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# Explicit Multi-Symplectic Methods for Hamiltonian Wave Equations

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**Abstract.** In this paper, based on the multi-symplecticity of concatenating symplectic Runge-Kutta-Nyström (SRKN) methods and symplectic Runge-Kutta-type methods for numerically solving Hamiltonian PDEs, explicit multi-symplectic schemes are constructed and investigated, where the nonlinear wave equation is taken as a model problem. Numerical comparisons are made to illustrate the effectiveness of our newly derived explicit multi-symplectic integrators.

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**Key words**: Hamiltonian wave equations, multi-symplectic integration, symplectic Runge-Kutta methods, symplectic Runge-Kutta-Nyström methods.

## 1 Introduction

Consider the following Hamiltonian partial differential equation (PDE),

$$K\partial_t z + L\partial_x z = \nabla_z S(z), \tag{1.1}$$

where $z \in \mathbb{R}^n$, $S: \mathbb{R}^n \mapsto \mathbb{R}$ is some smooth function and $K, L$ are two skew-symmetric constant $n \times n$ matrices. It is well-known that system (1.1) is multi-symplectic, i.e., its phase flow gives rise to the multi-symplectic conservation law

$$\partial_t \omega + \partial_x \kappa = 0, \tag{1.2}$$

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with

$$\omega = dz \wedge K dz, \qquad \kappa = dz \wedge L dz.$$

The local invariant (1.2) implies that symplecticity can vary over the spatial domain from time to time. But this variation is not arbitrary as the changes in time are exactly compensated by changes in space (see [9, 12], and references therein). Some very important PDEs can be rewritten in this form, particularly, including various wave equations (see, e.g., [2, 8, 9, 14] and references therein).

More recently, there has been growing interest in multi-symplectic integration for Hamiltonian PDEs (1.1), i.e., numerical integrators whose numerical flow gives rise to certain preservation of the local invariant (1.2). Now, for our study, we introduce a uniform grid $\{x_k, t_l\} \in \mathbb{R}^2$ with mesh length $h$ in the $x$-direction and mesh length $\tau$ in the $t$-direction, which will be used throughout the paper. According to the definition in [2], a numerical discretization for (1.1), i.e.,

$$K\partial_t^{k,l} z_k^l + L\partial_x^{k,l} z_k^l = (\nabla_z S(z_k^l))_k^l, \qquad z_k^l \approx z(x_k, t_l), \tag{1.3}$$

where $\partial_t^{k,l}$ and $\partial_x^{k,l}$ are discretizations of the derivatives $\partial_t$ and $\partial_x$, respectively, is called multi-symplectic, if it satisfies a discrete version of the multi-symplectic conservation law:

$$\partial_t^{k,l} \omega_k^l + \partial_x^{k,l} \kappa_k^l = 0, \tag{1.4}$$

where

$$\omega_k^l = dz_k^l \wedge K dz_k^l, \qquad \kappa_k^l = dz_k^l \wedge L dz_k^l,$$

and $dz_k^l$ satisfies the discrete variational equation

$$K\partial_t^{k,l} dz_k^l + L\partial_x^{k,l} dz_k^l = S''(z_k^l) dz_k^l. \tag{1.5}$$

Some progress has been made on multi-symplectic integration for various Hamiltonian PDEs (see, e.g., [1,5,6,9,11,14] and references therein). In particular, as one of the most important classes of multi-symplecitic integrators, the concatenation of symplectic Runge-Kutta (SRK) methods and symplectic partitioned Runge-Kutta (SPRK) methods is intensively studied in [5, 6, 11, 14]. However, since both SRK methods and SPRK methods are implicit (this means that in the numerical implementation some iteration methods must be utilized for the nonlinear case) with only a very few exceptional cases of lower order methods [15], multi-symplectic integrators constructed in this way are usually fully implicit (see, e.g., [11]). Clearly, this brings numerous difficulties for practical implementations due to the massive computational costs and for this reason, we are led to the challenging problem of systematically constructing efficient explicit multi-symplectic integrators.

As mentioned before, both SRK and SPRK are implicit, and concatenations of implicit methods inevitably produce implicit methods for numerically solving PDEs. Therefore, for our investigation, we naturally resort to another notable class of numerical methods, namely, Runge-Kutta Nyström (RKN) method (see [4, 7, 10, 15]), since which has been shown to be able to derive explicit symplectic integration algorithms for a wide class of Hamiltonian ODEs (see [13]). It has been known in [4] that if we use a SRKN method for one directional discretization [17] and a SRKN/SRK/SPRK method for the other, then we will obtain a multi-symplectic integrator. But unfortunately, it then turns out that even if we use explicit SRKN methods for both directional discretizations, the resulting multi-symplectic schemes are not necessarily explicit. Nonetheless, taking advantage of the fact that more types of methods are allowed for concatenation, and the explicitness of SRKN methods, we eventually achieve a class of explicit multi-symplectic schemes for the nonlinear scalar wave equation. In detail, the new methods are derived by means of concatenating symplectic Euler method and explicit SRKN methods of arbitrary order larger than 2. The results obtained are readily extended to some Hamiltonian PDEs other than nonlinear scalar wave equation.

As an example, we study in detail a two-parameter family of explicit multi-symplectic SRKN-SRK methods. It is first shown that the explicit schemes are conditionally stable, which is known to be crucial when numerically solving wave equations with explicit schemes. Then, we perform some numerical experiments with four different explicit schemes to test the effectiveness of our newly derived multi-symplectic integrators. Through comparisons, it is illustrated that the superiority of our novel integrators lies not only in the capability of long-time scale computation, but also in the good preservation of local/global energy.

The plan of the paper is as follows. In the next section, we present some preliminary knowledge on explicit SRKN methods and explicit SRKN methods of orders one through four are collected for the subsequent use. Section 3 provides the general framework based on which our multi-symplectic integration algorithms are constructed. In section 4, a two-parameter family of explicit multi-symplectic integrators is constructed and investigated. Section 5 is devoted to the numerical experiments.

## 2 Symplectic Runge-Kutta Nyström methods

Consider the Hamiltonian system

$$\dot{\mathbf{q}}=\mathbf{T}^{-1}\mathbf{p}, \qquad \dot{\mathbf{p}}=-\nabla_{\mathbf{q}}U(\mathbf{q}), \qquad \mathbf{p}\times\mathbf{q}\in\mathbb{R}^n\times\mathbb{R}^n, \tag{2.1}$$

where $\mathbf{T}\in\mathbb{R}^{n\times n}$ is a symmetric positive definite matrix. This system is equivalent to a second-order differential equation

$$\ddot{\mathbf{q}}=f(\mathbf{q}), \qquad f(\mathbf{q})=-\mathbf{T}^{-1}\nabla_{\mathbf{q}}U(\mathbf{q}). \tag{2.2}$$

An $r$-stage Runge-Kutta-Nyström method for (2.2) is read as

$$\begin{aligned} Q_i &= \mathbf{q}_k + c_i h \dot{\mathbf{q}}_k + h^2 \sum_{j=1}^{r} a_{ij} f(Q_j), \\ \mathbf{q}_{k+1} &= \mathbf{q}_k + h\dot{\mathbf{q}}_k + h^2 \sum_{i=1}^{r} \beta_i f(Q_i), \\ \dot{\mathbf{q}}_{k+1} &= \dot{\mathbf{q}}_k + h \sum_{i=1}^{r} b_i f(Q_i), \end{aligned} \tag{2.3}$$

where $\mathbf{q}_k$ and $\dot{\mathbf{q}}_k$ are the approximations to $\mathbf{q}(kh)$ and $\dot{\mathbf{q}}(kh)$, respectively, and $Q_i$ $(i=1,\cdots,r)$ are the internal stage values. In the sequel, we denote an $r$-stage RKN method (2.3) by the tetrad $\mathcal{N}_r = (A,b,c,\beta)$ with $A=(a_{ij})_{i,j=1}^r$, $b=(b_i)_{i=1}^r$, $c=(c_i)_{i=1}^r$ and $\beta=(\beta_i)_{i=1}^r$. $\mathcal{N}_r$ is said to be symplectic if $d\mathbf{q}_{k+1}\wedge d\dot{\mathbf{q}}_{k+1} = d\mathbf{q}_k \wedge d\dot{\mathbf{q}}_k$, which leads to

**Proposition 2.1.** (Suris [18]) If the coefficients of $\mathcal{N}_r$ satisfies the conditions

$$\beta_i = b_i(1-c_i), \quad i=1,\cdots,r, \tag{2.4}$$
$$b_i\beta_j - b_i a_{ij} = b_j \beta_i - b_j a_{ji}, \quad i,j=1,\cdots,r, \tag{2.5}$$

then it is symplectic.

It is observed from (2.3) that, if

$$a_{ij}=0, \quad \text{for } j\geq i,$$

then $\mathcal{N}_r$ is explicit and the symplectic conditions (2.4)-(2.5) reduce to

$$\begin{aligned} &\beta_i = b_i(1-c_i), \quad i=1,\cdots,r, \\ &b_i a_{ij} = b_i b_j (c_i - c_j), \quad j<i, \quad i=1,\cdots,r. \end{aligned} \tag{2.6}$$

If we require $b_i \neq 0$ $(i=1,\cdots,r)$, then the second condition in (2.6) can be further simplified to

$$a_{ij} = b_j(c_i - c_j), \quad j<i, \quad i=1,\cdots,r,$$

and the SRKN method $\mathcal{N}_r$ in this case can be formulated by the following Butcher's tableau:

$$\begin{array}{c|ccccc} c_1 & 0 & 0 & \cdots & 0 & 0 \\ c_2 & b_1(c_2-c_1) & 0 & \cdots & 0 & 0 \\ c_3 & b_1(c_3-c_1) & b_2(c_3-c_2) & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ c_r & b_1(c_r-c_1) & b_2(c_r-c_2) & \cdots & b_{r-1}(c_r-c_{r-1}) & 0 \\ \hline & b_1(1-c_1) & b_2(1-c_2) & \cdots & b_{r-1}(1-c_{r-1}) & b_r(1-c_r) \\ & b_1 & b_2 & \cdots & b_{r-1} & b_r \end{array}$$

From the above tableau, it can be seen that $b_i$ and $c_i$, $i=1,\cdots,r$, are the only free parameters for an explicit SRKN method. Furthermore, one can also see that if $c_i=c_{i-1}$ $(i=2,\cdots,r)$ or $b_i=0$ $(i=1,\cdots,r)$, then the $i$th stage is redundant, i.e., the method is reducible. Therefore, for the explicit SRKN methods given below, we would require that $c_i \neq c_{i-1}$ $(i=2,\cdots,r)$ and $b_i \neq 0$ $(i=1,\cdots,r)$.

In the following, we listed some explicit SRKN methods of order one through four for the subsequent use (see [13]).

1. 1-stage explicit SRKN methods:

$$\begin{array}{c|c} c_1 & 0 \\ \hline & 1-c_1 \\ & 1 \end{array}$$

where $c_1$ is a free parameter to be chosen arbitrarily. If $c_1 \neq 1/2$, then the method is of order 1. If $c_1=1/2$, then the method becomes a 1-stage explicit SRKN method of order 2, which is equivalent to the well-known Störmer-Verlet method (see, e.g., [15]).

2. 2-stage explicit SRKN methods of order 2:

$$\begin{array}{c|cc} \frac{1}{2}+\alpha & 0 & 0 \\ \frac{1}{2}+\beta & \beta & 0 \\ \hline & \frac{\beta}{\beta-\alpha}(\frac{1}{2}-\alpha) & \frac{-\alpha}{\beta-\alpha}(\frac{1}{2}-\beta) \\ & \frac{\beta}{\beta-\alpha} & \frac{-\alpha}{\beta-\alpha} \end{array}$$

where $\alpha$ and $\beta(\alpha\neq\beta)$ are two free parameters. For subsequent reference, we call this method $\mathrm{SRKN}_2(\alpha,\beta)$. It can be shown that $\mathrm{SRKN}_2(-1/2,1/2)$ is also equivalent to the Störmer-Verlet method. We remark that there are no real $\alpha$ and $\beta$ such that $\mathrm{SRKN}_2(\alpha,\beta)$ is of order 3.

3. 3-stage explicit SRKN methods:

$$\begin{array}{c|ccc} \frac{1}{2}+\alpha & 0 & 0 & 0 \\ \frac{1}{2}+\beta & \frac{\frac{1}{12}+\beta\gamma}{\gamma-\alpha} & 0 & 0 \\ \frac{1}{2}+\gamma & \frac{\frac{1}{12}+\beta\gamma}{\beta-\alpha} & -\frac{\frac{1}{12}+\alpha\gamma}{\beta-\alpha} & 0 \\ \hline & \frac{(\frac{1}{12}+\beta\gamma)(\frac{1}{2}-\alpha)}{(\beta-\alpha)(\gamma-\alpha)} & -\frac{(\frac{1}{12}+\alpha\gamma)(\frac{1}{2}-\beta)}{(\beta-\alpha)(\gamma-\beta)} & \frac{(\frac{1}{12}+\alpha\beta)(\frac{1}{2}-\gamma)}{(\gamma-\alpha)(\gamma-\beta)} \\ & \frac{\frac{1}{12}+\beta\gamma}{(\beta-\alpha)(\gamma-\alpha)} & -\frac{\frac{1}{12}+\alpha\gamma}{(\beta-\alpha)(\gamma-\beta)} & \frac{\frac{1}{12}+\alpha\beta}{(\gamma-\alpha)(\gamma-\beta)} \end{array}$$

where $\alpha,\beta,\gamma$ are three parameters to be chosen different from each other. It can be verified that the method is of order 3. In the sequel, we refer to this method as $\mathrm{SRKN}_3(\alpha,\beta,\gamma)$. Furthermore, one can check that $\mathrm{SRKN}_3(-\mu,0,\mu)$ is of order 4 (see [3] and [13]) if $\mu$ is chosen to be the real zero of $p(x)=48x^3-24x^2+1$, i.e.

$$\mu=\frac{1}{12}(2-\sqrt[3]{4}-\sqrt[3]{16})\approx -0.1756035959798288. \tag{2.7}$$

# 3 Multi-symplectic integration for Hamiltonian wave equations

In this section, we discuss the multi-symplectic integration for Hamiltonian PDEs (1.1) through concatenation of SRKN methods and SRK/SPRK methods. Throughout, we take the nonlinear scalar wave equation as a model problem, which is given by

$$\partial_{tt}u = \partial_{xx}u - G'(u), \quad (x,t) \in \Omega \subset \mathbb{R}^2, \tag{3.1}$$

where $G$ is some smooth function in $u$. Introduce $v = \partial_t u$ and $w = \partial_x u$, then a first order PDE system of the abstract form (1.1) equivalent to (3.1) is given by taking $z = (u,v,w)^T$ (see, e.g., [14]),

$$K = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad L = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix},$$

and the Hamiltonian

$$S(z) = \frac{1}{2}(v^2 - w^2) + G(u).$$

By (1.2), through straightforward calculation, the corresponding multi-symplectic conservation law for (3.1) is

$$\partial_t[du \wedge dv] - \partial_x[du \wedge dw] = 0. \tag{3.2}$$

Now, we are ready to derive the multi-symplectic integrator for (3.1). Henceforth, we customarily refer to an $s$-stage RK method by the triple $\mathcal{R}_s = (\widehat{A}, \widehat{b}, \widehat{c})$, where $\widehat{A} = (\widehat{a}_{\widehat{i}\widehat{j}})_{\widehat{i},\widehat{j}=1}^s$, $\widehat{b} = (\widehat{b}_{\widehat{i}})_{\widehat{i}=1}^s$ and $\widehat{c} = (\widehat{c}_{\widehat{i}})_{\widehat{i}=1}^s$ are, respectively, the coefficient matrix, weights and abscissae. As is well-known, $\mathcal{R}_s$ is symplectic if it satisfies (see [15])

$$\widehat{B}\widehat{A} + \widehat{A}^T\widehat{B} - \widehat{b}\widehat{b}^T = 0, \quad \widehat{B} = diag[\widehat{b}]. \tag{3.3}$$

We firstly apply an $r$-stage RKN method $\mathcal{N}_r$ for the temporal discretization and an $s$-stage RK method $\mathcal{R}_s$ for the spatial discretization, and get the following fully-discrete scheme for (3.1),

$$U_{k,\widehat{i}}^{l,i} = u_{k,\widehat{i}}^l + c_i \tau v_{k,\widehat{i}}^l + \tau^2 \sum_{j=1}^r a_{ij} \partial_{tt} U_{k,\widehat{i}}^{l,j}, \quad 1 \le i \le r, \ 1 \le \widehat{i} \le s, \tag{3.4}$$

$$u_{k,\widehat{i}}^{l+1} = u_{k,\widehat{i}}^l + \tau v_{k,\widehat{i}}^l + \tau^2 \sum_{i=1}^r \beta_i \partial_{tt} U_{k,\widehat{i}}^{l,i}, \quad 1 \le \widehat{i} \le s, \tag{3.5}$$

$$v_{k,\widehat{i}}^{l+1} = v_{k,\widehat{i}}^l + \tau \sum_{i=1}^r b_i \partial_{tt} U_{k,\widehat{i}}^{l,i}, \quad 1 \le \widehat{i} \le s, \tag{3.6}$$

$$U_{k,\widehat{i}}^{l,i} = u_k^{l,i} + h \sum_{\widehat{j}=1}^s \widehat{a}_{\widehat{i}\widehat{j}} W_{k,\widehat{j}}^{l,i}, \quad 1 \le i \le r, \ 1 \le \widehat{i} \le s, \tag{3.7}$$

$$u_{k+1}^{l,i} = u_k^{l,i} + h\sum_{\widehat{i}=1}^{s} \widehat{b}_{\widehat{i}} W_{k,\widehat{i}}^{l,i}, \qquad 1 \le i \le r, \tag{3.8}$$

$$W_{k,\widehat{i}}^{l,i} = w_k^{l,i} + h\sum_{\widehat{j}=1}^{s} \widehat{a}_{\widehat{i}\widehat{j}} \partial_{xx} U_{k,\widehat{j}}^{l,i}, \quad 1 \le i \le r, \ 1 \le \widehat{i} \le s, \tag{3.9}$$

$$w_{k+1}^{l,i} = w_k^{l,i} + h\sum_{\widehat{i}=1}^{s} \widehat{b}_{\widehat{i}} \partial_{xx} U_{k,\widehat{i}}^{l,i}, \quad 1 \le i \le r, \tag{3.10}$$

$$\partial_{tt} U_{k,\widehat{i}}^{l,i} = \partial_{xx} U_{k,\widehat{i}}^{l,i} - G'(U_{k,\widehat{i}}^{l,i}), \quad 1 \le i \le r, \ 1 \le \widehat{i} \le s, \tag{3.11}$$

where we have used the following notations:

$$U_{k,\widehat{i}}^{l,i} \approx u(x_k + \widehat{c}_{\widehat{i}} h, t_l + c_i \tau), \quad u_k^{l,i} \approx u(x_k, t_l + c_i \tau), \quad u_{k,\widehat{i}}^{l} \approx u(x_k + \widehat{c}_{\widehat{i}} h, t_l), \text{ etc.}$$

By a standard proof (see [4] and [16]) we have the following conditions which characterize the multi-symplecticity of above the RKN-RK method (3.4)-(3.11).

**Proposition 3.1.** If the method (3.4)-(3.11) satisfies the following coefficients conditions

$$\widehat{b}_{\widehat{i}} \widehat{b}_{\widehat{j}} = \widehat{b}_{\widehat{i}} \widehat{a}_{\widehat{i}\widehat{j}} + \widehat{b}_{\widehat{j}} \widehat{a}_{\widehat{j}\widehat{i}}, \tag{3.12}$$

$$\beta_i = b_i(1 - c_i), \tag{3.13}$$

$$b_i(\beta_j - a_{ij}) = b_j(\beta_i - a_{ji}), \tag{3.14}$$

for all $\widehat{i}$, $\widehat{j} = 1, \cdots, s$, and $i$, $j = 1, \cdots, r$, then it is multi-symplectic and gives rise to the following discrete multi-symplectic conservation law:

$$\tau \sum_{i=1}^{r} b_i \left[ du_{k+1}^{l,i} \wedge dw_{k+1}^{l,i} - du_k^{l,i} \wedge dw_k^{l,i} \right] - h \sum_{\widehat{i}=1}^{s} \widehat{b}_i \left[ du_{k,\widehat{i}}^{l+1} \wedge dv_{k,\widehat{i}}^{l+1} - du_{k,\widehat{i}}^{l} \wedge dv_{k,\widehat{i}}^{l} \right] = 0. \tag{3.15}$$

**Remark 3.1.** Proposition 3.1 shows that concatenation of the SRKN method and SRK method, applied respectively to the temporal and spatial discretizations, yields a multi-symplectic integrator for the wave equation (3.1). For the discretization, we can alternatively apply an SRK method in time and an SRKN method in space, and the obtained scheme can also be shown to be multi-symplectic in a similar way as above.

**Remark 3.2.** For the above concatenation, instead of the RK method $\mathcal{R}_s$, one can also use an $s$-stage PRK method $\mathcal{R}_s^{(1)} - \mathcal{R}_s^{(2)}$, whose coefficients are assumed to satisfy

$$\widehat{b}^{(1)} = \widehat{b}^{(2)} := \widehat{b}. \tag{3.16}$$

The resulting scheme is the same as (3.4)-(3.11), but with equations (3.7)-(3.10) replaced by

$$\begin{aligned}
&U^{l,i}_{k,\widehat{i}} = u^{l,i}_k + h\sum_{\widehat{j}=1}^{s} \widehat{a}^{(1)}_{\widehat{i}\widehat{j}} W^{l,i}_{k,\widehat{j}}, && 1\le i\le r,\ 1\le \widehat{i}\le s,\\
&u^{l,i}_{k+1} = u^{l,i}_k + h\sum_{\widehat{i}=1}^{s} \widehat{b}^{(1)}_{\widehat{i}} W^{l,i}_{k,\widehat{i}}, && 1\le i\le r,\\
&W^{l,i}_{k,\widehat{i}} = w^{l,i}_k + h\sum_{\widehat{j}=1}^{s} \widehat{a}^{(2)}_{\widehat{i}\widehat{j}} \partial_{xx} U^{l,i}_{k,\widehat{j}}, && 1\le i\le r,\ 1\le \widehat{i}\le s,\\
&w^{l,i}_{k+1} = w^{l,i}_k + h\sum_{\widehat{i}=1}^{s} \widehat{b}^{(2)}_{\widehat{i}} \partial_{xx} U^{l,i}_{k,\widehat{i}}, && 1\le i\le r.
\end{aligned}$$

It can be proved similarly that if the RKN-PRK method satisfies the coefficients conditions

$$\begin{aligned}
&\widehat{b}^{(1)}_{\widehat{i}}\widehat{b}^{(2)}_{\widehat{j}} = \widehat{b}^{(1)}_{\widehat{i}}\widehat{a}^{(2)}_{\widehat{i}\widehat{j}} + \widehat{b}^{(2)}_{\widehat{j}}\widehat{a}^{(1)}_{\widehat{j}\widehat{i}},\\
&\beta_i = b_i(1-c_i),\\
&b_i(\beta_j - a_{ij}) = b_j(\beta_i - a_{ji}),
\end{aligned}$$

for all $\widehat{i}, \widehat{j} = 1,\cdots,s$, and $i, j = 1,\cdots,r$, together with the assumption (3.16), then it is multi-symplectic and preserves the discrete multi-symplectic conservation law (3.15). That is, concatenation of the SPRK method and SRKN method also produces a multi-symplectic integrator. Here, for our discussion in the sequel, we remark that if we utilize the symplectic Euler method (which is a first-order SPRK method) for the spatial discretization, and eliminate the introduced variable $W^{l,i}_{k,\widehat{i}}$, we till get the second-order central difference for $u_{xx}$.

**Remark 3.3.** We emphasize that concatenation of SRK/SPRK methods with SRKN methods can also be used to derive multi-symplectic integrators for other kinds of Hamiltonian PDEs.

Next, we apply RKN methods for both directional discretizations of equation (3.1), i.e., a RKN method $\mathcal{N}_r = (A,b,c,\beta)$ in $t$-direction and a RKN method $\bar{\mathcal{N}}_s = (\bar{A},\bar{b},\bar{c},\bar{\beta})$ in $x$-direction, and get the following scheme:

$$U^{l,i}_{k,\bar{i}} = u^l_{k,\bar{i}} + c_i\tau v^l_{k,\bar{i}} + \tau^2\sum_{j=1}^{r} a_{ij}\partial_{tt}U^{l,j}_{k,\bar{i}}, \quad 1\le i\le r,\ 1\le \bar{i}\le s, \tag{3.17}$$

$$u^{l+1}_{k,\bar{i}} = u^l_{k,\bar{i}} + \tau v^l_{k,\bar{i}} + \tau^2\sum_{i=1}^{r} \beta_i\partial_{tt}U^{l,i}_{k,\bar{i}}, \quad 1\le \bar{i}\le s, \tag{3.18}$$

$$v^{l+1}_{k,\bar{i}} = v^l_{k,\bar{i}} + \tau\sum_{i=1}^{r} b_i\partial_{tt}U^{l,i}_{k,\bar{i}}, \quad 1\le \bar{i}\le s, \tag{3.19}$$

$$U^{l,i}_{k,\bar{i}} = u^{l,i}_k + \bar{c}_{\bar{i}} h w^{l,i}_k + h^2 \sum_{\bar{j}=1}^{s} \bar{a}_{\bar{i}\bar{j}} \partial_{xx} U^{l,i}_{k,\bar{j}}, \quad 1 \le i \le r,\ 1 \le \bar{i} \le s, \tag{3.20}$$

$$u^{l,i}_{k+1} = u^{l,i}_k + h w^{l,i}_k + h^2 \sum_{\bar{i}=1}^{s} \bar{\beta}_{\bar{i}} \partial_{xx} U^{l,i}_{k,\bar{i}}, \quad 1 \le i \le r, \tag{3.21}$$

$$w^{l,i}_{k+1} = w^{l,i}_k + h \sum_{\bar{i}=1}^{s} \bar{b}_{\bar{i}} \partial_{xx} U^{l,i}_{k,\bar{i}}, \quad 1 \le i \le r, \tag{3.22}$$

$$\partial_{tt} U^{l,i}_{k,\bar{i}} = \partial_{xx} U^{l,i}_{k,\bar{i}} - G'(U^{l,i}_{k,\bar{i}}), \quad 1 \le i \le r,\ 1 \le \bar{i} \le s. \tag{3.23}$$

The multi-symplecticity of the above RKN-RKN method is stated as follows.

**Proposition 3.2.** ([16]) If the method (3.17)-(3.22) satisfies the coefficient conditions

$$\beta_i = b_i(1-c_i), \tag{3.24}$$

$$b_i\beta_j - b_i a_{ij} = b_j \beta_i - b_j a_{ji}, \tag{3.25}$$

$$\bar{\beta}_{\bar{i}} = \bar{b}_{\bar{i}}(1-\bar{c}_{\bar{i}}), \tag{3.26}$$

$$\bar{b}_{\bar{i}}(\bar{\beta}_{\bar{j}} - \bar{a}_{\bar{i}\bar{j}}) = \bar{b}_{\bar{j}}(\bar{\beta}_{\bar{i}} - \bar{a}_{\bar{j}\bar{i}}), \tag{3.27}$$

for all $i, j=1,\cdots,r$, and $\bar{i}, \bar{j}=1,\cdots,s$, then it is multi-symplectic and gives rise to the discrete multi-symplectic conservation law

$$\tau \sum_{i=1}^{r} b_i \left[ du^{l,i}_{k+1} \wedge dw^{l,i}_{k+1} - du^{l,i}_k \wedge dw^{l,i}_k \right] - h \sum_{\bar{i}=1}^{s} \bar{b}_i \left[ du^{l+1}_{k,\bar{i}} \wedge dv^{l+1}_{k,\bar{i}} - du^{l}_{k,\bar{i}} \wedge dv^{l}_{k,\bar{i}} \right] = 0. \tag{3.28}$$

**Remark 3.4.** Proposition 3.2 shows that concatenation of SRKN-type methods can produce a multi-symplectic integrator for Hamiltonian wave equations. It is remarked that the above conclusion applies equally to other Hamiltonian PDEs. For example, consider the beam equation

$$u_{tt} + u_{xxxx} = V'(u), \tag{3.29}$$

where $V(u)$ is some smooth function in $u$, which is shown to be a multi-symplectic PDE of form (1.1) in [8]. Now, we apply an SRKN method $\mathcal{N}_r$ to the temporal discretization and an SRKN method $\mathcal{N}_s$ to the spatial discretization, and get the following multi-symplectic scheme:

$$U^{l,i}_{k,\bar{i}} = u^{l}_{k,\bar{i}} + c_i \tau \partial_t u^{l}_{k,\bar{i}} + \tau^2 \sum_{j=1}^{r} a_{ij} \partial_{tt} U^{l,j}_{k,\bar{i}}, \quad 1 \le i \le r,\ 1 \le \bar{i} \le s,$$

$$u^{l+1}_{k,\bar{i}} = u^{l}_{k,\bar{i}} + \tau \partial_t u^{l}_{k,\bar{i}} + \tau^2 \sum_{i=1}^{r} \beta_i \partial_{tt} U^{l,i}_{k,\bar{i}}, \quad 1 \le \bar{i} \le s,$$

$$
\begin{aligned}
&\partial_t u_{k,\bar{i}}^{l+1} = \partial_t u_{k,\bar{i}}^{l} + \tau \sum_{i=1}^{r} b_i \partial_{tt} U_{k,\bar{i}}^{l,i}, && 1 \le \bar{i} \le s,\\
&U_{k,\bar{i}}^{l,i} = u_k^{l,i} + \bar{c}_{\bar{i}} h \partial_x u_k^{l,i} + h^2 \sum_{\bar{j}=1}^{s} \bar{a}_{\bar{i}\bar{j}} W_{k,\bar{j}}^{l,i}, && 1 \le i \le r,\ 1 \le \bar{i} \le s,\\
&u_{k+1}^{l,i} = u_k^{l,i} + h \partial_x u_k^{l,i} + h^2 \sum_{\bar{i}=1}^{s} \bar{\beta}_{\bar{i}} W_{k,\bar{i}}^{l,i}, && 1 \le i \le r,\\
&\partial_x u_{k+1}^{l,i} = \partial_x u_k^{l,i} + h \sum_{\bar{i}=1}^{s} \bar{b}_{\bar{i}} W_{k,\bar{i}}^{l,i}, && 1 \le i \le r,\\
&W_{k,\bar{i}}^{l,i} = w_k^{l,i} + \bar{c}_{\bar{i}} h \partial_x w_k^{l,i} + h^2 \sum_{\bar{j}=1}^{s} \bar{a}_{\bar{i}\bar{j}} \partial_{xx} W_{k,\bar{j}}^{l,i}, && 1 \le i \le r,\ 1 \le \bar{i} \le s,\\
&w_{k+1}^{l,i} = w_k^{l,i} + h \partial_x w_k^{l,i} + h^2 \sum_{\bar{i}=1}^{s} \bar{\beta}_{\bar{i}} \partial_{xx} W_{k,\bar{i}}^{l,i}, && 1 \le i \le r,\\
&\partial_x w_{k+1}^{l,i} = \partial_x w_k^{l,i} + h \sum_{\bar{i}=1}^{s} \bar{b}_{\bar{i}} \partial_{xx} W_{k,\bar{i}}^{l,i}, && 1 \le i \le r,\\
&\partial_{tt} U_{k,\bar{i}}^{l,i} = -\partial_{xx} W_{k,\bar{i}}^{l,i} + V'(U_{k,\bar{i}}^{l,i}), && 1 \le i \le r,\ 1 \le \bar{i} \le s.
\end{aligned}
$$

# 4 A two-parameter family of explicit multi-symplectic integration algorithms

Clearly, based on the general framework provided in Section 3, a large number of novel multi-symplectic schemes can be constructed and more members are added to the known class of multi-symplectic integrators. Besides, as has been mentioned in Section 2, SRKN methods can be used to derive explicit symplectic schemes, one naturally expects that concatenation of explicit SRKN methods may produce explicit multi-symplectic schemes. But unfortunately, by straightforward calculations, it can be shown that this is not always the case; that is, even if we use explicit SRKN methods for both directional discretizations, the resulting multi-symplectic scheme is not necessarily explicit. Nevertheless, it is found that if in one direction, we apply the symplectic Euler method, which finally gives the second-order central difference (see Remark 3.2), and in the other direction, we apply an explicit SRKN method given in section 2, then the resulting scheme is explicit (here, "explicit" means that we don't utilize the fixed point iteration), which is also multi-symplectic according to Remark 3.2. As is widely recognized, it is not easy to construct explicit schemes for numerically solving PDEs, and the case will become more complicated when turn to the structure-preserving numerical integrators. Noting that the explicit SRKN methods utilized for the concatenation can reach order even higher than 4, those obtained schemes are of significant interests since they are high-order (at least in one direction) explicit and multi-symplectic methods. This is in sharp contrast to the multi-symplectic Runge-Kutta-type methods, where the methods are always fully implicit, especially in the high-order case (see [5,6,11,14]). Next, as an example, we present a two-parameter family explicit multi-symplectic scheme for wave equation (3.1). In space, we apply the symplectic Euler method and in time, we apply the method $\mathrm{SRKN}_2(\alpha,\beta)$. The resulting multi-symplectic scheme is formulated as follows:

$$
\begin{aligned}
&U_k^{l,1}=u_k^l+\left(\frac{1}{2}+\alpha\right)\tau v_k^l,\\
&(\partial_{xx}U)_k^{l,1}=\frac{U_{k+1}^{l,1}-2U_k^{l,1}+U_{k-1}^{l,1}}{h^2},\\
&U_k^{l,2}=u_k^l+\left(\frac{1}{2}+\beta\right)\tau v_k^l+\tau^2\beta[(\partial_{xx}U)_k^{l,1}-G'(U_k^{l,1})],\\
&(\partial_{xx}U)_k^{l,2}=\frac{U_{k+1}^{l,2}-2U_k^{l,2}+U_{k-1}^{l,2}}{h^2},\\
&u_k^{l+1}=u_k^l+\tau v_k^l+\tau^2\frac{\beta(1/2-\alpha)}{\beta-\alpha}\left[(\partial_{xx}U)_k^{l,1}-G'(U_k^{l,1})\right]-\tau^2\frac{\alpha(1/2-\beta)}{\beta-\alpha}\left[(\partial_{xx}U)_k^{l,2}-G'(U_k^{l,2})\right],\\
&v_k^{l+1}=v_k^l+\tau\frac{\beta}{\beta-\alpha}\left[(\partial_{xx}U)_k^{l,1}-G'(U_k^{l,1})\right]-\tau\frac{\alpha}{\beta-\alpha}\left[(\partial_{xx}U)_k^{l,2}-G'(U_k^{l,2})\right].
\end{aligned}
$$

In the sequel, we refer to the above scheme as $\mathrm{MSIA}_2(\alpha,\beta)$. It is easily seen that $\mathrm{MSIA}_2(\alpha,\beta)$ advances explicitly from $(u_k^l,v_k^l)$ to $(u_k^{l+1},\, v_k^{l+1})$. The method can be verified directly to be of order 2 in both space and time. For the concatenation, one can alternatively utilize method $\mathrm{SRKN}_3(\alpha,\beta,\gamma)$ for the temporal discretization and would achieve a three-parameter explicit multi-symplectic scheme $\mathrm{MSIA}_3(\alpha,\,\beta,\gamma)$, which is of order 3 in time (here if we choose $\alpha=-\mu$, $\beta=0$, $\gamma=\mu$ with $\mu$ given in (2.7), then it will be of order 4 in time). It is emphasized that all the above arguments apply equally to the case where the role of $x$ and $t$ is exchanged; i.e., we can use the symplectic Euler method for the temporal discretization while explicit SRKN methods for the spatial discretization. Now, it is clear that with different free parameters to be fixed, we can obtain a large number of novel numerical integrators, and most significantly, they are both explicit and multi-symplectic. In the rest of this section, we turn to another crucial issue for those constructed schemes above, namely, the stability. As is known, the attractiveness of explicit schemes obviously relies on the efficiency, but such efficiency is always at the cost of stability. Using the well-known Fourier method (see [7]), we now make some linear stability analyses for those explicit multi-symplectic schemes, and where we only take $\mathrm{MSIA}_2(\alpha,\beta)$ as an example. Results show that our newly derived integrators possess good stability properties which ensure their practicality.

Set $u_k^l=\hat{u}^l\exp\{\mathrm{i}\xi kh\}$, $v_k^l=\hat{v}^l\exp\{\mathrm{i}\xi kh\}$, $U_k^{l,1}=\hat{U}^{l,1}\exp\{\mathrm{i}\xi kh\}$, $U_k^{l,2}=\hat{U}^{l,2}\exp\{\mathrm{i}\xi kh\}$ etc., where $\xi\in\mathbb{R}$ and $\mathrm{i}=\sqrt{-1}$ and we also let $\theta=\tau/h$ be the ratio of step-sizes. Next, substituting the above expressions into scheme $\mathrm{MSIA}_2(\alpha,\beta)$ with nonlinear terms removed and after straightforward calculations, we get

$$\hat{U}^{l,1}=\hat{u}^l+\left(\frac{1}{2}+\alpha\right)\tau\hat{v}^l,$$
$$\hat{U}^{l,2}=\hat{u}^l+\left(\frac{1}{2}+\beta\right)\tau\hat{v}^l+\tau^2\beta\hat{U}^{l,1}[e^{\mathrm{i}\xi h}-2+e^{-\mathrm{i}\xi h}],$$
$$\hat{u}^{l+1}=\hat{u}^l+\tau\hat{v}^l+\tau^2\frac{\beta(1/2-\alpha)}{\beta-\alpha}\hat{U}^{l,1}[e^{\mathrm{i}\xi h}-2+e^{-\mathrm{i}\xi h}]-\tau^2\frac{\alpha(1/2-\beta)}{\beta-\alpha}\hat{U}^{l,2}[e^{\mathrm{i}\xi h}-2+e^{-\mathrm{i}\xi h}],$$
$$\hat{v}^{l+1}=v^l+\tau\frac{\beta}{\beta-\alpha}\hat{U}^{l,1}[e^{\mathrm{i}\xi h}-2+e^{-\mathrm{i}\xi h}]-\tau\frac{\alpha}{\beta-\alpha}\hat{U}^{l,2}[e^{\mathrm{i}\xi h}-2+e^{-\mathrm{i}\xi h}].$$

Then, by getting rid of $\hat{U}^{l,1}$ and $\hat{U}^{l,2}$, we further obtain

$$\begin{pmatrix}\hat{u}^{l+1}\\ \hat{v}^{l+1}\end{pmatrix}=G(\xi,\tau)\begin{pmatrix}\hat{u}^{l}\\ \hat{v}^{l}\end{pmatrix},$$

where $G(\xi,\tau)=(G_{ij})_{i,j=1}^2$ is the amplification matrix with

$$G_{11}=1-2\theta^2\sin^2\frac{\xi h}{2}+16\frac{\alpha\beta(\beta-1/2)}{\beta-\alpha}\theta^4\sin^4\frac{\xi h}{2},$$
$$G_{12}=\tau-\tau(1+4\alpha\beta)\theta^2\sin^2\frac{\xi h}{2}+16\tau\frac{\alpha\beta(1/2+\alpha)(\beta-1/2)}{\beta-\alpha}\theta^4\sin^4\frac{\xi h}{2},$$
$$G_{21}=-4\frac{\theta^2}{h}\sin^2\frac{\xi h}{2}-16\frac{\alpha\beta}{\beta-\alpha}\frac{\theta^4}{h}\sin^4\frac{\xi h}{2},$$
$$G_{22}=1-2\theta^2\sin^2\frac{\xi h}{2}-16\frac{\alpha\beta(1/2+\alpha)}{\beta-\alpha}\theta^4\sin^4\frac{\xi h}{2}.$$

The eigenvalues of $G(\xi,\tau)$ satisfy the equation

$$\lambda^2-(G_{11}+G_{22})\lambda+(G_{11}G_{22}-G_{21}G_{12})=0, \tag{4.1}$$

where it can be easily verified that $G_{11}G_{22}-G_{12}G_{21}=1$, and hence equation (4.1) becomes

$$\lambda^2-(G_{11}+G_{22})\lambda+1=0. \tag{4.2}$$

Obviously, the roots $\lambda_i$ $(i=1,2)$ of equation (4.2) satisfy $|\lambda_i|\le 1$ $(i=1,2)$ iff $|G_{11}+G_{22}|\le 2$ and the method satisfies the von Neumann condition, which is known to be a necessary condition of stability (see [7]). Then, one can solve the above inequality for specific $\alpha$ and $\beta$ to find the conditions satisfied by $\theta$, which gives the necessary condition of stability, and then from which one can further deduce the sufficient conditions of stability by refining. Next, we take the method MSIA$_2(-1/4,1/4)$ as an example and the subsequent arguments apply equally to other $\alpha$ and $\beta$. The amplification matrix then becomes

$$G(\sigma,\tau):=G(\xi,\tau)=\begin{pmatrix}1-2\theta^2\sin^2\frac{\sigma}{2}+\frac{1}{2}\theta^4\sin^4\frac{\sigma}{2} & \tau-\tau\frac{3}{4}\theta^2\sin^2\frac{\sigma}{2}+\tau\frac{1}{8}\theta^4\sin^4\frac{\sigma}{2}\\ -4\frac{1}{h}\theta^2\sin^2\frac{\sigma}{2}+2\frac{1}{h}\theta^4\sin^4\frac{\sigma}{2} & 1-2\theta^2\sin^2\frac{\sigma}{2}+\frac{1}{2}\theta^4\sin^4\frac{\sigma}{2}\end{pmatrix},$$

where we have set $\sigma=\xi h$. From $|G_{11}+G_{22}|\leq 2$, we get

$$\Big|2-4\theta^2\sin^2\frac{\sigma}{2}+\theta^4\sin^4\frac{\sigma}{2}\Big|\leq 2,$$

which is equivalent to

$$\Big|\theta\sin\frac{\sigma}{2}\Big|\leq 2. \tag{4.3}$$

Clearly, if we choose $0<\theta<2$, then the inequality (4.3) is satisfied. Now, we show that it also gives a sufficient condition for the stability of $\mathrm{MSIA}_2(-1/4,1/4)$. In fact, it can be seen that when $0<\theta<2$ and $\sigma\neq 2n\pi$ with $n$ being an arbitrary integer, $G(\sigma,\tau)$ has two different eigenvalues and when $\sigma=2n\pi$,

$$G(\sigma,\tau)=\begin{pmatrix} 1 & \tau \\ 0 & 1 \end{pmatrix}=I+\mathcal{O}(\tau),$$

and therefore we know that when $0<\theta<2$, the method $\mathrm{MSIA}_2(-1/4,1/4)$ is linearly stable. It is emphasized that we can argue similarly for $\mathrm{MSIA}_3(\alpha,\beta,\gamma)$, but we will not explore more details here.

## 5 Numerical experiments

In order to test the effectiveness of the newly derived explicit multi-symplectic integrators, we perform some numerical experiments. For the numerics, we are mainly concerned about the long-time behaviors and preservation of local/global energy, which are known to be the eminent properties of multi-symplectic integrators.

The local energy conservation law of the Hamiltonian PDE (1.1) is (see, e.g., [5,14])

$$\partial_t E(z)+\partial_x F(z)=0, \tag{5.1}$$

with

$$E(z)=S(z)-\frac{1}{2}z^T L\partial_x z, \qquad F(z)=\frac{1}{2}z^T L\partial_t z,$$

and for the wave equation (3.1) we have

$$E(z)=\frac{1}{2}(v^2+w^2)+G(u), \qquad F(z)=-vw.$$

Integrating (5.1) over the $(k,l)$-cell gives

$$\int_{x_k}^{x_{k+1}}\int_{t_l}^{t_{l+1}}\left(\frac{\partial E}{\partial t}+\frac{\partial F}{\partial x}\right)dtdx=0,$$

which further implies

$$\int_{x_k}^{x_{k+1}}[E(z(x,t_{l+1}))-E(z(x,t_l))]dx+\int_{t_l}^{t_{l+1}}[F(z(x_{k+1},t))-F(z(x_k,t))]dt=0. \tag{5.2}$$

For the multi-symplectic RKN-RK scheme (3.4)-(3.11), we define

$$(E_{le})_{k,l} = h\sum_{\widehat{i}=1}^{s}\widehat{b}_{\widehat{i}}\left(E_{k,\widehat{i}}^{l+1} - E_{k,\widehat{i}}^{l}\right) + \tau\sum_{i=1}^{r} b_i\left(F_{k+1}^{l,i} - F_{k}^{l,i}\right),$$

to be an approximation to the above integral (5.2), where we have made use of the obvious abbreviations

$$E_{k,\widehat{i}}^{l} = \frac{1}{2}\left({v_{k,\widehat{i}}^{l}}^{2} + {w_{k,\widehat{i}}^{l}}^{2}\right) + G\left(u_{k,\widehat{i}}^{l}\right), \qquad F_{k}^{l,i} = -v_{k}^{l,i} w_{k}^{l,i}.$$

We refer to [14] for a similar definition for multi-symplectic Gauss-Legendre RK methods. Clearly, we still need to introduce some compatible auxiliary systems to replenish the missing values of $w_{k,\widehat{i}}^{l}$ and $v_{k}^{l,i}$, and which can be conducted in a similar manner as having been done in [14]. Next, we define

$$(E_{le}^{*})_{k,l} = \frac{(E_{le})_{k,l}}{\tau h}$$

to denote the discretization error of the local energy conservation law (LECL) (5.1), and let

$$(Error_{le})_{l} = \max_{k} |(E_{le}^{*})_{k,l}| \tag{5.3}$$

to be the error of LECL depending only on the time-steps.

The spatial interval to be considered is $[-\mathrm{L}/2,\mathrm{L}/2]$ with $\mathrm{L}=120$, and we always assume the periodic boundary condition $u(-\mathrm{L}/2,t) = u(\mathrm{L}/2,t)$ to exclude the boundary effects. Then, it is easy to deduce from (5.2) that

$$\frac{d}{dt}\mathcal{E}(t) := \frac{d}{dt}\int_{-\mathrm{L}/2}^{\mathrm{L}/2} E(x,t)\,dx = 0.$$

We define $\mathcal{E}(t)$, being some constant, as the global energy and let

$$\mathcal{E}_{\mathrm{L}}^{l} = h\sum_{k}\sum_{\widehat{i}=1}^{s}\widehat{b}_{\widehat{i}} E_{k,\widehat{i}}^{l}$$

be the discrete global energy at some fixed time-step $t_l$, which is obviously an approximation to the integral

$$\mathcal{E}(t_l) := \int_{-\mathrm{L}/2}^{\mathrm{L}/2} E(x,t_l)\,dx.$$

Now, define

$$(\mathcal{E}rror_{te})_{l} = \mathcal{E}_{\mathrm{L}}^{l} - \mathcal{E}_{\mathrm{L}}^{0}, \tag{5.4}$$

it depicts the error propagation of the conservation of global energy.

We also use

$$(error_u)_l = \max_k |\breve{u}_k^l - u_k^l| \tag{5.5}$$

to represent the maximum error of the scheme at the time-step $t_l$. Here, $\breve{u}_k^l$ and $u_k^l$ are the exact solution and numerical solution at $(x_k, t_l)$, respectively.

In the following, we take in (3.1) the potential function $G(u) = 1 - \cos u$, which gives the well-known Sine-Gordon equation

$$u_{tt} = u_{xx} - \sin u. \tag{5.6}$$

We only consider the so-called *breather solution* for (5.6),

$$u(x,t) = -4\tan^{-1}\left[\frac{m}{\sqrt{1-m^2}}\frac{\sin(t\sqrt{1-m^2}+c_2)}{\cosh(mx+c_1)}\right], \tag{5.7}$$

where we take $m = 0.2$, $c_1 = 0$, $c_2 = -10\sqrt{1-m^2}$. The initial conditions employed are

$$u(x,0) = -4\tan^{-1}\left[\frac{m}{\sqrt{1-m^2}}\frac{\sin(c_2)}{\cosh(mx+c_1)}\right], \tag{5.8}$$

and

$$v(x,0) = \frac{\partial}{\partial t}\left\{-4\tan^{-1}\left[\frac{m}{\sqrt{1-m^2}}\frac{\sin(t\sqrt{1-m^2}+c_2)}{\cosh(mx+c_1)}\right]\right\}_{t=0}. \tag{5.9}$$

For comparisons, we implement four different schemes for the experiment, which are referred to as scheme I, II, III & IV and described as follows:

(i). Scheme I is the well-known leap-frog scheme for the wave equation

$$\frac{u_k^{l+1} - 2u_k^l + u_k^{l-1}}{\tau^2} = \frac{u_{k+1}^l - 2u_k^l + u_{k-1}^l}{h^2} - G'(u_k^l),$$

which is also known to be multi-symplectic (see, e.g., [8] and [11]).

(ii). Scheme II is the multi-symplectic SRKN-SRK method $\mathrm{MSIA}_2(\alpha,\beta)$ constructed in Section 3.

(iii). Scheme III is given by

$$\begin{aligned}
u_k^{l+1} &= u_k^l + \tau v_k^l + \frac{1}{2}\tau^2\left[\frac{u_{k+1}^l - 2u_k^l + u_{k-1}^l}{h^2} - G'(u_k^l)\right],\\
U_k^{l,2} &= u_k^l + \frac{1}{2}\tau v_k^l,\\
v_k^{l+1} &= v_k^l + \tau\left[\frac{U_{k+1}^{l,2} - 2U_k^{l,2} + U_{k-1}^{l,2}}{h^2} - G'(U_k^{l,2})\right],
\end{aligned}$$

Table 1: Numerical results for scheme I, III & IV.

| $\tau\backslash h$ | scheme | $l$ | $(error_u)_l$ | $(Error_{le})_l$ | $(\mathcal{E}rror_{te})_l$ |
|---|---|---|---|---|---|
| $\tau=0.01$ | I | 500 | 1.30e-5 | 2.56e-3 | -3.33e-3 |
| $h=0.2$ | III | 500 | 2.51e-5 | 9.14e-3 | 3.13e-7 |
| | IV | 500 | 1.62e-4 | 2.63e-3 | -3.22e-3 |
| $\tau=0.02$ | I | 250 | 1.19e-5 | 5.06e-3 | -6.72e-3 |
| $h=0.2$ | III | 250 | 6.37e-5 | 1.82e-2 | 4.15e-6 |
| | IV | 250 | 1.51e-4 | 5.12e-3 | -6.61e-3 |
| $\tau=0.02$ | I | 250 | 9.82e-6 | 5.05e-3 | -3.36e-3 |
| $h=0.1$ | III | 250 | 5.40e-5 | 7.29e-2 | 2.07e-6 |
| | IV | 250 | 3.75e-5 | 5.07e-3 | -3.35e-3 |
| $\tau=0.01$ | I | 500 | 9.84e-6 | 2.55e-3 | -1.67e-3 |
| $h=0.1$ | III | 500 | 1.50e-5 | 3.65e-2 | 1.57e-7 |
| | IV | 500 | 4.09e-5 | 2.57e-3 | -1.65e-3 |

which is a method-of-line, and can be obtained by using the second-order central difference for the Laplace operator and the following 2nd order RK method in time,

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 0 & 1 \end{array}$$

Since the RK method utilized is not symplectic, scheme III is not multi-symplectic.

(iv). Scheme IV is a modified leap-frog scheme:

$$\frac{u_k^{l+1}-2u_k^l+u_k^{l-1}}{\tau^2}=\frac{u_{k+1}^l-2u_k^l+u_{k-1}^l}{h^2}-G'\left(\frac{u_{k+1}^l+u_{k-1}^l}{2}\right).$$

We note that all of the above schemes are explicit, conditionally stable and of second order in both space and time. We run those different schemes on the same computer. The first result is on the maximum error of the numerical solution, the error of LECL and the error of global energy after $l$ time-steps. Data given in Tables 1 and 2 show the averagely superiority of scheme II. Particularly, scheme II preserves the LECL prominently better than the other three.

Next, we plot the maximum error $(error_u)_l$, the error of LECL $(Error_{le})_l$ and the error of global energy $(\mathcal{E}rror_{te})_l$ as functions of the time-step. These results are given in Figs. 1-3, respectively, and are all obtained by using $\tau=0.01$ and $h=0.2$. From Fig. 1, it can be seen that there is no evident difference in maximum solution error for scheme I, scheme II and scheme III, but scheme IV displays a quick amplification of error. And they all show the process of accumulation of global errors and reasonable oscillations.

Fig. 2 shows the numerical error of LECL as a function of the time-step. The multi-symplectic RKN-RK method, i.e., scheme II is better than the other three. In fact, the error

Table 2: Numerical results for scheme II ($MSIA_2(\alpha,\beta)$).

| $\tau\backslash h$ | $\alpha,\ \beta$ | $l$ | $(error_u)_l$ | $(Error_{le})_l$ | $(\mathcal{E}rror_{te})_l$ |
|---|---|---|---|---|---|
| $\tau=0.01$ | $-\sqrt{2}/4,\ \sqrt{2}/4$ | 500 | 1.64e-5 | 1.01e-4 | 2.67e-6 |
| $h=0.2$ | $-1/4, 1/4$ | 500 | 1.20e-5 | 1.00e-4 | -3.08e-6 |
| | $-1/8, 1/8$ | 500 | 1.23e-5 | 9.95e-5 | -8.51e-6 |
| | $-1/8, 3/8$ | 500 | 1.09e-5 | 9.99e-5 | -5.38e-6 |
| $\tau=0.02$ | $-\sqrt{2}/4,\ \sqrt{2}/4$ | 250 | 2.50e-5 | 1.04e-4 | 1.07e-5 |
| $h=0.2$ | $-1/4, 1/4$ | 250 | 1.29e-5 | 1.01e-4 | -1.23e-5 |
| | $-1/8, 1/8$ | 250 | 2.32e-5 | 9.84e-5 | -3.41e-5 |
| | $-1/8, 3/8$ | 250 | 1.63e-5 | 1.00e-4 | -2.15e-5 |
| $\tau=0.02$ | $-\sqrt{2}/4,\ \sqrt{2}/4$ | 250 | 1.52e-5 | 5.32e-5 | 5.34e-6 |
| $h=0.1$ | $1/4, 1/4$ | 250 | 6.64e-6 | 5.02e-5 | -6.15e-6 |
| | $-1/8, 1/8$ | 250 | 1.76e-5 | 4.72e-5 | -1.70e-5 |
| | $-1/8, 3/8$ | 250 | 1.01e-5 | 4.89e-5 | -1.07e-5 |
| $\tau=0.01$ | $-\sqrt{2}/4,\ \sqrt{2}/4$ | 500 | 6.31e-6 | 5.09e-5 | 1.33e-6 |
| $h=0.1$ | $-1/4, 1/4$ | 500 | 3.30e-6 | 5.02e-5 | -1.54e-6 |
| | $-1/8, 1/8$ | 500 | 5.89e-6 | 4.95e-5 | -4.26e-6 |
| | $-1/8, 3/8$ | 500 | 4.15e-6 | 4.99e-5 | -2.69e-6 |

of scheme II is not of the same magnitude than that of the others, which is approximately second-order in $\tau$.

Fig. 3 exhibits the numerical error of the global energy, i.e., $(\mathcal{E}rror_{te})_l$. For scheme I, scheme II and scheme IV, the errors do not show numerical amplifications. But the errors of scheme I and scheme IV only reach the magnitude of $10^{-3}$, while for scheme II, it is $10^{-6}$. Though the error of scheme III is in the scale of $10^{-5}$, it exhibits an obvious linear growth process.

We also run the scheme $MSIA_2(-1/4,1/4)$ with different spatial and temporal step-sizes. Fig. 4 is for the numerical error of LECL with different step-sizes. One can see that the change of error has less relation to the change of temporal step-size $\tau$ and stays reasonable oscillation for a long time. Fig. 5 is for the maximum solution error, which is seen to be consistent with the theoretical analysis that the method is of accuracy $\mathcal{O}(\tau^2+h^2)$. Moreover, Fig. 6 is about the error of global energy, which can be seen to be of order $\tau^2 h$, for when the spatial step-size $h$ increases two times, the error also increases two times, and if the temporal step-size $\tau$ increases two times, the error goes up four times.

Finally, we apply the multi-symplectic SRKN-SRK method $MSIA_3(-\mu,0,\mu)$ with $\mu=(2-\sqrt[3]{4}-\sqrt[3]{16})/12$ for the breather solution. Here, we still take $\tau=0.01$ and $h=0.2$. The numerical result is plotted in Fig. 7, which is shown to give a good simulation.

All the numerical phenomena in this section reveal that the superiority of the explicit multi-symplectic RKN-RK method lies not only in the conservation of multi-symplectic geometric structure, but also in the good preservation of some crucial conservative properties in physics.

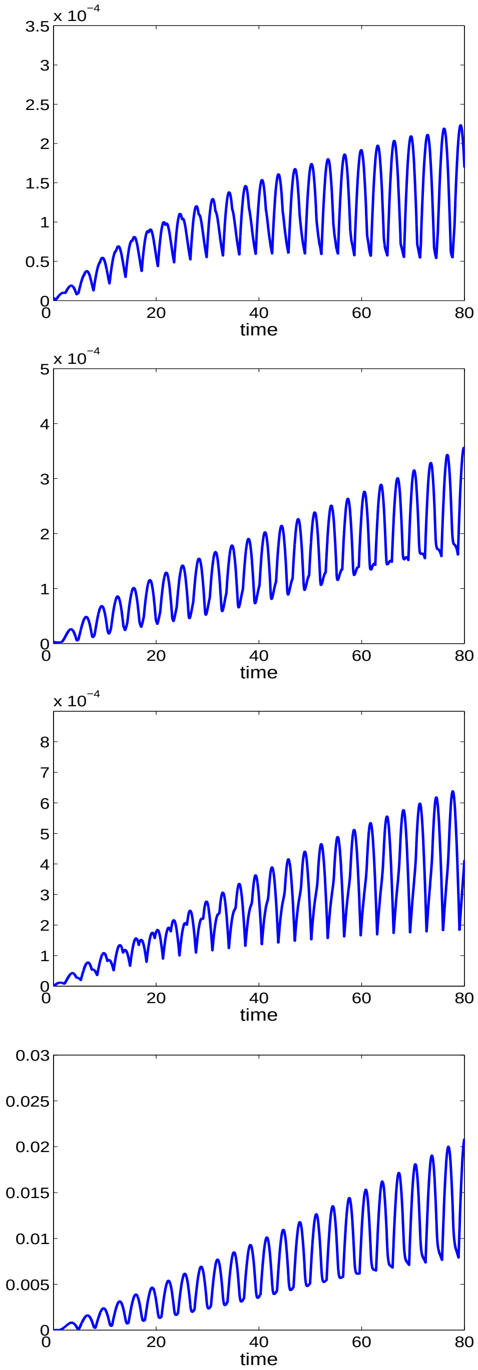


Figure 1: Maximum solution error $(error_u)_l$ as a function of the time-step $t_l$ for different schemes: Top is for scheme I; second is for scheme II with $\alpha=-1/4$, $\beta=1/4$; third is for scheme III; bottom is for scheme IV.

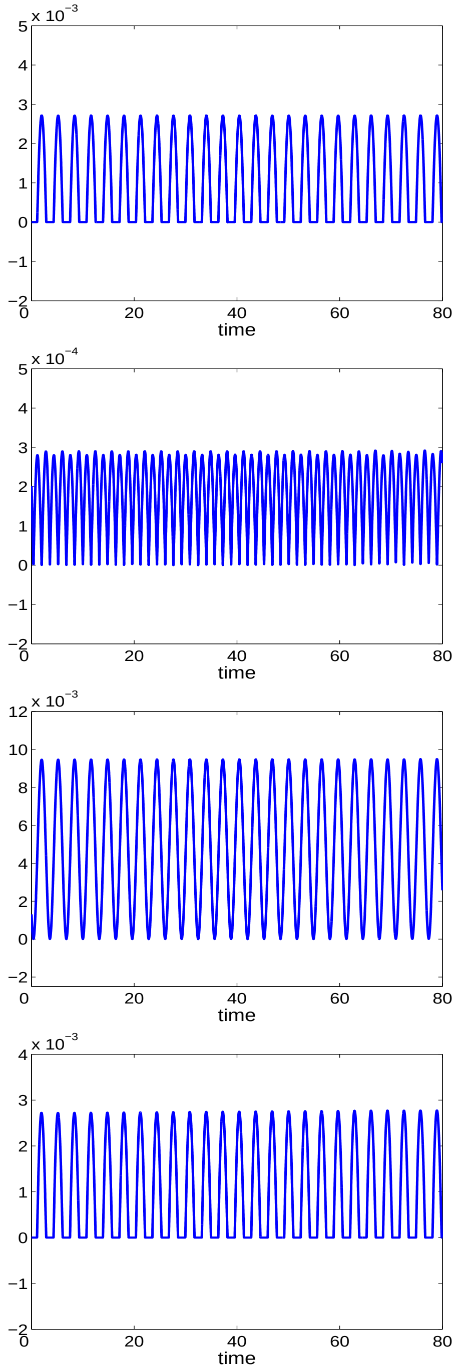


Figure 2: Numerical error of LECL, i.e., $(Error_{le})_l$ as a function of the time-step $t_l$ for different schemes: Top is for scheme I; second is for scheme II with $\alpha=-1/4$, $\beta=1/4$; third is for scheme III; bottom is for scheme IV.

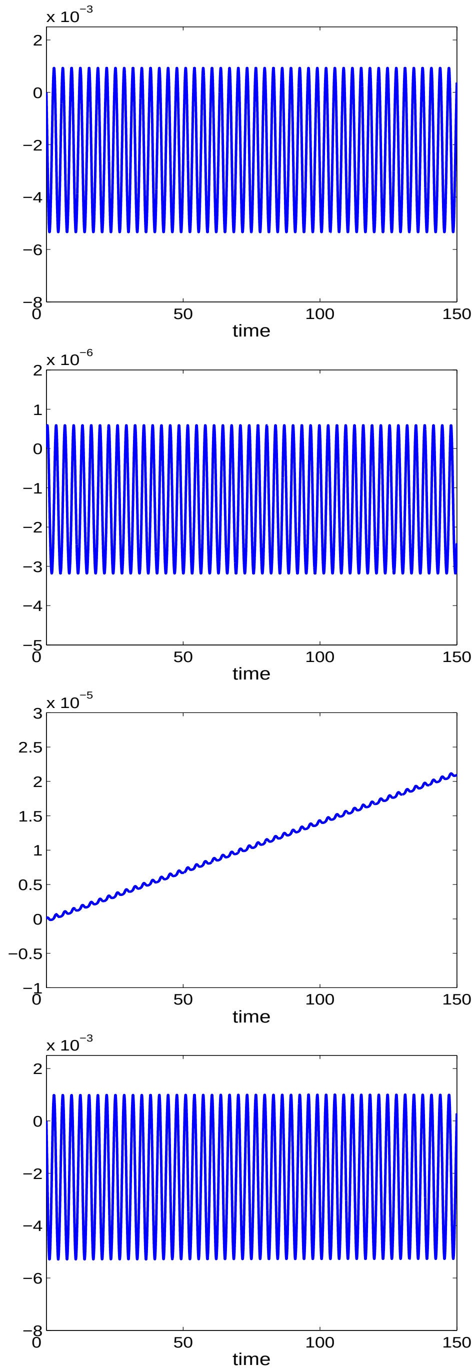


Figure 3: Numerical error of global energy, i.e., $(\mathcal{E}rror_{te})_l$ as a function of the time-step $t_l$ for different schemes: Top is for scheme I; second is for scheme II with $\alpha=-1/4$, $\beta=1/4$; third is for scheme III; bottom is for scheme IV.

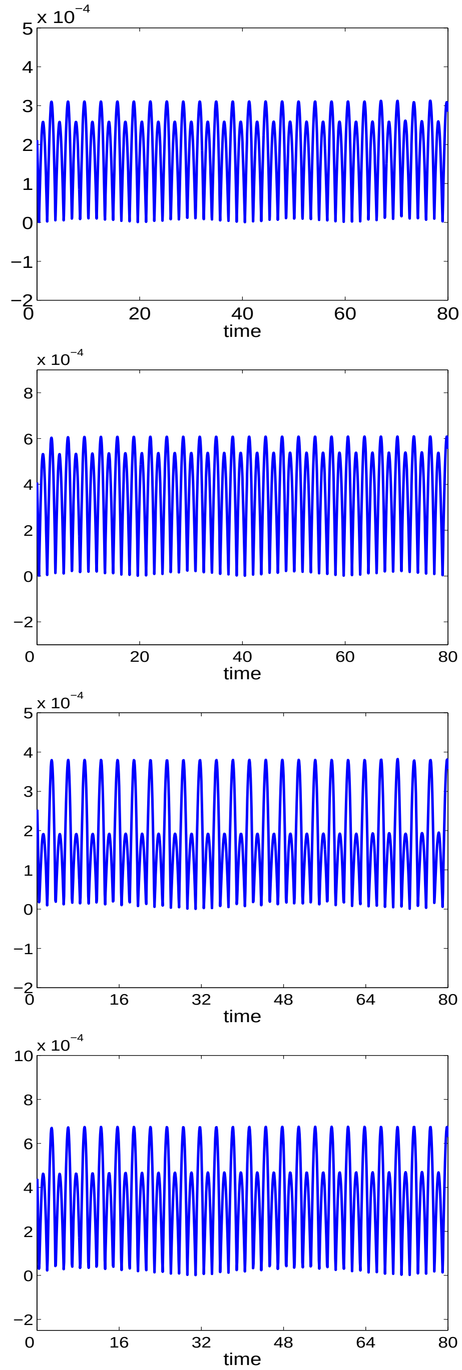


Figure 4: Error of LECL, i.e., $(Error_{le})_l$ for scheme II ($\alpha=-1/4$, $\beta=1/4$) with different spatial and temporal step-sizes: Top is for $\tau=0.04$ and $h=0.2$; second is for $\tau=0.04$ and $h=0.4$; third is for $\tau=0.08$ and $h=0.2$; bottom is for $\tau=0.08$ and $h=0.4$.

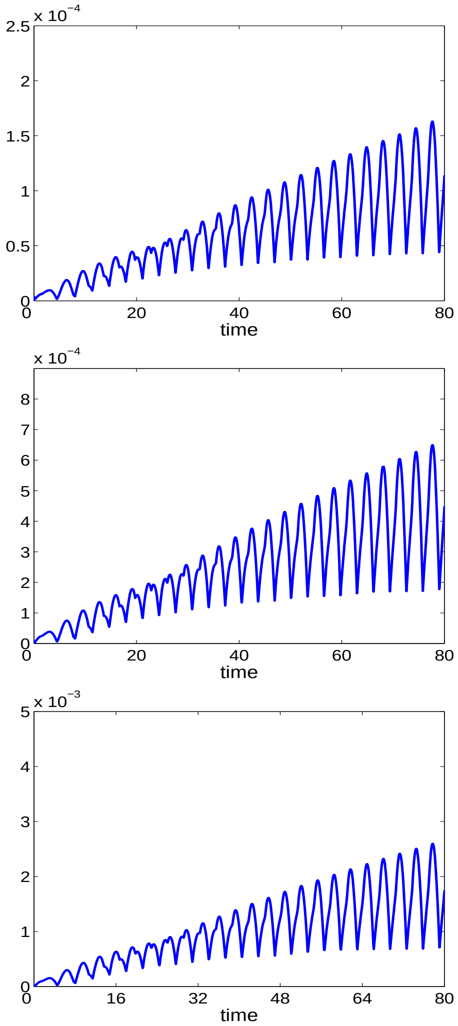


Figure 5: Maximum solution error $(error_u)_l$ for scheme II $(\alpha=-1/4,\ \beta=1/4)$ with different spatial and temporal step-sizes: Top is for $\tau=0.02$ and $h=0.1$; middle is for $\tau=0.04$ and $h=0.2$; bottom is for $\tau=0.08$ and $h=0.4$.

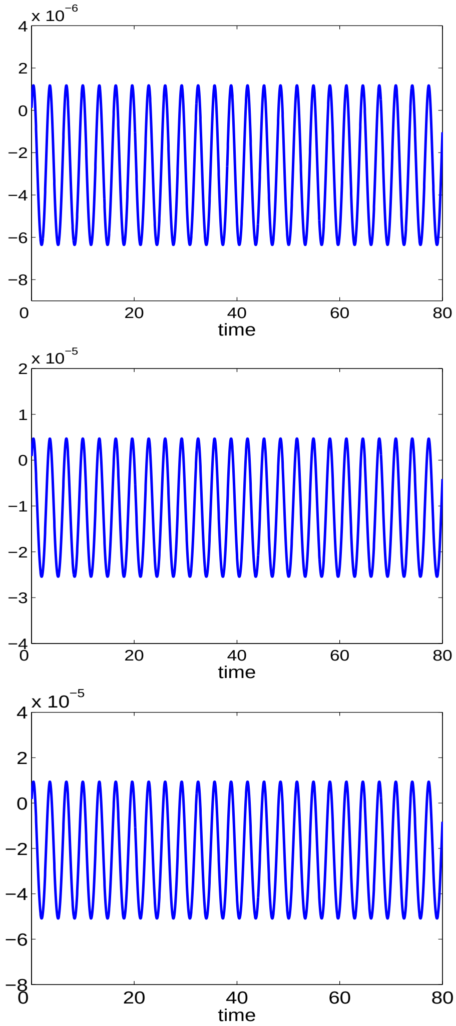


Figure 6: Error of global energy, i.e., $(\mathcal{E}rror_{te})_l$ for scheme II $(\alpha=-1/4,\ \beta=1/4)$ with different spatial and temporal step-sizes: Top is for $\tau=0.02$ and $h=0.1$; middle is for $\tau=0.04$ and $h=0.1$; bottom is for $\tau=0.04$ and $h=0.2$.

# 6 Conclusions

The present paper considers the systematic construction of explicit multi-symplectic integration algorithms by means of concatenating symplectic Runge-Kutta-Nyström methods and symplectic Runge-Kutta-type methods. Based on a general framework provided in this paper, we construct a class of high-order explicit multi-symplectic schemes for the nonlinear scalar wave equation. Clearly, our results are readily extended to some other Hamiltonian PDEs. Furthermore, the newly derived explicit methods are shown

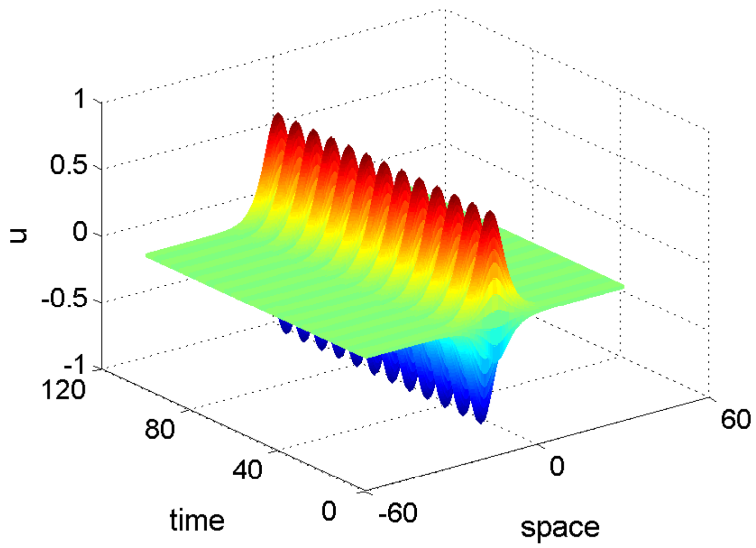


Figure 7: The breather solution of $\mathrm{MSIA}_3(-\mu,0,\mu)$ with $\mu=(2-\sqrt[3]{4}-\sqrt[3]{16})/12$.

to possess good stability properties which ensures their practicality. Through numerical comparisons, it is illustrated that the superiority of the newly derived integrators lies not only in the capability of long-time scale computation, but also in the good preservation of local/global energy. We believe that more efficient multi-symplectic integrators can be constructed based on the general framework present in this paper, since it allows more types of methods for concatenation, including SRK methods, SPRK methods and SRKN methods. Further research will be conducted on this aspect, and pertinent results will be reported elsewhere in the future.

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### References

[1] U. M. Ascher and R. I. McLachlan, Multisymplectic box schemes and the Korteweg-de Vries equation, Appl. Numer. Math., 48 (2004), 255-269.
[2] T. J. Bridges and S. Reich, Multi-symplectic integrators: Numerical schemes for Hamiltonian PDEs that conserve symplecticity, Phys. Lett. A, 284 (2001), 491-504.
[3] E. Forest and R. D. Ruth, Fourth order symplectic integration, Physica D, 43 (1990), 105-117.

[4] J. Hong, A survey of multi-symplectic Runge-Kutta type methods for Hamiltonlian partial differential equations, in: T. Li and P. Zhang (Eds.), Frontiers and Prospects of Contemporary Applied Mathematics, Series in Contemporary Applied Mathematics, Higher Education Press, Word Scientific Beijing, Vol. 6, 2005, pp. 71-113.

[5] J. Hong and C. Li, Multi-symplectic Runge-Kutta methods for nonlinear Dirac equations, J. Comput. Phys., 211 (2006), 448-472.

[6] J. Hong, H. Liu and G. Sun, The multi-symplecticity of partitioned Runge-Kutta methods for Hamiltonian PDEs, Math. Comput., 75(253) (2006), 167-181.

[7] A. Iserles, A First Course in the Numerical Analysis of Differential Equations, Cambridge Texts in Applied Mathematics, Cambridge University Press, Cambridge, 1996.

[8] S. Jiang, C. Li, H. Liu and K. Zhang, A multi-symplectic integration algorithm for some Hamiltonian PDEs, preprint, 2006.

[9] B. Leimkuhler and S. Reich, Simulating Hamiltonian Dynamics, Cambridge University Press, Cambridge, 2004.

[10] X. Liu, Y. Qi, J. He and P. Ding, Recent progress in symplectic algorithms for use in quantum systems, Commun. Comput. Phys., 2 (2007), 1-53.

[11] H. Liu and K. Zhang, Multi-symplectic Runge-Kutta-type methods for Hamiltonian wave equations, IMA J. Numer. Anal., 26 (2006), 252-271.

[12] J. M. Marsden, G. P. Patrick and S. Shkoller, Multisymplectic geometry, variational integrators, and nonlinear PDEs, Commun. Math. Phys., 199(2) (1999), 351-395.

[13] D. Okunbor and R. D. Skeel, Explicit canonical methods for Hamiltonian systems, Math. Comput., 59(200) (1992), 439-455.

[14] S. Reich, Multi-symplectic Runge-Kutta collocation methods for Hamiltonian wave equations, J. Comput. Phys., 157 (2000), 473-499.

[15] J. M. Sanz-Serna and M. P. Calvo, Numerical Hamiltonian Problems, Chapman and Hall, London, 1994.

[16] Y. Sun, Multi-sympleciticity of Nyström methods, preprint, 2004.

[17] G. Sun, A simple way of constructing symplectic Runge-Kutta methods, J. Comput. Math., 18 (2000), 61-68.

[18] Y. B. Suris, The canonicity of mappings generated by Runge-Kutta type methods when integrating the system $\ddot{x} = -\partial U/\partial x$, Zh. Vychisl. Mat. i Mat. Fiz., 29 (1989), 202-211; U.S.S.R. Comput. Math. Math. Phys., 29 (1989), 138-144 (English translation).