THE MULTI-SYMPLECTICITY OF PARTITIONED RUNGE-KUTTA METHODS FOR HAMILTONIAN PDEs

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Abstract In this article we consider partitioned Runge-Kutta (PRK) methods for Hamiltonian partial differential equations (PDEs), and present some sufficient conditions for multi-symplecticity of PRK methods of Hamiltonian PDEs.

Key words : Partitioned Runge-Kutta method ; Multi-symplecticity ; Hamiltonian partial differential equation.

AMS subject classification : 65M06, 65M99, 65N06, 65N99

1. Introduction

It has been widely recognized that the symplectic integrator has the numerical superiority when applied to solving Hamiltonian ODEs. A systemic theory of symplectic integrators for Hamiltonian ODEs has been established by some authors. The Runge-Kutta methods play an important role in numerically solving differential equations (see [1, 3, 4, 6, 9-19] and references therein). The symplectic condition of Runge-Kutta methods was founded independently by Lasagni, Sanz-Serna and Suris in 1988 (see [6, 13, 15, 18] and references therein). The numerical analysis has been investigated and developed by some authors (see [4, 6, 10, 13, 19] and references therein). Some characterizations of symplectic partitioned Runge-Kutta method, which are very useful for the construction of symplectic schemes for solving numerical Hamiltonian problems, were obtained by Sanz-Serna in [14], Sun in [16, 17] and Suris in [19], and recently discussed by Marsden and West in [11]. Reich in [12] considered Hamiltonian wave equations, and showed that the Gauss-Legendre discretization applied to the scalar wave equation (and Schrödinger equation) both in time and space direction, leads to a multi-symplectic integrator (also see [9]) . Motivated by ref. [6, 12, 14, 16, 17, 19], questions we considered are : are there any multi-symplectic partitioned Runge-Kutta methods for Hamiltonian PDEs ? what is the characterization of multi-symplectic partitioned Runge-Kutta methods for the general case of Hamiltonian PDEs ? The answer to the first question is obviously affirmative. The last question is closely related to the construction of higher order multi-symplectic schemes for Hamiltonian PDEs. In this article we consider the general case of Hamiltonian PDEs, and investigate the multi-symplecticity of partitioned Runge-Kutta methods, then present some conditions for multi-symplectic partitioned Runge-Kutta methods. In the rest of this section we introduce some basic concepts on multi-symplectic discretization and multi-symplecticity of Hamiltonian PDEs, and give

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an extension version of Reich's result on the multi-symplecticity of Gauss-Legendre methods for the general case of Hamiltonian PDEs. In section 2 we present conditions for multi-symplecticity of partitioned Runge-Kutta methods when applied to a Hamiltonian PDE. In section 3, the multi-symplecticity of partitioned Runge-Kutta methods for the wave equation is discussed. In section 4 we investigate conservative properties of energy and momentum for Runge-Kutta methods of linear Hamiltonian PDEs. In what follows we assume that all numerical methods proposed are numerically solvable, and only focus on the multi-symplecicitity of methods.

Consider the Hamiltonian partial differential equation

$$Mz_t + Kz_x = \nabla_z S(z), \quad (x,t) \in \Omega \subset R^2, \tag{1}$$

where M and K are skew-symmetric matrices, and S is a real smooth function of variable z. As well-known, some very important partial differential equations can be rewritten in this form (see [2, 7, 8, 12] and references therein). The following is its multi-symplectic conservation law

$$\frac{\partial \omega(U,V)}{\partial t} + \frac{\partial \kappa(U,V)}{\partial x} = 0, \tag{2}$$

where

$$\omega(U,V) = U^T M^T V, \qquad \kappa(U,V) = U^T K^T V,$$

$U(x,t)$ and $V(x,t)$ are solutions of the variational equation

$$M dz_t + K dz_x = D_{zz} S(z) dz. \tag{3}$$

In order to study the multi-symplecticity (2)-preserving Runge-Kutta method, we introduce an uniform grid $(x_j, t_k) \in R^2$ with mesh-length Δt in the t direction and mesh-length Δx in the x direction. The value of the function $\psi(x,t)$ at the mesh point (x_j, t_k) is denoted by $\psi_{j,k}$. The equation (1), (2) and (3) can be, respectively, schemed numerically as

$$\boxed{\begin{aligned} &M\partial_t^{j,k} z_{j,k} + K\partial_x^{j,k} z_{j,k} = (\nabla_z S_{j,k})_{j,k}, && (4)\\ &\partial_t^{j,k}\omega_{j,k} + \partial_x^{j,k}\kappa_{j,k} = 0, && (5)\\ &M\partial_t^{j,k}(dz)_{j,k} + K\partial_x^{j,k}(dz)_{j,k} = (D_{zz}^{j,k} S_{j,k})(dz)_{j,k}, && (6)\end{aligned}}$$

where $S_{j,k} = S(z_{j,k}, x_j, t_k)$,

$$\omega_{j,k} =< MU_{j,k}, V_{j,k} > \quad \kappa_{j,k} =< KU_{j,k}, V_{j,k} >,$$

$U_{j,k}$ and $V_{j,k}$ are solutions of (6), and $\partial_t^{j,k}$, $\partial_x^{j,k}$ are discretizations of the derivatives ∂_t and ∂_x respectively. The following definition is from [2]

Definition 1 *The numerical scheme (4) is called multi-symplectic if (5) is a discrete conservation law of (4).*

To simplify notations, let the starting point (x_0, t_0)=$(0,0)$ in numerical methods proposed throughout this paper. The Runge-Kutta method for the equation (1) is the following

$$\boxed{\begin{array}{lr}
Z_{mk} = z_m^{\mathbf{0}} + \Delta t \sum_{j=1}^{r} a_{kj} \partial_t Z_{mj}, & (7) \\
z_m^{\mathbf{1}} = z_m^{\mathbf{0}} + \Delta t \sum_{k=1}^{r} b_k \partial_t Z_{mk}, & (8) \\
Z_{mk} = z_{\mathbf{0}}^{k} + \Delta x \sum_{n=1}^{s} \tilde{a}_{mn} \partial_x Z_{nk}, & (9) \\
z_{\mathbf{1}}^{k} = z_{\mathbf{0}}^{k} + \Delta x \sum_{m=1}^{s} \tilde{b}_m \partial_x Z_{mk}, & (10) \\
M \partial_t Z_{mk} + K \partial_x Z_{mk} = \nabla_z S(Z_{mk}), & (11)
\end{array}}$$

where notations are used as follows $Z_{mk} \approx z(c_m \Delta x, d_k \Delta t)$, $z_m^{\mathbf{0}} \approx z(c_m \Delta x, 0)$, $\partial_t Z_{mj} \approx \partial_t z(c_m \Delta x, d_k \Delta t)$, $\partial_x Z_{mj} \approx \partial_x z(c_m \Delta x, d_k \Delta t)$, $z_m^{\mathbf{1}} \approx z(c_m \Delta x, \Delta t)$. $z_{\mathbf{0}}^{k} \approx z(0, d_k \Delta t)$, $z_{\mathbf{1}}^{k} \approx z(\Delta x, d_k \Delta t)$, and

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

Corresponding variational equations to (7-11) respectively are

$$\boxed{\begin{array}{lr}
dZ_{mk} = dz_m^{\mathbf{0}} + \Delta t \sum_{j=1}^{r} a_{kj} d(\partial_t Z_{mj}), & (12) \\
dz_m^{\mathbf{1}} = dz_m^{\mathbf{0}} + \Delta t \sum_{k=1}^{r} b_k d(\partial_t Z_{mk}), & (13) \\
dZ_{mk} = dz_{\mathbf{0}}^{k} + \Delta x \sum_{n=1}^{s} \tilde{a}_{mn} d(\partial_x Z_{nk}), & (14) \\
dz_{\mathbf{1}}^{k} = dz_{\mathbf{0}}^{k} + \Delta x \sum_{m=1}^{s} \tilde{b}_m d(\partial_x Z_{mk}), & (15) \\
M \partial_t dZ_{mk} + K \partial_x dZ_{mk} = D_{zz} S(Z_{mk}) dZ_{mk}, & (16)
\end{array}}$$

where $D_{zz} S(Z_{mk})$ is a symmetric matrix.

Theorem 1 *If in the method (7-11)*

$$b_k b_j - b_k a_{kj} - b_j a_{jk} = 0 \tag{17}$$

$$\text{and} \quad \tilde{b}_m \tilde{b}_n - \tilde{b}_m \tilde{a}_{mn} - \tilde{b}_n \tilde{a}_{nm} = 0 \tag{18}$$

hold for $k, j = 1, 2, \cdots, r$ and $m, n = 1, 2, \cdots, s$, then the method (7-11) is multi-symplectic with the conservation law

$$\begin{array}{l}
\Delta x \sum_{m=1}^{s} \tilde{b}_m ((\widetilde{dz_m^{\mathbf{1}}})^T M^T (dz_m^{\mathbf{1}}) - (\widetilde{dz_m^{\mathbf{0}}})^T M^T (dz_m^{\mathbf{0}})) \\
+ \Delta t \sum_{k=1}^{r} b_k ((\widetilde{dz_{\mathbf{1}}^{k}})^T K^T (dz_{\mathbf{1}}^{k}) - (\widetilde{dz_{\mathbf{0}}^{k}})^T K^T (dz_{\mathbf{0}}^{k})) = 0,
\end{array} \tag{19}$$

where

$$\begin{array}{ll}
 & \{\widetilde{dz_m^{\mathbf{1}}}, \widetilde{dz_m^{\mathbf{0}}}, \widetilde{dz_{\mathbf{1}}^{k}}, \widetilde{dz_{\mathbf{0}}^{k}}, d\widetilde{Z_{mk}}, d(\widetilde{\partial_x Z_{mk}}), d(\widetilde{\partial_t Z_{mk}})\} \\
\text{and} & \{dz_m^{\mathbf{1}}, dz_m^{\mathbf{0}}, dz_{\mathbf{1}}^{k}, dz_{\mathbf{0}}^{k}, dZ_{mk}, d(\partial_x Z_{mk}), d(\partial_t Z_{mk})\}
\end{array}$$

are solutions of the variational equation (12-16).

Proof. Let

$$\{\widetilde{dz_m^{\mathbf{1}}}, \widetilde{dz_m^{\mathbf{0}}}, \widetilde{dz_{\mathbf{1}}^k}, \widetilde{dz_{\mathbf{0}}^k}, \widetilde{dZ_{mk}}, d(\widetilde{\partial_x Z_{mk}}), d(\widetilde{\partial_t Z_{mk}})\}$$

$$\{dz_m^{\mathbf{1}}, dz_m^{\mathbf{0}}, dz_{\mathbf{1}}^k, dz_{\mathbf{0}}^k, dZ_{mk}, d(\partial_x Z_{mk}), d(\partial_t Z_{mk})\}$$

are solutions of the variational equation (12-16). It follows from (12-16) and (17-18) that

$$\begin{aligned}&(\widetilde{dz_m^{\mathbf{1}}})^T M^T (dz_m^{\mathbf{1}}) - (\widetilde{dz_m^{\mathbf{0}}})^T M^T (dz_m^{\mathbf{0}})\\ &= \Delta t \textstyle\sum_{k=1}^r b_k (d(\widetilde{\partial_t Z_{mk}})^T M^T (dZ_{mk}) + (\widetilde{dZ_{mk}})^T M^T d(\partial_t Z_{mk}))\\ &+(\Delta t)^2 \textstyle\sum_{j,k=1}^r (b_k b_j - b_k a_{kj} - b_j a_{jk}) d(\widetilde{\partial_t Z_{mk}})^T M^T d(\partial_t Z_{mk})\\ &= \Delta t \textstyle\sum_{k=1}^r b_k (d(\widetilde{\partial_t Z_{mk}})^T M^T (dZ_{mk}) + (\widetilde{dZ_{mk}})^T M^T d(\partial_t Z_{mk})),\end{aligned} \tag{20}$$

and

$$\begin{aligned}&(\widetilde{dz_{\mathbf{1}}^k})^T K^T (dz_{\mathbf{1}}^k) - (\widetilde{dz_{\mathbf{0}}^k})^T K^T (dz_{\mathbf{0}}^k)\\ &= \Delta x \textstyle\sum_{m=1}^s \tilde{b}_m (d(\widetilde{\partial_x Z_{mk}})^T K^T (dZ_{mk}) + (\widetilde{dZ_{mk}})^T K^T d(\partial_x Z_{mk})).\end{aligned} \tag{21}$$

Using (16) and the symmetry of the matrix $D_{zz}S(Z_{mk})$ produce

$$\begin{aligned}&d(\widetilde{\partial_t Z_{mk}})^T M^T (dZ_{mk}) + (\widetilde{dZ_{mk}})^T M^T d(\partial_t Z_{mk})\\ &+d(\widetilde{\partial_x Z_{mk}})^T K^T (dZ_{mk}) + (\widetilde{dZ_{mk}})^T K^T d(\partial_x Z_{mk}) = 0\end{aligned} \tag{22}$$

Combining (20), (21) and (22), the proof of theorem is completed.

Remark 1 *This theorem can be extended to the Hamiltonian partial differential equation with varying coefficients*

$$M(x) z_t + K(t) z_x = \nabla_z S(z, x, t), \tag{23}$$

where $M(x)$ and $K(t)$ are skew-symmetric matrices and smooth in x and t respectively, $S(z, x, t)$ is a smooth real function.

The following corollary is a natural extension of the result in [12]

Corollary 1 *If in (7-11), the method applied to both time direction and space direction is of Gauss-Legendre, then the method (7-11) is a multi-symplectic integrator.*

2. Partitioned Runge-Kutta methods

We consider the blocked Hamiltonian partial differential equation

$$\begin{pmatrix} M_1 & M_0 \\ -M_0^T & M_2 \end{pmatrix} \begin{pmatrix} p_t \\ q_t \end{pmatrix} + \begin{pmatrix} K_1 & K_0 \\ -K_0^T & K_2 \end{pmatrix} \begin{pmatrix} p_x \\ q_x \end{pmatrix} = \begin{pmatrix} \nabla_p S(p,q) \\ \nabla_q S(p,q) \end{pmatrix}, \tag{24}$$

where M_τ, K_τ $(\tau = 1, 2)$ are $\alpha \times \alpha$ skew-symmetric matrices, M_0, K_0 are $\alpha \times \alpha$ matrices, $S(p, q)$ is a smooth real function in $p = (p_1, p_2, \cdots, p_\alpha)^T$ and $q = (q_1, q_2, \cdots, q_\alpha)^T$.

The corresponding multi-symplectic conservation law is :

$$\frac{\partial \omega(U, V)}{\partial t} + \frac{\partial \kappa(U, V)}{\partial x} = 0, \tag{25}$$

where

$$\omega(U,V)=U^T\begin{pmatrix} M_1 & M_0\\ -M_0^T & M_2\end{pmatrix}^T V,\qquad\qquad \kappa(U,V)=U^T\begin{pmatrix} K_1 & K_0\\ -K_0^T & K_2\end{pmatrix}^T V,$$

$U(x,t)$ and $V(x,t)$ are solutions of the variational equation

$$\begin{pmatrix} M_1 & M_0\\ -M_0^T & M_2\end{pmatrix} dz_t+\begin{pmatrix} K_1 & K_0\\ -K_0^T & K_2\end{pmatrix} dz_x=D_{zz}S(z)dz \tag{26}$$

and $z=(p_1,p_2,\cdots,p_\alpha,q_1,q_2,\cdots,q_\alpha)^T$. Now we apply partitioned Runge-Kutta method to the equation (24).

$$\boxed{\begin{aligned}
P_{mk}&=p_m^{\mathbf{0}}+\Delta t\textstyle\sum_{j=1}^r a_{kj}^{(1)}\partial_t P_{mj}, &(27)\\
Q_{mk}&=q_m^{\mathbf{0}}+\Delta t\textstyle\sum_{j=1}^r a_{kj}^{(2)}\partial_t Q_{mj}, &(28)\\
p_m^{\mathbf{1}}&=p_m^{\mathbf{0}}+\Delta t\textstyle\sum_{k=1}^r b_k^{(1)}\partial_t P_{mk}, &(29)\\
q_m^{\mathbf{1}}&=q_m^{\mathbf{0}}+\Delta t\textstyle\sum_{k=1}^r b_k^{(2)}\partial_t Q_{mk}, &(30)\\
P_{mk}&=p_{\mathbf{0}}^k+\Delta x\textstyle\sum_{n=1}^s \tilde{a}_{mn}^{(1)}\partial_x P_{nk}, &(31)\\
Q_{mk}&=q_{\mathbf{0}}^k+\Delta x\textstyle\sum_{n=1}^s \tilde{a}_{mn}^{(2)}\partial_x Q_{nk}, &(32)\\
p_{\mathbf{1}}^k&=p_{\mathbf{0}}^k+\Delta x\textstyle\sum_{m=1}^s \tilde{b}_m^{(1)}\partial_x P_{mk}, &(33)\\
q_{\mathbf{1}}^k&=q_{\mathbf{0}}^k+\Delta x\textstyle\sum_{m=1}^s \tilde{b}_m^{(2)}\partial_x Q_{mk}, &(34)\\
\begin{pmatrix} M_1 & M_0\\ -M_0^T & M_2\end{pmatrix}\begin{pmatrix}\partial_t P_{mk}\\ \partial_t Q_{mk}\end{pmatrix}&+\begin{pmatrix} K_1 & K_0\\ -K_0^T & K_2\end{pmatrix}\begin{pmatrix}\partial_x P_{mk}\\ \partial_x Q_{mk}\end{pmatrix}=\begin{pmatrix}\nabla_p S(P_{mk},Q_{mk})\\ \nabla_q S(P_{mk},Q_{mk})\end{pmatrix}, &(35)
\end{aligned}}$$

where we make use of notations

$$\begin{aligned}
p_m^{\mathbf{0}}&\approx p(c_m\Delta x,0), & p_m^{\mathbf{1}}&\approx p(c_m\Delta x,\Delta t),\\
p_{\mathbf{0}}^k&\approx p(0,d_k\Delta t), & p_{\mathbf{1}}^k&\approx p(\Delta x,d_k\Delta t),\\
q_m^{\mathbf{0}}&\approx q(c_m\Delta x,0), & q_m^{\mathbf{1}}&\approx q(c_m\Delta x,\Delta t),\\
q_{\mathbf{0}}^k&\approx q(0,d_k\Delta t), & q_{\mathbf{1}}^k&\approx q(\Delta x,d_k\Delta t),\\
P_{mk}&\approx p(c_m\Delta x,d_k\Delta t), & Q_{mk}&\approx q(c_m\Delta x,d_k\Delta t),\\
\partial_t P_{mk}&\approx \tfrac{\partial p}{\partial t}(c_m\Delta x,d_k\Delta t), & \partial_x P_{mk}&\approx \frac{\partial p}{\partial x}(c_m\Delta x,d_k\Delta t),\\
\partial_t Q_{mk}&\approx \tfrac{\partial q}{\partial t}(c_m\Delta x,d_k\Delta t), & \partial_x Q_{mk}&\approx \frac{\partial q}{\partial x}(c_m\Delta x,d_k\Delta t)
\end{aligned}$$

under the assumption that

$$\sum_{n=1}^s \tilde{a}_{mn}^{(1)}=\sum_{n=1}^s \tilde{a}_{mn}^{(2)}=c_m,\qquad \sum_{j=1}^r a_{kj}^{(1)}=\sum_{j=1}^r a_{kj}^{(2)}=d_k. \tag{36}$$

The corresponding system of variation equations of this method to (27-35) to (6) is

$$dP_{mk}=dp_m^{\mathbf{0}}+\Delta t\textstyle\sum_{j=1}^r a_{kj}^{(1)}d\partial_t P_{mj}, \tag{37}$$

$$dQ_{mk} = dq_m^{\mathbf{0}} + \Delta t \sum_{j=1}^{r} a_{kj}^{(2)} d\partial_t Q_{mj}, \tag{38}$$

$$dp_m^{\mathbf{1}} = dp_m^{\mathbf{0}} + \Delta t \sum_{k=1}^{r} b_k^{(1)} d\partial_t P_{mk}, \tag{39}$$

$$dq_m^{\mathbf{1}} = dq_m^{\mathbf{0}} + \Delta t \sum_{k=1}^{r} b_k^{(2)} d\partial_t Q_{mk}, \tag{40}$$

$$dP_{mk} = dp_{\mathbf{0}}^k + \Delta x \sum_{n=1}^{s} \tilde{a}_{mn}^{(1)} d\partial_x P_{nk}, \tag{41}$$

$$dQ_{mk} = dq_{\mathbf{0}}^k + \Delta x \sum_{n=1}^{s} \tilde{a}_{mn}^{(2)} d\partial_x Q_{nk}, \tag{42}$$

$$dp_{\mathbf{1}}^k = dp_{\mathbf{0}}^k + \Delta x \sum_{m=1}^{s} \tilde{b}_m^{(1)} d\partial_x P_{mk}, \tag{43}$$

$$dq_{\mathbf{1}}^k = dq_{\mathbf{0}}^k + \Delta x \sum_{m=1}^{s} \tilde{b}_m^{(2)} d\partial_x Q_{mk}, \tag{44}$$

$$M d(\partial_t Z_{mk}) + K d(\partial_x Z_{mk}) = A_{mk} d(Z_{mk}), \tag{45}$$

where

$$d(Z_{mk}) = \begin{pmatrix} dP_{mk} \\ dQ_{mk} \end{pmatrix},$$
$$d(\partial_t Z_{mk}) = \begin{pmatrix} d\partial_t P_{mk} \\ d\partial_t Q_{mk} \end{pmatrix},$$
$$d(\partial_x Z_{mk}) = \begin{pmatrix} d\partial_x P_{mk} \\ d\partial_x Q_{mk} \end{pmatrix},$$
$$A_{mk} = \begin{pmatrix} D_{pp}S(P_{mk}, Q_{mk}) & D_{pq}S(P_{mk}, Q_{mk}) \\ D_{qp}S(P_{mk}, Q_{mk}) & D_{qq}S(P_{mk}, Q_{mk}) \end{pmatrix},$$
$$M = \begin{pmatrix} M_1 & M_0 \\ -M_0^T & M_2 \end{pmatrix}, \qquad K = \begin{pmatrix} K_1 & K_0 \\ -K_0^T & K_2 \end{pmatrix}.$$

Obviously, A_{mk} is a symmetric matrix. Now we let

$$\{dp_m^{\mathbf{1}},\, dp_m^{\mathbf{0}},\, dp_{\mathbf{1}}^k,\, dp_{\mathbf{0}}^k,\, dP_{mk},\, d\partial_t P_{mk},\, d\partial_x P_{mk},\, dq_m^{\mathbf{1}},\, dq_m^{\mathbf{0}},\, dq_{\mathbf{1}}^k,\, dq_{\mathbf{0}}^k,\, dQ_{mk},\, d\partial_t Q_{mk},\, d\partial_x Q_{mk}\}$$
$$\{\widetilde{dp_m^{\mathbf{1}}},\, \widetilde{dp_m^{\mathbf{0}}},\, \widetilde{dp_{\mathbf{1}}^k},\, \widetilde{dp_{\mathbf{0}}^k},\, \widetilde{dP_{mk}},\, \widetilde{d\partial_t P_{mk}},\, \widetilde{d\partial_x P_{mk}},\, \widetilde{dq_m^{\mathbf{1}}},\, \widetilde{dq_m^{\mathbf{0}}},\, \widetilde{dq_{\mathbf{1}}^k},\, \widetilde{dq_{\mathbf{0}}^k},\, \widetilde{dQ_{mk}},\, \widetilde{d\partial_t Q_{mk}},\, \widetilde{d\partial_x Q_{mk}}\}$$

be solutions of the variational equations (37-45), and

$$\delta_t \omega_m = (\widetilde{dp_m^{\mathbf{1}}}^T, \widetilde{dq_m^{\mathbf{1}}}^T) M^T \begin{pmatrix} dp_m^{\mathbf{1}} \\ dq_m^{\mathbf{1}} \end{pmatrix} - (\widetilde{dp_m^{\mathbf{0}}}^T, \widetilde{dq_m^{\mathbf{0}}}^T) M^T \begin{pmatrix} dp_m^{\mathbf{0}} \\ dq_m^{\mathbf{0}} \end{pmatrix}, \tag{46}$$

$$\delta_x \kappa^k = (\widetilde{dp_{\mathbf{1}}^k}^T, \widetilde{dq_{\mathbf{1}}^k}^T) K^T \begin{pmatrix} dp_{\mathbf{1}}^k \\ dq_{\mathbf{1}}^k \end{pmatrix} - (\widetilde{dp_{\mathbf{0}}^k}^T, \widetilde{dq_{\mathbf{0}}^k}^T) K^T \begin{pmatrix} dp_{\mathbf{0}}^k \\ dq_{\mathbf{0}}^k \end{pmatrix}. \tag{47}$$

By a straightforward calculation, we have

$$\begin{aligned}
\delta_t \omega_m &= \Delta t \sum_{k=1}^{r} ((\widetilde{dP_{mk}}^T, \widetilde{dQ_{mk}}^T) M^T \begin{pmatrix} b_k^{(1)} d\partial_t P_{mk} \\ b_k^{(2)} d\partial_t Q_{mk} \end{pmatrix} \\
&+ (b_k^{(1)} \widetilde{d\partial_t P_{mk}}^T, b_k^{(2)} \widetilde{d\partial_t Q_{mk}}^T) M^T \begin{pmatrix} dP_{mk} \\ dQ_{mk} \end{pmatrix}), \\
&+ (\Delta t)^2 \sum_{j,k=1}^{r} ((b_k^{(1)} a_{kj}^{(1)} + b_j^{(1)} a_{jk}^{(1)} - b_k^{(1)} b_j^{(1)}) d(\widetilde{\partial_t P_{mj}})^T M_1 d(\partial_t P_{mk}) \\
&+ (b_k^{(2)} a_{kj}^{(2)} + b_j^{(2)} a_{jk}^{(2)} - b_k^{(2)} b_j^{(2)}) d(\widetilde{\partial_t Q_{mj}})^T M_2 d(\partial_t Q_{mk}) \\
&+ (b_k^{(2)} a_{kj}^{(1)} + b_j^{(1)} a_{jk}^{(2)} - b_k^{(2)} b_j^{(1)}) d(\widetilde{\partial_t P_{mj}})^T M_0 d(\partial_t Q_{mk}) \\
&+ (b_j^{(2)} b_k^{(1)} - b_j^{(2)} a_{jk}^{(1)} - b_k^{(1)} a_{kj}^{(2)}) d(\widetilde{\partial_t Q_{mj}})^T M_0 d(\partial_t P_{mk}))
\end{aligned} \tag{48}$$

and

$$\begin{array}{rl}\delta_x\kappa^k & =\Delta x\sum_{m=1}^{s}((\widetilde{dP_{mk}}^T,\widetilde{dQ_{mk}}^T)K^T\left(\begin{array}{c}\tilde{b}_k^{(1)}d\partial_xP_{mk}\\ \tilde{b}_k^{(2)}d\partial_xQ_{mk}\end{array}\right)\\ & +(\tilde{b}_k^{(1)}d\widetilde{\partial_xP_{mk}}^T,\tilde{b}_k^{(2)}d\widetilde{\partial_xQ_{mk}}^T)K^T\left(\begin{array}{c}dP_{mk}\\ dQ_{mk}\end{array}\right)),\\ & +(\Delta x)^2\sum_{m,n=1}^{s}((\tilde{b}_m^{(1)}\tilde{a}_{mn}^{(1)}+\tilde{b}_n^{(1)}\tilde{a}_{nm}^{(1)}-\tilde{b}_m^{(1)}\tilde{b}_n^{(1)})d\widetilde{(\partial_xP_{nk})}^TK_1d(\partial_xP_{mk})\\ & +(\tilde{b}_m^{(2)}\tilde{a}_{mn}^{(2)}+\tilde{b}_n^{(2)}\tilde{a}_{nm}^{(2)}-\tilde{b}_m^{(2)}\tilde{b}_n^{(2)})d\widetilde{(\partial_xQ_{nk})}^TK_2d(\partial_xQ_{mk})\\ & +(\tilde{b}_m^{(2)}\tilde{a}_{mn}^{(1)}+\tilde{b}_n^{(1)}\tilde{a}_{nm}^{(2)}-\tilde{b}_m^{(2)}\tilde{b}_n^{(1)})d\widetilde{(\partial_xP_{nk})}^TK_0d(\partial_xQ_{mk})\\ & +(\tilde{b}_n^{(2)}\tilde{b}_m^{(1)}-\tilde{b}_m^{(1)}\tilde{a}_{mn}^{(2)}-\tilde{b}_n^{(2)}\tilde{a}_{nm}^{(1)})d\widetilde{(\partial_xQ_{nk})}^TK_0d(\partial_xP_{mk}).\end{array}\tag{49}$$

If for $k=1,2,\cdots,r$ and $m=1,2,\cdots,s$

$$b_k^{(1)}=b_k^{(2)}=b_k,\quad \tilde{b}_m^{(1)}=\tilde{b}_m^{(2)}=\tilde{b}_m.\tag{50}$$

Then the corresponding multi-symplectic conservation law of the method (27-35) to (5) is

$$\Delta x\sum_{m=1}^{s}\tilde{b}_m\delta_t\omega_m+\Delta t\sum_{k=1}^{r}b_k\delta_x\kappa^k=0.\tag{51}$$

Consequently, in this case, it is sufficient for (51), which holds, that

$$I_1=0\qquad\text{and}\qquad I_2=0,\tag{52}$$

where

$$\begin{array}{rl}I_1 & =(\Delta t)^2\sum_{j,k=1}^{r}((b_k^{(1)}a_{kj}^{(1)}+b_j^{(1)}a_{jk}^{(1)}-b_k^{(1)}b_j^{(1)})d\widetilde{(\partial_tP_{mj})}^TM_1d(\partial_tP_{mk})\\ & +(b_k^{(2)}a_{kj}^{(2)}+b_j^{(2)}a_{jk}^{(2)}-b_k^{(2)}b_j^{(2)})d\widetilde{(\partial_tQ_{mj})}^TM_2d(\partial_tQ_{mk})\\ & +(b_k^{(2)}a_{kj}^{(1)}+b_j^{(1)}a_{jk}^{(2)}-b_k^{(2)}b_j^{(1)})d\widetilde{(\partial_tP_{mj})}^TM_0d(\partial_tQ_{mk})\\ & +(b_j^{(2)}b_k^{(1)}-b_j^{(2)}a_{jk}^{(1)}-b_k^{(1)}a_{kj}^{(2)})d\widetilde{(\partial_tQ_{mj})}^TM_0d(\partial_tP_{mk}))\end{array}\tag{53}$$

and

$$\begin{array}{rl}I_2 & =(\Delta x)^2\sum_{m,n=1}^{s}((\tilde{b}_m^{(1)}\tilde{a}_{mn}^{(1)}+\tilde{b}_n^{(1)}\tilde{a}_{nm}^{(1)}-\tilde{b}_m^{(1)}\tilde{b}_n^{(1)})d\widetilde{(\partial_xP_{nk})}^TK_1d(\partial_xP_{mk})\\ & +(\tilde{b}_m^{(2)}\tilde{a}_{mn}^{(2)}+\tilde{b}_n^{(2)}\tilde{a}_{nm}^{(2)}-\tilde{b}_m^{(2)}\tilde{b}_n^{(2)})d\widetilde{(\partial_xQ_{nk})}^TK_2d(\partial_xQ_{mk})\\ & +(\tilde{b}_m^{(2)}\tilde{a}_{mn}^{(1)}+\tilde{b}_n^{(1)}\tilde{a}_{nm}^{(2)}-\tilde{b}_m^{(2)}\tilde{b}_n^{(1)})d\widetilde{(\partial_xP_{nk})}^TK_0d(\partial_xQ_{mk})\\ & +(\tilde{b}_n^{(2)}\tilde{b}_m^{(1)}-\tilde{b}_m^{(1)}\tilde{a}_{mn}^{(2)}-\tilde{b}_n^{(2)}\tilde{a}_{nm}^{(1)})d\widetilde{(\partial_xQ_{nk})}^TK_0d(\partial_xP_{mk})).\end{array}\tag{54}$$

We let

$$\begin{array}{rcl}(\mu_1)_{kj} & = & b_k^{(1)}a_{kj}^{(1)}+b_j^{(1)}a_{jk}^{(1)}-b_k^{(1)}b_j^{(1)},\\ (\mu_2)_{kj} & = & b_k^{(2)}a_{kj}^{(2)}+b_j^{(2)}a_{jk}^{(2)}-b_k^{(2)}b_j^{(2)},\\ (\mu_3)_{kj} & = & b_k^{(2)}a_{kj}^{(1)}+b_j^{(1)}a_{jk}^{(2)}-b_k^{(2)}b_j^{(1)},\\ (\nu_1)_{mn} & = & \tilde{b}_m^{(1)}\tilde{a}_{mn}^{(1)}+\tilde{b}_n^{(1)}\tilde{a}_{nm}^{(1)}-\tilde{b}_m^{(1)}\tilde{b}_n^{(1)},\\ (\nu_2)_{mn} & = & \tilde{b}_m^{(2)}\tilde{a}_{mn}^{(2)}+\tilde{b}_n^{(2)}\tilde{a}_{nm}^{(2)}-\tilde{b}_m^{(2)}\tilde{b}_n^{(2)},\\ (\nu_3)_{mn} & = & \tilde{b}_m^{(2)}\tilde{a}_{mn}^{(1)}+\tilde{b}_n^{(1)}\tilde{a}_{nm}^{(2)}-\tilde{b}_m^{(2)}\tilde{b}_n^{(1)}.\end{array}$$

Then the following result is concluded

Theorem 2 *In the method (27-35), suppose that (36) and (50) hold. The method (27-35) is multi-symplectic, with discrete multi-symplectic law (51), if one of following conditions holds*

1. *for* $\tau = 1, 2, 3$

$$(\mu_\tau)_{kj} = 0 \ (k, j = 1, 2, \cdots r) \quad \text{and} \quad (\nu_\tau)_{mn} = 0 \ (m, n = 1, 2, \cdots, s), \tag{55}$$

when $M_\lambda \neq 0$, $K_\lambda \neq 0$ *(*$\lambda = 1, 2$*),* $M_0 \neq 0$ *and* $K_0 \neq 0$;

2. *for* $\tau = 1, 2, 3$,

$$(\mu_1)_{kj} = (\mu_2)_{kj} = 0 \, (k, j = 1, 2, \cdots r)(\text{resp.} \, (\mu_\tau)_{kj} = 0 \ (k, j = 1, 2, \cdots r)), \tag{56}$$

$$(\nu_\tau)_{mn} = 0 \, (m, n = 1, 2, \cdots, s)(\text{resp.} \, (\nu_1)_{mn} = (\nu_2)_{mn} = 0 \, (m, n = 1, 2, \cdots, s)), \tag{57}$$

when $M_0 = 0$ *(resp.* $K_0 = 0$*);*

3. *for* $\tau = 1, 2$, $(\mu_\tau)_{kj} = 0 \, (k, j = 1, 2, \cdots r)$ *and* $(\nu_\tau)_{mn} = 0 \, (m, n = 1, 2, \cdots, s)$, *when* $M_0 = 0$ *and* $K_0 = 0$*;*

4. $(\mu_3)_{kj} = (\nu_3)_{mn} = 0$, *for* $k, j = 1, 2, \cdots, r$; $m, n = 1, 2, \cdots, s$, *when* $M_\tau = K_\tau = 0$ *for* $\tau = 1, 2$. *(This is a typical multi-symplectic partitioned condition);*

5. *for* $\tau = 1, 2$, $(\mu_3)_{kj} = (\nu_\tau)_{mn} = 0$, *for* $k, j = 1, 2, \cdots, r$; $m, n = 1, 2, \cdots, s$, *when* $M_\sigma = K_0 = 0$ *for* $\sigma = 1, 2$;

6. *for* $\tau = 1, 2$, $(\mu_\tau)_{kj} = (\nu_3)_{mn} = 0$, *for* $k, j = 1, 2, \cdots, r$; $m, n = 1, 2, \cdots, s$, *when* $M_0 = K_\sigma = 0$ *for* $\sigma = 1, 2$;

7. $(\mu_1)_{kj} = (\nu_3)_{mn} = 0$, *for* $k, j = 1, 2, \cdots, r$; $m, n = 1, 2, \cdots, s$, *when* $M_0 = M_2 = K_\sigma = 0$ *for* $\sigma = 1, 2$;

8. $(\mu_3)_{kj} = (\nu_1)_{mn} = 0$, *for* $k, j = 1, 2, \cdots, r$; $m, n = 1, 2, \cdots, s$, *when* $M_\sigma = K_0 = K_2 = 0$ *for* $\sigma = 1, 2$.

Now we give some remarks.

Remark 2 *In Theorem 2 we list only eight conditions for multi-symplecticity of partitioned Runge-Kutta method of (27-35). By using* $I_1 = 0$ *and* $I_2 = 0$, *we can conclude more conditions for multi-symplectic partitioned Runge-Kutta methods. This theorem can be extended naturally to the case of Hamiltonian partial differential equation with varying coefficients.*

Remark 3 *It is trivial and apparent to extend Theorem 1 and Theorem 2 to the Hamiltonian partial differential equation with higher spatial dimension*

$$Mz_t + \sum_{\tau=1}^{\iota} K_\tau z_{x_\tau} = \nabla_z S(z), \tag{58}$$

where $\iota \geq 2$, M *and* K_τ *(*$\tau = 1, 2, \cdots, \iota$*) are skew-symmetric matrices, and* S *is a smooth function.*

Remark 4 *In Theorem 2 the condition 1 implies* $a_{kj}^{(1)} = a_{kj}^{(2)}$ *for* $k, j = 1, 2, \cdots r$ *and* $\tilde{a}_{mn}^{(1)} = \tilde{a}_{mn}^{(2)}$ *for* $m, n = 1, 2, \cdots, s$*. In fact, in this case only one symplectic Runge-Kutta method is applied in each direction.*

Remark 5 *Consider the nonlinear Schrödinger equation*

$$i\frac{\partial\psi}{\partial t} + \frac{\partial^2\psi}{\partial x^2} + |\psi|^2\psi = 0, \tag{59}$$

Let $\psi(x,t) = u(x,t) + iv(x,t)$*. Then the equation (59) is read as*

$$\left\{ \begin{array}{l} -\frac{\partial v}{\partial t} + \frac{\partial^2 u}{\partial x^2} + (u^2+v^2)u = 0 \\ \frac{\partial u}{\partial t} + \frac{\partial^2 v}{\partial x^2} + (u^2+v^2)v = 0. \end{array} \right. \tag{60}$$

We take $z = (u, v, u_x, v_x)^T$*, then the equation (6) can be rewritten as the following*

$$M\frac{\partial z}{\partial t} + K\frac{\partial z}{\partial x} = \nabla_z S(z,t), \tag{61}$$

where

$$M = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad K = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix},$$
$$S(z,t) = -\tfrac{1}{4}(u^2+v^2)^2 - \tfrac{1}{2}(u_x^2+v_x^2).$$

The equation (61) accords with the case of condition 7 in Theorem 2 . Thus the partitioned Runge-Kutta (27-35) method can be applied to the equation (61). The numerical experiments of multi-symplectic method applied to equation (59) has been given in the ref.[7,9].

Remark 6 *We consider the nonlinear Dirac equation*

$$\psi_t = A\psi_x + if(|\psi_1|^2 - |\psi_2|^2)B\psi, \tag{62}$$

where $\psi = (\psi_1, \psi_2)^T$*,* $i = \sqrt{-1}$*,* $f(s)$ *is a real function of a real variable* s *and matrices* A *and* B *are* $\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$ *and* $\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$ *respectively,* $\varphi = (\varphi_1, \varphi_2)^T$ *is sufficiently smooth. Let* $\psi_j = u_j + iv_j$ $(j = 1, 2)$ *and* $z = (u_1, v_1, u_2, v_2)^T$*. Then the equation (62) can be written as*

$$Mz_t + Kz_x = \nabla_z S(z), \tag{63}$$

where

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

and

$$S(z) = \frac{-1}{2}F(u_1^2 + v_1^2 - u_2^2 - v_2^2),$$

where the real smooth function $F(\zeta)$ *satisfies that* $\frac{d}{d\zeta}F(\zeta) = f(\zeta)$*.*

The equation (63) is in the case of condition (6) in Theorem 2.

Now we denote $z = (u_1, u_2, v_1, v_2)$, the equation (62) can be rewritten as

$$\hat{M}\hat{z}_t + \hat{K}\hat{z}_x = \nabla_{\hat{z}} S(\hat{z}), \tag{64}$$

where

$$\hat{M} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, \quad \hat{K} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}.$$

The equation (64) is in the case of condition (4) in Theorem 2.

3. Hamiltonian wave equations

In this section we consider the scalar wave equation

$$u_{tt} = u_{xx} - G'(u), \quad (x,t) \in \Omega \subset R^2, \tag{65}$$

where $G: R \to R$ is a smooth function. The investigation on symplectic integration for the equation (65) can be found in [4, 10] and references therein.

Let $\hat{z} = (u, p, v, w)^T$, $u_t = v$, $u_x = w$, Then the equation (65) can be written as

$$M\hat{z}_t + K\hat{z}_x = \nabla_{\hat{z}} S(\hat{z}), \tag{66}$$

where

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

The case 4 in Theorem 2 is suitable for the equation (66).

In [12], the following result is given by Reich

Proposition 1 *Let (65) be discretized in space and in time by a pair of Gauss-Legendre collocation methods with s, r, respectively, stages. Then the resulting discretization is a multi-symplectic integrator.*

A similar result is proven in [9] for the nonlinear Schrödinger equation. the multi-symplecticity of Preissman type scheme and the multi-symplectic structure for the wave equation have been discussed in [20]. Now we investigate the multi-symplecticity of partitioned Runge-Kutta method for the equation (65) by using the multi-symplectic conservation law (see [12])

$$\partial_t(du \wedge du_t) = \partial_x(du \wedge du_x). \tag{67}$$

The partitioned Runge-Kutta method applied to the equation (65) is

$$
\boxed{\begin{aligned}
U_{mk} &= u_{\mathbf{0}}^k + \Delta x \textstyle\sum_{n=1}^s \tilde{a}_{mn}^{(1)} \partial_x U_{nk}, && (68)\\
W_{mk} &= u_{\mathbf{0}}^k + \Delta x \textstyle\sum_{n=1}^s \tilde{a}_{mn}^{(2)} \partial_x W_{nk}, && (69)\\
U_{mk} &= u_m^{\mathbf{0}} + \Delta t \textstyle\sum_{j=1}^r a_{kj}^{(1)} \partial_t U_{mj}, && (70)\\
V_{mk} &= v_m^{\mathbf{0}} + \Delta t \textstyle\sum_{j=1}^r a_{kj}^{(2)} \partial_t V_{mj}, && (71)\\
u_{\mathbf{1}}^k &= u_{\mathbf{0}}^k + \Delta x \textstyle\sum_{m=1}^s \tilde{b}_m^{(1)} \partial_x U_{mk}, && (72)\\
w_{\mathbf{1}}^k &= w_{\mathbf{0}}^k + \Delta x \textstyle\sum_{m=1}^s \tilde{b}_m^{(2)} \partial_x W_{mk}, && (73)\\
u_m^{\mathbf{1}} &= u_m^{\mathbf{0}} + \Delta t \textstyle\sum_{k=1}^r b_k^{(1)} \partial_t U_{mk}, && (74)\\
v_m^{\mathbf{1}} &= v_m^{\mathbf{0}} + \Delta t \textstyle\sum_{k=1}^r b_k^{(2)} \partial_t V_{mk}, && (75)\\
\partial_t U_{mk} &= V_{mk},\ \partial_x U_{mk} = W_{mk}, && (76)\\
\partial_t V_{mk} &= \partial_x W_{mk} - G'(U_{mk}), && (77)
\end{aligned}}
$$

under the assumption that

$$
\textstyle\sum_{j=1}^r a_{kj}^{(1)} = \sum_{j=1}^r a_{kj}^{(2)} = d_k, \tag{78}
$$

$$
\textstyle\sum_{n=1}^s \tilde{a}_{mn}^{(1)} = \sum_{n=1}^s \tilde{a}_{mn}^{(2)} = c_m. \tag{79}
$$

Here notations are in the following sense, $U_{mk} \approx u(c_m\Delta x, d_k\Delta t)$, $\partial_t U_{mk} \approx \partial_t u(c_m\Delta x, d_k\Delta t)$, $\partial_x U_{mk} \approx \partial_x u(c_m\Delta x, d_k\Delta t)$, $u_{\mathbf{0}}^k \approx u(0, d_k\Delta t)$, $u_{\mathbf{1}}^k \approx u(\Delta x, d_k\Delta t)$, $u_m^{\mathbf{0}} \approx u(c_m\Delta x, 0)$, $u_m^{\mathbf{1}} \approx u(c_m\Delta x, \Delta t)$.

Theorem 3 *In the method (68-77), assume that (78), (79) and*

$$
b_k^{(1)} = b_k^{(2)} = b_k,\ \tilde{b}_m^{(1)} = \tilde{b}_m^{(2)} = \tilde{b}_m, \tag{80}
$$

$$
\tilde{b}_m^{(1)}\tilde{b}_n^{(2)} - \tilde{b}_m^{(1)}\tilde{a}_{mn}^{(2)} - \tilde{b}_n^{(2)}\tilde{a}_{nm}^{(1)} = 0, \tag{81}
$$

$$
b_k^{(1)}b_j^{(2)} - b_k^{(1)}a_{kj}^{(2)} - b_j^{(2)}a_{jk}^{(1)} = 0 \tag{82}
$$

hold for $m, n = 1, 2, \cdots, s; k, j = 1, 2, \cdots, s$. Then the method (68-77) is multi-symplectic with a discrete multi-symplectic conservation law

$$
\Delta t \sum_{k=1}^r b_k(du_{\mathbf{1}}^k \wedge dw_{\mathbf{1}}^k - du_{\mathbf{0}}^k \wedge dw_{\mathbf{0}}^k) = \Delta x \sum_{m=1}^s \tilde{b}_m(du_m^{\mathbf{1}} \wedge dv_m^{\mathbf{1}} - du_m^{\mathbf{0}} \wedge dw_m^{\mathbf{0}}). \tag{83}
$$

Proof. It follows from (68-77) and the conditions (78) - (82) that

$$
\begin{aligned}
&du_{\mathbf{1}}^k \wedge dw_{\mathbf{1}}^k - du_{\mathbf{0}}^k \wedge dw_{\mathbf{0}}^k\\
&= \Delta x \textstyle\sum_{m=1}^s \tilde{b}_m(dU_{mk} \wedge d(\partial_x W_{mk}))
\end{aligned} \tag{84}
$$

and

$$
\begin{aligned}
&du_m^{\mathbf{1}} \wedge dv_m^{\mathbf{1}} - du_m^{\mathbf{0}} \wedge dv_m^{\mathbf{0}}\\
&= \Delta t \textstyle\sum_{k=1}^r b_k(dU_{mk} \wedge d(\partial_t V_{mk})).
\end{aligned} \tag{85}
$$

On the other hand, (77) implies

$$
dU_{mk} \wedge d(\partial_x W_{mk}) = dU_{mk} \wedge d(\partial_t V_{mk}). \tag{86}
$$

From (84), (85) and (86), the discrete conservation law (83) is concluded. This completes the proof.

Remark 7 *(76) and (77) imply that (78) and (79), in essence, are not necessary for the characterization (80-82) of multi-symplectic partitioned Runge-Kutta methods (68-77).*

4. The conservation of energy and momentum

It has been shown, by S. Reich in [12] (also see [2, 9]), that multi-symplectic Gauss-Legendre schemes preserve both the discrete energy and momentum conservation laws exactly for linear Hamiltonian PDEs. In this section we show that the scheme (7-11) preserves the discrete energy and momentum conservation laws exactly for linear Hamiltonian PDEs

$$Mz_t + Kz_x = \nabla_z S(z), \tag{87}$$

where M and K are skew-symmetric matrices, and $S(z) = \frac{1}{2}z^T Az$, A is a symmetric matrix. The equation (87) has the energy conservation law

$$\begin{aligned} \partial_t E(z) + \partial_x F(z) &= 0, & (88)\\ \partial_t I(z) + \partial_x G(z) &= 0, & (89) \end{aligned}$$

where

$$\begin{aligned} E(z) &= \frac{1}{2}z^T Az - \frac{1}{2}\partial_x z^T K^T z,\\ F(z) &= \frac{1}{2}\partial_t z^T K^T z,\\ G(z) &= \frac{1}{2}z^T Az - \frac{1}{2}\partial_t z^T M^T z,\\ I(z) &= \frac{1}{2}\partial_x z^T M^T z. \end{aligned}$$

Theorem 4 *Under the assumptions of Theorem 1, if the matrices of RK methods in the method (7-11) are invertible, then the method (7-11) has a discrete energy conservation law*

$$\Delta x \sum_{m=1}^{s} \tilde{b}_m (E(z_m^{\mathbf{1}}) - E(z_m^{\mathbf{0}})) + \Delta t \sum_{k=1}^{r} b_k (F(z_{\mathbf{1}}^k) - F(z_{\mathbf{0}}^k)) = 0 \tag{90}$$

and a discrete momentum conservation law

$$\Delta x \sum_{m=1}^{s} \tilde{b}_m (I(z_m^{\mathbf{1}}) - I(z_m^{\mathbf{0}})) + \Delta t \sum_{k=1}^{r} b_k (G(z_{\mathbf{1}}^k) - G(z_{\mathbf{0}}^k)) = 0. \tag{91}$$

Proof. First of all, we introduce the system

$$\begin{aligned} \partial_x Z_{mk} &= (\partial_x z)_m^{\mathbf{0}} + \Delta t \sum_{j=1}^{r} a_{kj} \partial_t (\partial_x Z_{mj}), & (92)\\ (\partial_x z)_m^{\mathbf{1}} &= (\partial_x z)_m^{\mathbf{0}} + \Delta t \sum_{k=1}^{r} b_k \partial_t (\partial_x Z_{mk}), & (93) \end{aligned}$$

$$\partial_t Z_{mk} = (\partial_t z)_{\mathbf{0}}^k + \Delta x \sum_{n=1}^{s} \tilde{a}_{mn} \partial_x (\partial_t Z_{nk}), \tag{94}$$

$$(\partial_x z)_{\mathbf{1}}^k = (\partial_x z)_{\mathbf{0}}^k + \Delta x \sum_{m=1}^{r} \tilde{b}_m \partial_x (\partial_t Z_{mk}), \tag{95}$$

where $(\partial_x z)_m^{\mathbf{0}}$ and $(\partial_t z)_{\mathbf{0}}^k$ satisfy

$$z_m^{\mathbf{0}} = z_0^{\mathbf{0}} + \Delta x \sum_{n=1}^{s} \tilde{a}_{mn} (\partial_x z)_n^{\mathbf{0}}, \tag{96}$$

$$z_{\mathbf{0}}^k = z_{\mathbf{0}}^k + \Delta t \sum_{j=1}^{r} a_{kj} (\partial_t z)_{\mathbf{0}}^k, \tag{97}$$

respectively, and

$$\partial_t (\partial_x Z_{mk}) \approx \partial_{tx} z(c_m \Delta x, d_k \Delta t),$$

$$\partial_x (\partial_t Z_{mk}) \approx \partial_{xt} z(c_m \Delta x, d_k \Delta t).$$

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

$$\partial_t (\partial_x Z_{mk}) = \partial_x (\partial_t Z_{mk}). \tag{98}$$

In fact, (9), (92) and (96) imply that

$$Z_{mk} = z_{\mathbf{0}}^k + z_m^{\mathbf{0}} - z_0^{\mathbf{0}} + \Delta x \Delta t \sum_{j=1}^{r} \sum_{n=1}^{s} a_{kj} \tilde{a}_{mn} \partial_t (\partial_x Z_{nj}). \tag{99}$$

Similar, (7), (94) and (97) imply that

$$Z_{mk} = z_m^{\mathbf{0}} + z_{\mathbf{0}}^k - z_0^{\mathbf{0}} + \Delta x \Delta t \sum_{j=1}^{r} \sum_{n=1}^{s} a_{kj} \tilde{a}_{mn} \partial_x (\partial_t Z_{nj}). \tag{100}$$

From (99) and (100), we conclude that (98) holds for $m = 1, 2, \cdots, s$ and $k = 1, 2, \cdots, r$.

From the assumptions, we have

$$\begin{array}{l} \frac{1}{2}(z_{\mathbf{1}}^k)^T K^T (\partial_t z)_{\mathbf{1}}^k = \frac{1}{2}(z_{\mathbf{0}}^k)^T K^T (\partial_t z)_{\mathbf{0}}^k \\ + \frac{\Delta x}{2} \sum_{m=1}^{s} \tilde{b}_m (Z_{mk})^T K^T \partial_x (\partial_t Z_{mk}) + \frac{\Delta x}{2} \sum_{m=1}^{s} \tilde{b}_m \partial_x (Z_{mk})^T K^T (\partial_t Z_{mk}), \end{array} \tag{101}$$

therefore,

$$\frac{F(z_{\mathbf{1}}^k) - F(z_{\mathbf{0}}^k)}{\Delta x} = \frac{1}{2} \sum_{m=1}^{s} \tilde{b}_m (Z_{mk})^T K^T \partial_x (\partial_t Z_{mk}) + \frac{1}{2} \sum_{m=1}^{s} \tilde{b}_m \partial_x (Z_{mk})^T K^T (\partial_t Z_{mk}). \tag{102}$$

A similar (but little bit tedious) calculation leads to

$$\frac{E(z_m^{\mathbf{1}}) - E(z_m^{\mathbf{0}})}{\Delta t} = -\frac{1}{2} \sum_{k=1}^{r} b_k (Z_{mk})^T K^T \partial_t (\partial_x Z_{mk}) - \frac{1}{2} \sum_{k=1}^{r} b_k \partial_x (Z_{mk})^T K^T (\partial_t Z_{mk}). \tag{103}$$

This means that (90) holds. Analogously, we show that (91) holds. The proof is finished.

Remark 8 *The discrete conservation of energy and momentum for (27-35) can be discussed in a similar way, but with tedious calculation.*

5. Conclusion Theorem 1 tells us that concatenating two symplectic Runge-Kutta methods probably produce a multi-symplectic integrator with order that we need. Theorem 2 provides theoretically much more constructing ways of multi-symplectic integrators by using partitioned Runge-Kutta methods. For example, a multi-symplectic integrator of the wave equation can be produced by using the Lobatto IIIA-IIIB pair to discrete the equation both in time and in space directions.

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