \alpha) = \begin{pmatrix} y_1 - \Phi_{h,\tau}(y_0, \alpha) \\ T(y_1) - T(y_0) \end{pmatrix},$$

then the system (28) is equivalent to $\varphi(h, \tau, y_1, \alpha) = 0$.

From (27), we know that $\varphi(0, 0, y_1, \alpha) = 0$ for every y_1 and α. The Jacobian of φ with respect to (y_1, α) is

$$\frac{\partial \varphi}{\partial (y_1, \alpha)}(h, \tau, y_1, \alpha) = \begin{pmatrix} I & -\frac{\partial \Phi_{h,\tau}}{\partial \alpha}(y_0, \alpha) \\ \nabla^\top T(y_1) & 0 \end{pmatrix} \tag{29}$$

with I being the identity matrix of dimension $3s + 2r$. By using the formula on the determinant of a block matrix, we get

$$\det\left(\frac{\partial \varphi}{\partial (y_1, \alpha)}(h, \tau, y_1, \alpha)\right) = \det\left(\nabla^\top T(y_1) \cdot \frac{\partial \Phi_{h,\tau}}{\partial \alpha}(y_0, \alpha)\right).$$

Since

$$T(y_1) = \left[\frac{1}{2} b^\top \mathrm{diag}(w^1) w^1 + \frac{1}{2} b^\top \mathrm{diag}(v^1) v^1 + b^\top V(u^1)\right] h - \tilde{b}^\top \mathrm{diag}(v_1) w_1 \tau,$$

it holds that

$$(\nabla T(y_1))^\top = \Big(b^\top P'_{u^1}(u^1) h, \quad \frac{1}{2} b^\top (\mathrm{diag}(v^1) v^1)'_{v^1} h, \quad \frac{1}{2} b^\top (\mathrm{diag}(w^1) w^1)'_{w^1} h,$$
$$- \tilde{b}^\top (\mathrm{diag}(v_1) w_1)'_{v_1} \tau, \quad -\tilde{b}^\top (\mathrm{diag}(v_1) w_1)'_{w_1} \tau\Big).$$

Therefore, when $h = 0$ and $\tau = 0$, $(\nabla T(y_1))^\top$ is the zero vector for any α, and thus the rank of the matrix (29) is $3s + 2r$.

Due to singularity of the matrix (29) when $h = 0$ and $\tau = 0$, the implicit function theorem cannot be applied directly to prove the solvability of the nonlinear system (28). In [13], the existence of the parameter α^* for the EQUIP method is proved with the aid of the Lyapunov-Schmidt decomposition method. This decomposition method restricts the nonlinear system to the complement of the null space and the range of the Jacobian. Thus one gets two subsystems whose Jacobians are nonsingular and then the implicit function theorem is applicable.

Before we give the existence of α^*, we first state the solvability of the first system in (28), which could be proved similarly as in [30, Theorem 3.1].

Lemma 4.1. *If $h \leqslant \tau^2$ and the RK matrix $\tilde{A}$ is nonsingular, then for $|\alpha| \leqslant \alpha_0$, $h \leqslant h_0$ and $\tau \leqslant \tau_0$ with α_0, h_0 and τ_0 small enough, there exists a solution $Y(\alpha)$ of the first system in (28).*

Similar as in [13], the following assumptions are made to give the existence of α^*:

(S_1) $h \leqslant \tau^2$;
(S_2) The function G is analytic in a cube $\mathcal{Q} = [-\alpha_0, \alpha_0] \times [-h_0, h_0] \times [-\tau_0, \tau_0]$;
(S_3) $G(0, h, \tau) = c_0 \tau^d + \mathcal{O}(\tau^{d+1}), \quad c_0 \neq 0,$
$G(\alpha, h, \tau) = c(\alpha) \tau^{d-m} + \mathcal{O}(\tau^{d+1-m}), \quad c(\alpha) \neq 0.$

The following lemma gives the existence and expansion of α^*, whose proof follows that of [13, Theorem 3.2] for EQUIP methods of Hamiltonian ODEs.

Lemma 4.2. *Under assumptions (S_1)-(S_3), there exists a function $\alpha^* = \alpha^*(h, \tau)$ defined in a rectangle $(-h_0, h_0) \times (-\tau_0, \tau_0)$, such that*

(i) $G(\alpha^*(h, \tau), h, \tau) = 0$, *for all $h \in (-h_0, h_0)$ and $\tau \in (-\tau_0, \tau_0)$;*
(ii) $\alpha^*(h, \tau) = \mathrm{const} \cdot \tau^m + \mathcal{O}(\tau^{m+1})$ *for some integer m.*

Proof. From (S_2) and (S_3), the expansion of G around $(0,0,0)$ is

$$G(\alpha,h,\tau)=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\sum_{k=0}^{\infty}\frac{1}{i!j!k!}\cdot\frac{\partial^{i+j+k}G}{\partial\alpha^i\partial h^j\partial\tau^k}(0,0,0)\alpha^i h^j\tau^k. \tag{30}$$

By (S_1), there exists a constant β $(0<\beta<1)$ such that $h=\beta\tau^2$. Substituting this into (30) leads to

$$\begin{aligned}G(\alpha,h,\tau)=G(\alpha,h(\tau),\tau)&=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\sum_{k=0}^{\infty}\frac{\beta^j}{i!j!k!}\cdot\frac{\partial^{i+j+k}G}{\partial\alpha^i\partial h^j\partial\tau^k}(0,0,0)\alpha^i\tau^{2j+k}\\ &=\sum_{j=0}^{\infty}\sum_{k=0}^{\infty}\frac{\beta^j}{j!k!}\cdot\frac{\partial^{j+k}G}{\partial h^j\partial\tau^k}(0,0,0)\tau^{2j+k}+\sum_{i=1}^{\infty}\sum_{j=0}^{\infty}\sum_{k=0}^{\infty}\frac{\beta^j}{i!j!k!}\cdot\frac{\partial^{i+j+k}G}{\partial\alpha^i\partial h^j\partial\tau^k}(0,0,0)\alpha^i\tau^{2j+k}.\end{aligned}$$

From (S_3), the above equation can be rewritten as

$$G(\alpha,h(\tau),\tau)=\sum_{2j+k\geqslant d}\frac{\beta^j}{j!k!}\cdot\frac{\partial^{j+k}G}{\partial h^j\partial\tau^k}(0,0,0)\tau^{2j+k}+\sum_{i=1}^{\infty}\sum_{2j+k\geqslant d-m}\frac{\beta^j}{i!j!k!}\cdot\frac{\partial^{i+j+k}G}{\partial\alpha^i\partial h^j\partial\tau^k}(0,0,0)\alpha^i\tau^{2j+k}.$$

In order to find a solution $\alpha^*=\alpha^*(h(\tau),\tau)$ in the form of $\alpha^*(h(\tau),\tau)=\eta(\tau)\tau^m$ with $\eta(\tau)$ being a real-valued function of τ, we consider the change of variables $\alpha=\eta\tau^m$,

$$\begin{aligned}&G(\alpha,h(\tau),\tau)\\ &=\sum_{2j+k\geqslant d}\frac{\beta^j}{j!k!}\cdot\frac{\partial^{j+k}G}{\partial h^j\partial\tau^k}(0,0,0)\tau^{2j+k}+\sum_{i=1}^{\infty}\sum_{2j+k\geqslant d-m}\frac{\beta^j}{i!j!k!}\cdot\frac{\partial^{i+j+k}G}{\partial\alpha^i\partial h^j\partial\tau^k}(0,0,0)\eta^i\tau^{mi+2j+k}\\ &=\sum_{2j+k=d}\frac{\beta^j}{j!k!}\cdot\frac{\partial^{j+k}G}{\partial h^j\partial\tau^k}(0,0,0)\tau^d+\mathcal{O}(\tau^{d+1})+\sum_{2j+k=d-m}\frac{\beta^j}{j!k!}\cdot\frac{\partial^{1+j+k}G}{\partial\alpha\partial h^j\partial\tau^k}(0,0,0)\eta\tau^d+\mathcal{O}(\tau^{d+1})\\ &=\tau^d\left[\sum_{2j+k=d}\frac{\beta^j}{j!k!}\cdot\frac{\partial^{j+k}G}{\partial h^j\partial\tau^k}(0,0,0)+\sum_{2j+k=d-m}\frac{\beta^j}{j!k!}\cdot\frac{\partial^{1+j+k}G}{\partial\alpha\partial h^j\partial\tau^k}(0,0,0)\eta+\mathcal{O}(\tau)\right].\end{aligned}$$

Denoting by $\tilde{G}(\eta,\tau)$ the formula in the above bracket. If $\tau\neq 0$, then $G(\alpha,h(\tau),\tau)=0$ if and only if $\tilde{G}(\eta,\tau)=0$. Therefore, we apply the implicit function theorem to $\tilde{G}(\eta,\tau)=0$. By (S_3), both $\sum_{2j+k=d}\frac{\beta^j}{j!k!}\cdot\frac{\partial^{j+k}G}{\partial h^j\partial\tau^k}(0,0,0)$ and $\sum_{2j+k=d-m}\frac{\beta^j}{j!k!}\cdot\frac{\partial^{1+j+k}G}{\partial\alpha\partial h^j\partial\tau^k}(0,0,0)$ are not equal to zero. Let

$$\eta_0=-\frac{\sum_{2j+k=d}\frac{\beta^j}{j!k!}\cdot\frac{\partial^{j+k}G}{\partial h^j\partial\tau^k}(0,0,0)}{\sum_{2j+k=d-m}\frac{\beta^j}{j!k!}\cdot\frac{\partial^{1+j+k}G}{\partial\alpha\partial h^j\partial\tau^k}(0,0,0)},\quad \tau_0=0,$$

then, $\tilde{G}(\eta_0,\tau_0)=0$. The functions $\tilde{G}(\eta,\tau)$, $\tilde{G}_\eta(\eta,\tau)$ and $\tilde{G}_\tau(\eta,\tau)$ are continuous in the neighborhood of the point (η_0,τ_0), moreover,

$$\tilde{G}_\eta(\eta_0,\tau_0)=\sum_{2j+k=d-m}\frac{\beta^j}{j!k!}\cdot\frac{\partial^{1+j+k}G}{\partial\alpha\partial h^j\partial\tau^k}(0,0,0)\neq 0.$$

Hence the implicit function theorem ensures the existence of a function $\eta=\eta(\tau)$ such that $\tilde{G}(\eta(\tau),\tau)=0$.

From the equation

$$\tilde{G}(\eta,\tau)=\sum_{2j+k=d}\frac{\beta^j}{j!k!}\frac{\partial^{j+k}G}{\partial h^j\partial\tau^k}(0,0,0)+\sum_{2j+k=d-m}\frac{\beta^j}{j!k!}\frac{\partial^{1+j+k}G}{\partial\alpha\partial h^j\partial\tau^k}(0,0,0)\eta+\mathcal{O}(\tau)=0,$$

the solution of $G(\alpha,\tau)=0$ takes the form

$$\alpha^*(h(\tau),\tau)=\eta(\tau)\tau^m=-\frac{\sum_{2j+k=d-m}\frac{\beta^j}{j!k!}\frac{\partial^{j+k}G}{\partial h^j\partial\tau^k}(0,0,0)}{\sum_{2j+k=d-m}\frac{\beta^j}{j!k!}\frac{\partial^{1+j+k}G}{\partial\alpha\partial h^j\partial\tau^k}(0,0,0)}\tau^m+\mathcal{O}(\tau^{m+1}),$$

which completes the proof. □

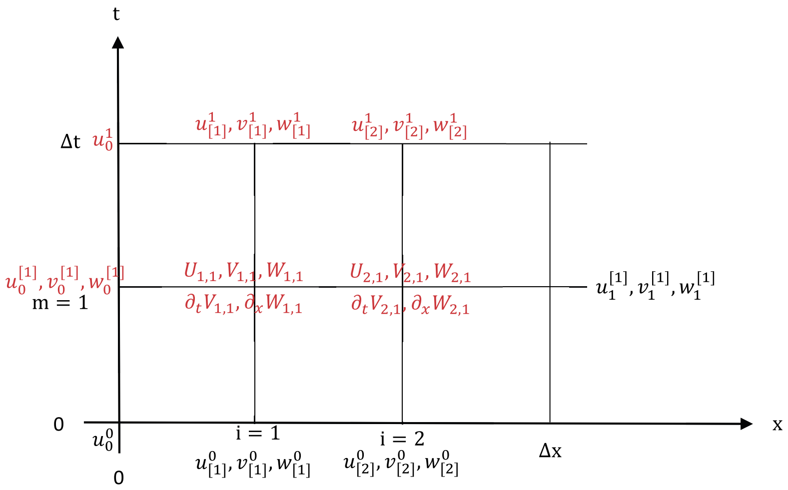

Fig. 1. A uniform grid and the unknowns in grid points.

From Lemmas 4.1 and 4.2, we obtain the main result.

Theorem 4.1. *Let assumptions* (S_1), (S_2) *and* (S_3) *be satisfied and let the RK matrix* $\tilde{A}$ *be nonsingular. Then the system (28) is solved uniquely, i.e., there exists a unique solution* $(Y^\top, \alpha^*)$.

The assumption (S_1) and the nonsingularity of $\tilde{A}$ in Theorem 4.1 can be replaced by $\tau \leqslant h^2$ and the nonsingularity of A, respectively. In fact, from [30] if the RK matrix A is nonsingular, the conclusion of Lemma 4.1 still holds. And in the proof of Lemma 4.2, by considering the change of variables $\alpha(h) = \zeta(h)h^m$, we can still get the solvability of the second equation of (28) with respect to α. The following corollary states the result.

Corollary 4.1. *Let assumptions* (S_2) *and* (S_3) *be satisfied. Then two kinds of conditions on step sizes and nonsigularities, each of which guarantees the solvability of the system (28), are as follows:*

(1) $h \leqslant \tau^2$ *and* $\tilde{A}$ *is nonsingular,*
(2) $\tau \leqslant h^2$ *and* A *is nonsingular.*

5. Numerical experiments

In this section, we present some numerical experiments to show the effectiveness in energy-preserving of the proposed EQUIP multi-symplectic methods. We consider the sine-Gordon equation (i.e., $V(u) = -\cos(u)$ in (5)):

$$\begin{aligned} \partial_{tt}u &= \partial_{xx}u - \sin(u), \quad (x,t) \in (-L/2, L/2) \times (0, T], \\ u(-L/2,t) &= u(L/2,t), \quad t \in [0, T], \end{aligned} \tag{31}$$

with initial conditions:

$$\begin{aligned} u(x,0) &= 4\tan^{-1}\left(\frac{e^{x-L/6}}{\sqrt{1-\beta^2}}\right) + 4\tan^{-1}\left(\frac{e^{-x-L/6}}{\sqrt{1-\beta^2}}\right), \\ \partial_t u(x,0) &= \frac{\partial}{\partial t}\left[4\tan^{-1}\left(\frac{e^{x-L/6-\beta t}}{\sqrt{1-\beta^2}}\right) + 4\tan^{-1}\left(\frac{e^{-x-L/6-\beta t}}{\sqrt{1-\beta^2}}\right)\right]\Bigg|_{t=0}. \end{aligned} \tag{32}$$

On an infinite domain, these initial conditions could yield a soliton solution and an anti-soliton solution moving with speed $\pm\beta$ respectively. We set $\beta = 0.5$, $L = 100$ and $T = 200$.

5.1. Numerical method

The numerical solution of (31)-(32) is obtained by using the EQUIP multi-symplectic method with $r = 1$ (midpoint in time) and $s = 2$ (fourth order Gauss collocation method in space) with a temporal step size $\Delta t = 0.1$ and a spatial step size $\Delta x = 1$ (see Example 3.1). Below the implementation of this method is provided in details for the sake of clarity.

First, in each domain composed of Δt and Δx, by letting $s = 2$, $r = 1$ in (10) with Butcher tableaux in Example 3.1, we obtain a nonlinear system with the discrete ECL (12)-(13):

$$
\begin{aligned}
&U_{1,1} = u_0^{[1]} + \Delta x \left(\frac{1}{4} W_{1,1} + \left(\frac{1}{4} - \frac{\sqrt{3}}{6} - \alpha \right) W_{2,1} \right), \\
&U_{2,1} = u_0^{[1]} + \Delta x \left(\left(\frac{1}{4} + \frac{\sqrt{3}}{6} + \alpha \right) W_{1,1} + \frac{1}{4} W_{2,1} \right), \\
&W_{1,1} = w_0^{[1]} + \Delta x \left(\frac{1}{4} \partial_x W_{1,1} + \left(\frac{1}{4} - \frac{\sqrt{3}}{6} - \alpha \right) \partial_x W_{2,1} \right), \\
&W_{2,1} = w_0^{[1]} + \Delta x \left(\left(\frac{1}{4} + \frac{\sqrt{3}}{6} + \alpha \right) \partial_x W_{1,1} + \frac{1}{4} \partial_x W_{2,1} \right), \\
&u_1^{[1]} = u_0^{[1]} + \frac{\Delta x}{2} (W_{1,1} + W_{2,1}), \\
&w_1^{[1]} = w_0^{[1]} + \frac{\Delta x}{2} (\partial_x W_{1,1} + \partial_x W_{2,1}), \\
&U_{1,1} = u_{[1]}^0 + \frac{\Delta t}{2} V_{1,1}, \\
&U_{2,1} = u_{[2]}^0 + \frac{\Delta t}{2} V_{2,1}, \\
&V_{1,1} = v_{[1]}^0 + \frac{\Delta t}{2} \partial_t V_{1,1}, \\
&V_{2,1} = v_{[2]}^0 + \frac{\Delta t}{2} \partial_t V_{2,1}, \\
&u_{[1]}^1 = u_{[1]}^0 + \Delta t V_{1,1}, \\
&u_{[2]}^1 = u_{[2]}^0 + \Delta t V_{2,1}, \\
&v_{[1]}^1 = v_{[1]}^0 + \Delta t \partial_t V_{1,1}, \\
&v_{[2]}^1 = v_{[2]}^0 + \Delta t \partial_t V_{2,1}, \\
&\partial_t V_{1,1} - \partial_x W_{1,1} = -\sin(U_{1,1}), \\
&\partial_t V_{2,1} - \partial_x W_{1,1} = -\sin(U_{2,1}), \\
&\frac{\Delta x}{4} \Big((w_{[1]}^1)^2 + (w_{[2]}^1)^2 + (v_{[1]}^1)^2 + (v_{[2]}^1)^2 - 2\cos(u_{[1]}^1) - 2\cos(u_{[2]}^1) \Big) - \Delta t v_1^{[1]} w_1^{[1]} \\
&= \frac{\Delta x}{4} \Big((w_{[1]}^0)^2 + (w_{[2]}^0)^2 + (v_{[1]}^0)^2 + (v_{[2]}^0)^2 - 2\cos(u_{[1]}^0) - 2\cos(u_{[2]}^0) \Big) - \Delta t v_0^{[1]} w_0^{[1]},
\end{aligned}
\tag{33}
$$

which has 20 unknowns $U_{1,1}, U_{2,1}, V_{1,1}, V_{2,1}, W_{1,1}, W_{2,1}, \partial_t V_{1,1}, \partial_t V_{2,1}, \partial_x W_{1,1}, \partial_x W_{2,1}, u_0^{[1]}, w_0^{[1]}, v_0^{[1]}, u_{[1]}^1, u_{[2]}^1, v_{[1]}^1, v_{[2]}^1, w_{[1]}^1, w_{[2]}^1$ and α. Since (33) only contains 17 equations, it still needs three more equations. To this end, letting $u_0^0 = u(0, 0)$, we add the following equations to the above system (33) (see for instance [19, Section 3]),

$$
\begin{aligned}
&u_0^{[1]} = u_0^0 + \frac{\Delta t}{2} v_0^{[1]}, \\
&u_{[1]}^1 = u_0^1 + \Delta x \left(\frac{1}{4} w_{[1]}^1 + \left(\frac{1}{4} - \frac{\sqrt{3}}{6} - \alpha \right) w_{[2]}^1 \right), \\
&u_{[2]}^1 = u_0^1 + \Delta x \left(\left(\frac{1}{4} + \frac{\sqrt{3}}{6} + \alpha \right) w_{[1]}^1 + \frac{1}{4} w_{[2]}^1 \right), \\
&u_0^1 = u_0^0 + \Delta t v_0^{[1]},
\end{aligned}
\tag{34}
$$

where $u_0^1 \approx u(0, \Delta t)$ is another unknown. Therefore, we have the nonlinear system (33)-(34) with 21 unknowns (see Fig. 1).

Next, considering the periodic boundary condition, in each time level we put together the above individual nonlinear system through space axis (including $M = 100$ grid points), which leads to a nonlinear system with 2100 unknowns. Denoting by X the unknowns, this nonlinear system can be rewritten as $F(X) = 0$, which is solved by using Newton iteration method with tolerance $\epsilon = 10^{-15}$.

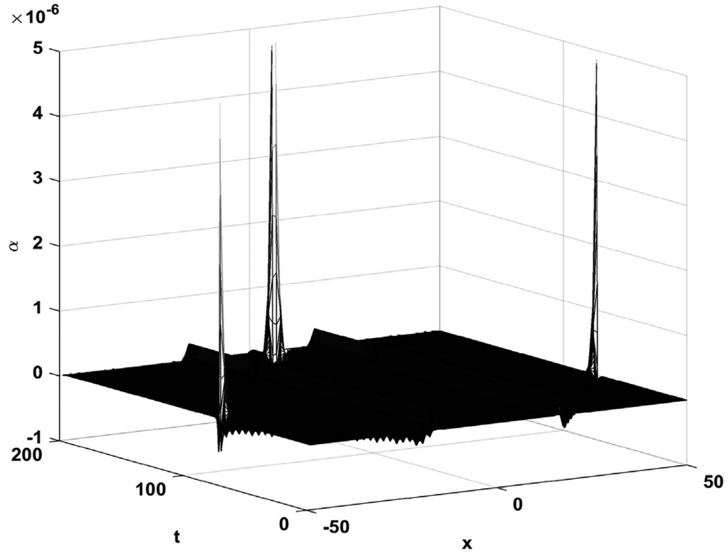

Fig. 2. Values of α in the EQUIP multi-symplectic method at (x,t)-plane $[-50,\ 50] \times [0,\ 200]$ with $h = 1$ and $\tau = 0.1$.

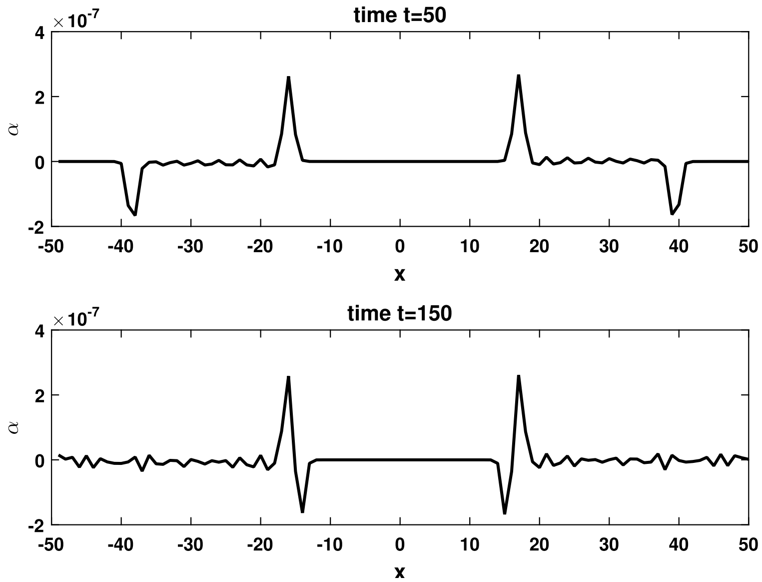

Fig. 3. Values of α in the EQUIP multi-symplectic method at two fixed moments $t = 50$ and $t = 150$.

5.2. Numerical results

Fig. 2 presents the values of the parameter α in the EQUIP multi-symplectic method on (x,t)-plane [-50, 50]× [0, 200], which make the method preserve energy. Fig. 3 shows the values of such parameter in details, for the selected moments $t = 50$ and $t = 150$. Numerical results indicate that the parameter sequence exists at every calculation grid and has the absolute values closed to zero (about $10^{-7} \sim 10^{-8}$). Fig. 4 is the cross-section plots of the wave $u(x,t)$ at some selected moments during the time interval $[0, 200]$.

We compare the errors of the total energy $\mathcal{E}(t)$ by using the multi-symplectic Gauss collocation (denoted by MSRK) method and the EQUIP multi-symplectic (denoted by α-MSRK) method, which are shown in Fig. 5. Numerical results show that in the conservation of the total energy $\mathcal{E}(t)$, the error of the MSRK method is of about 10^{-3}, while the error of the α-MSRK method is of about 10^{-12}. Both the MSRK method and the α-MSRK method conserve the total momentum $\mathcal{I}(t)$ exactly, since it is a quadratic invariant.

Fig. 6 shows the comparison of the error in the local discrete ECL (12)-(13) of the MSRK method and the α-MSRK method, in the time intervals $[0, 30]$ and $[150, 170]$, respectively. Observe that the α-MSRK method (about 10^{-13}) conserves the discrete ECL better than the MSRK method (about 10^{-3}).

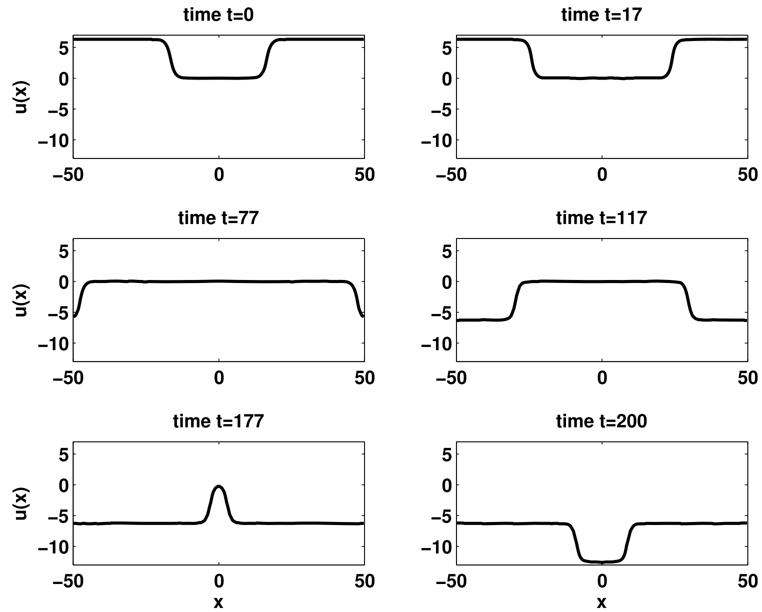

Fig. 4. Time evolution of solution during the time interval t ∈ [0, 200].

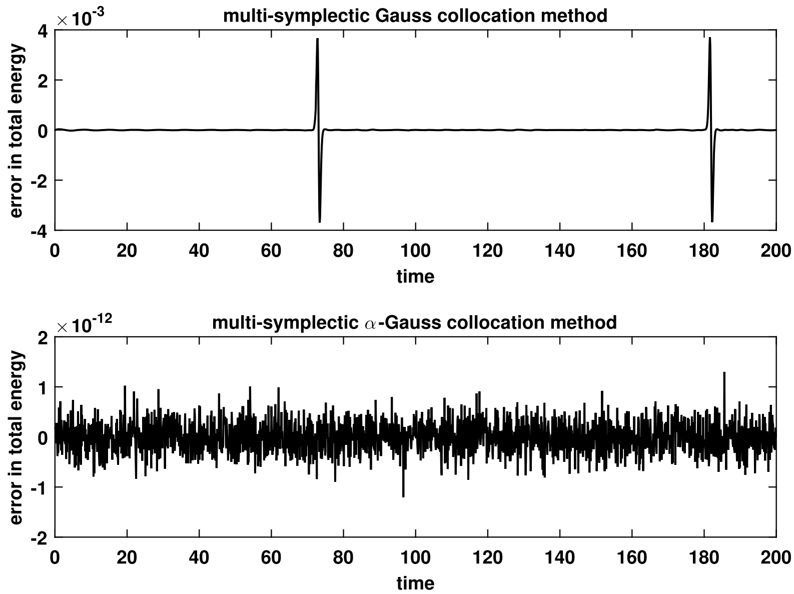

Fig. 5. Comparison of numerical errors in the global energy for both the MSRK method and the α-MSRK method over the time interval [0, 200].

Next, we will report the error in the numerical solution. Since the exact solution of this problem (31) with initial conditions (32) is not known explicitly, we use the numerical solution with a smaller time step size $\Delta t_0 = 0.01$ as the reference solution (denoted by $u_{\Delta t_0}$) to estimate the error.

The pointwise error is defined by

$$e_{\Delta t}(x_i, t^n) = |u_{\Delta t}(x_i, t^n) - u_{\Delta t_0}(x_i, t^n)|,$$

where the step size Δt takes the values 0.1, 0.08, 0.05, 0.02 as different step sizes, and $t^n = n\Delta t_0$ $(1 \le n \le N,\ N = 200/\Delta t_0)$. Fig. 7 shows the corresponding pointwise errors at some selected moments during the time interval [0, 200].

The discrete maximal (L^∞) and average (L^2) errors are defined as

$$L^\infty(t^n) = \max_{1\le i\le M} |e_{\Delta t}(x_i, t^n)|,$$

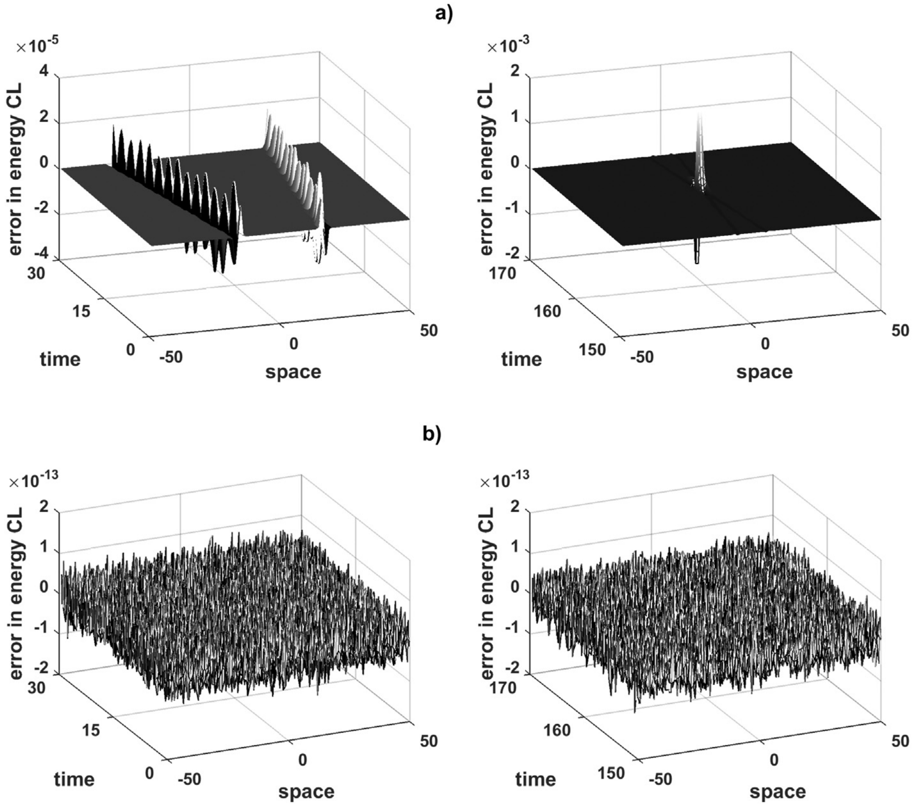

Fig. 6. Comparison of numerical errors in the local energy for both the MSRK method and the α-MSRK method over the time intervals [0, 30] and [150, 170].

Table 1
Values of errors at some selected times in [0, 200] for different temporal step sizes.

t	L^∞-error				L^2-error			
	$\Delta t = 0.1$	$\Delta t = 0.08$	$\Delta t = 0.05$	$\Delta t = 0.02$	$\Delta t = 0.1$	$\Delta t = 0.08$	$\Delta t = 0.05$	$\Delta t = 0.02$
1	9.46E–04	7.24E–04	2.25E–04	7.25E–05	2.73E–03	2.01E–04	1.11E–04	3.53E–04
17	4.69E–03	4.23E–03	3.62E–03	2.51E–03	1.95E–02	1.88E–02	1.81E–02	1.12E–02
77	2.43E–02	1.70E–02	7.67E–03	3.70E–03	6.34E–02	4.20E–02	4.20E–02	2.39E–02
117	1.94E–02	1.61E–02	5.18E–03	4.25E–03	7.34E–02	4.77E–02	4.77E–02	2.25E–02
177	2.09E–02	1.75E–02	7.09E–03	3.84E–03	8.34E–02	6.68E–02	6.68E–02	2.85E–02
200	3.48E–02	2.11E–02	8.29E–03	5.55E–03	1.40E–01	9.02E–02	9.02E–02	3.77E–02

$$L^2(t^n) = \left(\Delta x \sum_{1 \le i \le M} |e_{\Delta t}(x_i, t^n)|^2 \right)^{1/2}.$$

Fig. 8 and Fig. 9 present the curves of solution errors in L^∞- and L^2-norms in the time interval [0, 200] when $\Delta t = 0.1$, 0.08, 0.05 and 0.02, respectively.

Table 1 shows the values of solution errors at some selected moments during the time interval [0, 200] for different temporal step sizes.

5.3. Comparison of computational costs

When we implement the numerical experiments to solve the problem with the periodic boundary condition by using the EQUIP multi-symplectic method, the major costs result from the discretization of the PDE. The nonlinear system to be solved in each domain $(0, \Delta x) \times (0, \Delta t)$ has $(5s+3)r + 3s + 2$ unknowns. When $\alpha = 0$, namely, the standard multi-symplectic RK method is applied, the nonlinear system has $(5s+2)r$ unknowns. Therefore when Newton iteration method is applied, the Jacobian matrix has dimension $(5s+2)r$ for the case of $\alpha = 0$, while it has dimension $(5s+3)r + 3s + 2$ for the case of $\alpha = \alpha^*$. After assembling the individual Jacobian matrix through space axis (including $M = 100$ grid points), we obtain the matrices with $M(5s+2)r$ and $M((5s+3)r + 3s + 2)$ dimensions respectively. These matrices have approximately sparse

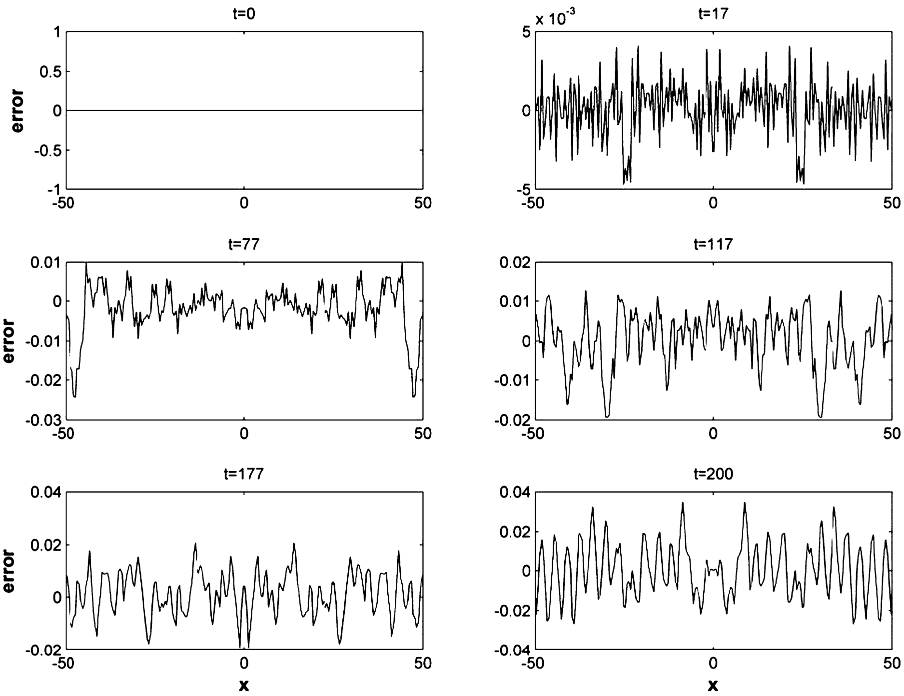

Fig. 7. Time evolution of the error for $\Delta t = 0.1$.

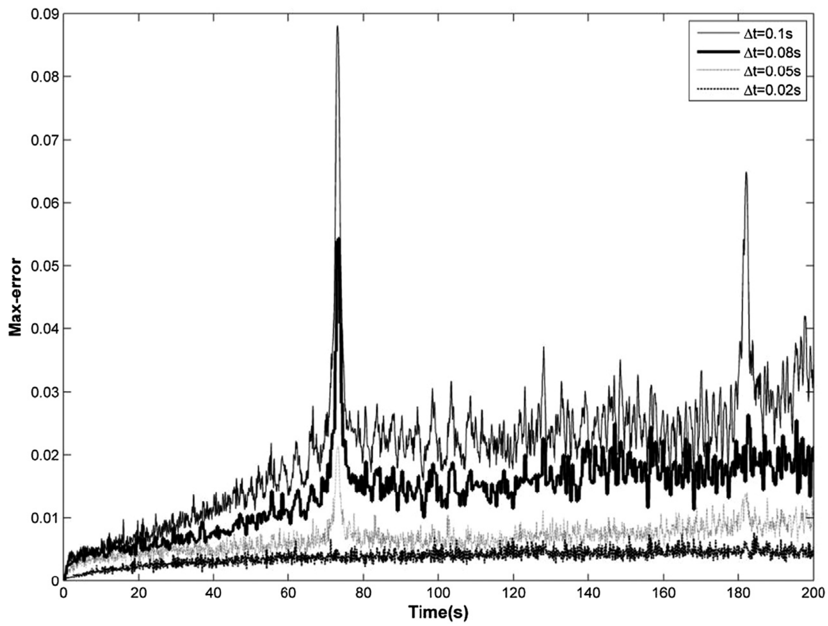

Fig. 8. Errors in L^∞-norm during the time interval [0, 200] for different temporal step sizes.

band structure with bandwidth $(5s+2)r+2$ and $(5s+3)r+3s+4$, respectively. Gauss elimination method is used in each iteration of Newton iteration method to solve a system of linear equations. If we denote d the bandwidth and N the dimension of the matrix, the calculation cost by using Gauss elimination method is as follows:

$$\begin{aligned}\text{Cost} &= [(N-d)d^2 + d^3/3](\text{forward}) + (Nd - d^2/2)(\text{backward}) \\ &= Nd^2 - 2d^3/3 + Nd - d^2/2.\end{aligned}$$

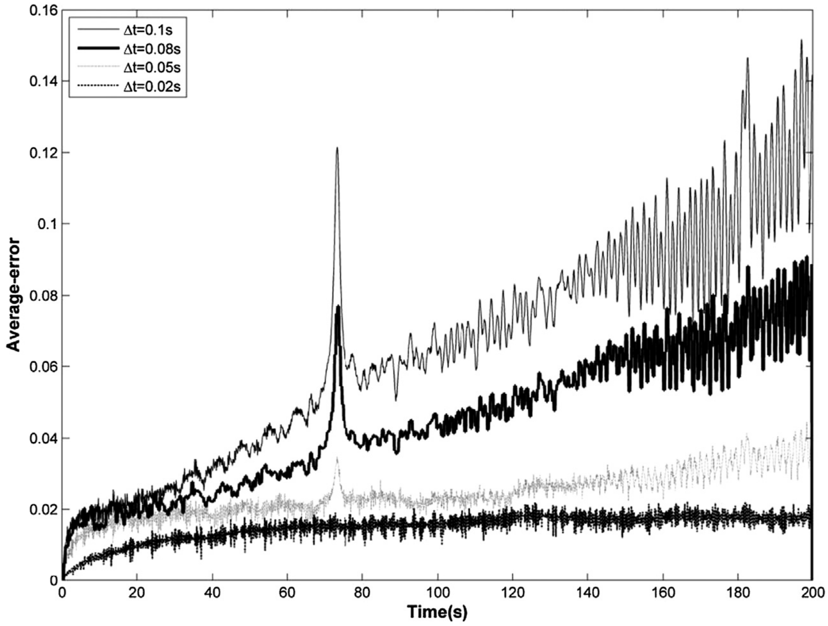

Fig. 9. Errors in L^2-norm during the time interval $[0, 200]$ for different temporal step sizes.

Table 2
Computer costs for the cases of $\alpha = 0$ and $\alpha = \alpha^*$.

Computer type	$\alpha = 0$	$\alpha = \alpha^*$
Core two Duo	$1091.47s$	$3283.46s$
Fourth generation core i5	$482.3s$	$1320.8s$

If $N \gg d$, then $\text{Cost} \approx Nd^2 + Nd \approx Nd^2$. Therefore, the costs of these two methods are approximately $M((5s+2)r+2)^2$ and $M((5s+3)r+2s+4)^2$, respectively. By comparing these two costs, we know that the larger s and r are, the smaller the difference in dimensions of the Jacobian matrices is. We compare the computational time needed to solve the sine-Gordon equation (31)-(32) by using the EQUIP multi-symplectic method with $r = 1$ and $s = 2$ in the cases of $\alpha = 0$ and $\alpha = \alpha^*$. In the numerical experiments, we have used Gauss elimination method to solve the linear system in each step of Newton iterations. We notice from Table 2 that the costs in numerical experiments coincide approximately with the above theoretical results.

6. Concluding remarks

We propose a family of EQUIP multi-symplectic methods for the Hamiltonian wave equation. These methods are multi-symplectic perturbations of the classical multi-symplectic methods with the free parameter α. The existence of a parameter such that the methods are energy-preserving in a weaker sense is proved. This weaker sense means that the parameter depends on the step sizes and the initial data, which says that the energy conservation property may fail if one changes the step sizes or the initial data. Numerical experiments show the effectiveness of the proposed method, and the preservation of both multi-symplecticity and energy. This work considers only energy-preserving property together with multi-symplecticity, a research on multi-symplectic method preserving both energy and momentum, and possible further invariants, will be the subject of future investigations.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

Jialin Hong and Chuchu Chen are supported by National Natural Science Foundation of China (Nos. 91630312, 11711530017, 11871068 and 11971470). Chol Sim and Kwang Sonwu are supported by Academy of Mathematics and Systems Science, Chinese Academy of Sciences.

References

[1] E. Hairer, C. Lubich, G. Wanner, Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations, eprint of the second (2006) edition Springer Series in Computational Mathematics, vol. 31, Springer, Heidelberg, 2010.

[2] K. Feng, M. Qin, Symplectic Geometric Algorithms for Hamiltonian Systems, Zhejiang Science and Technology Publishing House/Springer, Hangzhou/Heidelberg, 2010, translated and revised from the Chinese original, with a foreword by Feng Duan. https://doi.org/10.1007/978-3-642-01777-3.

[3] J.M. Sanz-Serna, Runge-Kutta schemes for Hamiltonian systems, BIT 28 (4) (1988) 877–883, https://doi.org/10.1007/BF01954907. URL https://doi.org/10.1007/BF01954907.

[4] K. Feng, Difference schemes for Hamiltonian formalism and symplectic geometry, J. Comput. Math. 4 (3) (1986) 279–289.

[5] J.E. Marsden, M. West, Discrete mechanics and variational integrators, Acta Numer. 10 (2001) 357–514, https://doi.org/10.1017/S096249290100006X. URL https://doi.org/10.1017/S096249290100006X.

[6] M. Calvo, M.P. Laburta, J.I. Montijano, L. Rández, Runge-Kutta projection methods with low dispersion and dissipation errors, Adv. Comput. Math. 41 (1) (2015) 231–251, https://doi.org/10.1007/s10444-014-9355-2. URL https://doi.org/10.1007/s10444-014-9355-2.

[7] O. Gonzalez, Time integration and discrete Hamiltonian systems, J. Nonlinear Sci. 6 (5) (1996) 449–467, https://doi.org/10.1007/s003329900018. URL https://doi.org/10.1007/s003329900018.

[8] L. Brugnano, F. Iavernaro, D. Trigiante, Hamiltonian boundary value methods (energy preserving discrete line integral methods), JNAIAM. J. Numer. Anal. Ind. Appl. Math. 5 (1–2) (2010) 17–37.

[9] L. Brugnano, F. Iavernaro, Line Integral Methods for Conservative Problems, Monographs and Research Notes in Mathematics, CRC Press, Boca Raton, FL, 2016.

[10] Z. Ge, J.E. Marsden, Lie-Poisson Hamilton-Jacobi theory and Lie-Poisson integrators, Phys. Lett. A 133 (3) (1988) 134–139, https://doi.org/10.1016/0375-9601(88)90773-6.

[11] C. Kane, J.E. Marsden, M. Ortiz, Symplectic-energy-momentum preserving variational integrators, J. Math. Phys. 40 (7) (1999) 3353–3371, https://doi.org/10.1063/1.532892.

[12] J.C. Simo, N. Tarnow, K.K. Wong, Exact energy-momentum conserving algorithms and symplectic schemes for nonlinear dynamics, Comput. Methods Appl. Mech. Engrg. 100 (1) (1992) 63–116, https://doi.org/10.1016/0045-7825(92)90115-Z.

[13] L. Brugnano, F. Iavernaro, D. Trigiante, Energy- and quadratic invariants–preserving integrators based upon Gauss collocation formulae, SIAM J. Numer. Anal. 50 (6) (2012) 2897–2916, https://doi.org/10.1137/110856617.

[14] D. Wang, A. Xiao, X. Li, Parametric symplectic partitioned Runge-Kutta methods with energy-preserving properties for Hamiltonian systems, Comput. Phys. Commun. 184 (2) (2013) 303–310, https://doi.org/10.1016/j.cpc.2012.09.012.

[15] L. Brugnano, G. Gurioli, F. Iavernaro, Analysis of energy and quadratic invariant preserving (EQUIP) methods, J. Comput. Appl. Math. 335 (2018) 51–73, https://doi.org/10.1016/j.cam.2017.11.043.

[16] Y. Gong, J. Cai, Y. Wang, Some new structure-preserving algorithms for general multi-symplectic formulations of Hamiltonian PDEs, J. Comput. Phys. 279 (2014) 80–102, https://doi.org/10.1016/j.jcp.2014.09.001.

[17] J. Hong, H. Liu, G. Sun, The multi-symplecticity of partitioned Runge-Kutta methods for Hamiltonian PDEs, Math. Comp. 75 (253) (2006) 167–181, https://doi.org/10.1090/S0025-5718-05-01793-X.

[18] J. Hong, Y. Sun, Generating functions of multi-symplectic RK methods via DW Hamilton-Jacobi equations, Numer. Math. 110 (4) (2008) 491–519, https://doi.org/10.1007/s00211-008-0170-x.

[19] S. Reich, Multi-symplectic Runge-Kutta collocation methods for Hamiltonian wave equations, J. Comput. Phys. 157 (2) (2000) 473–499, https://doi.org/10.1006/jcph.1999.6372.

[20] Y. Wang, J. Hong, Multi-symplectic algorithms for Hamiltonian partial differential equations, Commun. Appl. Math. Comput. 27 (2) (2013) 163–230.

[21] J. Hong, C. Li, Multi-symplectic Runge-Kutta methods for nonlinear Dirac equations, J. Comput. Phys. 211 (2) (2006) 448–472, https://doi.org/10.1016/j.jcp.2005.06.001.

[22] J. Hong, X. Liu, C. Li, Multi-symplectic Runge-Kutta-Nyström methods for nonlinear Schrödinger equations with variable coefficients, J. Comput. Phys. 226 (2) (2007) 1968–1984, https://doi.org/10.1016/j.jcp.2007.06.023. URL https://doi.org/10.1016/j.jcp.2007.06.023.

[23] J. Hong, S. Jiang, C. Li, Explicit multi-symplectic methods for Klein-Gordon-Schrödinger equations, J. Comput. Phys. 228 (9) (2009) 3517–3532, https://doi.org/10.1016/j.jcp.2009.02.006. URL https://doi.org/10.1016/j.jcp.2009.02.006.

[24] J. Hong, S. Jiang, C. Li, Accuracy of classical conservation laws for Hamiltonian PDEs under Runge-Kutta discretizations, Numer. Math. 112 (1) (2009) 1–23, https://doi.org/10.1007/s00211-008-0204-4.

[25] J. Hong, S. Jiang, C. Li, H. Liu, Explicit multi-symplectic methods for Hamiltonian wave equations, Commun. Comput. Phys. 2 (4) (2007) 662–683.

[26] H. Liu, K. Zhang, Multi-symplectic Runge-Kutta-type methods for Hamiltonian wave equations, IMA J. Numer. Anal. 26 (2) (2006) 252–271, https://doi.org/10.1093/imanum/dri042.

[27] D. Cohen, E. Hairer, C. Lubich, Conservation of energy, momentum and actions in numerical discretizations of non-linear wave equations, Numer. Math. 110 (2) (2008) 113–143, https://doi.org/10.1007/s00211-008-0163-9.

[28] L. Brugnano, F. Iavernaro, D. Trigiante, Energy and quadratic invariants preserving integrators of Gaussian type, AIP Conf. Proc. 1281 (1) (2010) 227–230, https://doi.org/10.1063/1.3498430.

[29] E. Hairer, G. Wanner, Solving ordinary differential equations. II, in: Stiff and Differential-Algebraic Problems, second revised edition, paperback, in: Springer Series in Computational Mathematics, vol. 14, Springer-Verlag, Berlin, 2010.

[30] J. Hong, C. Sim, X. Yin, Solvability of concatenated Runge-Kutta equations for second-order nonlinear PDEs, J. Comput. Appl. Math. 245 (2013) 232–241, https://doi.org/10.1016/j.cam.2012.12.014.