Generating functions of multi-symplectic PRK methods via DW Hamilton-Jacobi equations *

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Abstract

In this paper we investigate Donder-Weyl (DW) Hamilton-Jacobi equations and establish the connection between DW Hamilton-Jacobi equations and multi-symplectic Hamiltonian systems. Based on the study of DW Hamilton-Jacobi equations, we present the generating functions for multi-symplectic partitioned Runge-Kutta (PRK) methods.

Keywords Multi-Symplectic Partitioned Runge-Kutta Methods, Generating Functions, DW Hamilton-Jacobi Equations.

1 Introduction

Hamilton-Jacobi theory was presented and developed by W. Hamilton in the 1820s for problems in wave optics and geometrical optics. Then the idea was extended to problems in dynamics in 1834, and in 1837 C.G.J. Jacobi applied the method to the general problems of classical variational calculus. One of most important results on Hamilton-Jacobi theory is Jacobi's theorem, which reduces solving Hamiltonian equations to finding a complete integral of first-order partial differential equations (PDEs), so called Hamilton-Jacobi equations. It is noticed, the solution of Hamilton-Jacobi equations, function S can be related to any symplectic map ([12]), therefore S gains a name — generating function. For any symplectic transformation, theoretically, it is possible to find the function S such that the transformation can be expressed with S. The explicit expression of generating functions for symplectic Runge-Kutta (RK) methods and symplectic partitioned Runge-Kutta (PRK) methods have been presented in [7]. However, the generating function is

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not unique. By changing coordinate variables, any symplectic transformation can be generated by various generating functions. This provides various ways for constructing symplectic numerical algorithms. Based on Hamilton-Jacobi theory, the symplectic numerical algorithms of higher order — generating function method is discussed by several authors via computing the approximate solution of Hamilton-Jacobi equations and taking the truncation of approximate solution. The systematical development of generating function method is due to [2] and its more applications are obtained in the numerical computation for source free systems ([14]) and Birkhoffian systems ([15]).

In recent years, researchers have paid much more attentions to geometric integrators for the system of differential equations. In the study of Hamiltonian PDEs, the presentation of multi-symplectic Hamiltonian formulation and multi-symplectic structure suggests a new way to compute Hamiltonian PDEs ([1, 8]). Compared with traditional approach, which regards Hamiltonian PDEs as the infinite dimensional Hamiltonian systems based on symplectic geometry, the multi-symplectic geometry theory treats Hamiltonian PDEs as the finite dimensional multi-symplectic Hamiltonian systems by the use of bundle coordinates. In multi-symplectic geometry theory, the base space consists of independent spatial variables and tempotal variables, the bundle space consists of dependent functions with fiber coordinates and all the first derivatives of dependent functions form the 1-jet bundle space. The new geometric integrators are called multi-symplectic numerical algorithms, which preserve the discrete multi-symplectic conservation laws. Under certain conditions on coefficients, it has been proved, the discretization for Hamiltonian PDEs by using RK methods and PRK methods both in temporal direction and spatial direction is multi-symplectic ([5, 11]), and the variational integrators based on discrete variational principles are multi-symplectic ([9]). For Hamiltonian PDEs, an analogue of Hamilton-Jacobi equations is called Donder-Weyl (DW) Hamilton-Jacobi equations ([6]). To our knowledge, up to now there have not been any references which made use of DW Hamilton-Jacobi equations to study multi-symplectic numerical algorithms and establish generating function theory. The purpose of this paper is to present the generating functions of multi-symplectic PRK methods by means of the investigation of DW Hamilton-Jacobi equations.

This paper is organized as follows. In the next section, we recall the Hamilton-Jacobi theory for Hamiltonian ODEs and study the generating functions of symplectic PRK methods. In the third section, we introduce and investigate DW Hamilton-Jacobi equations for Hamiltonian PDEs. The generating functions of multi-symplectic PRK methods for multi-symplectic Hamiltonian systems are presented in the fourth section. We conclude the paper in section 5.

2 Hamilton-Jacobi theory for Hamiltonian ODEs

In classical variational calculus and analytical mechanics, finding the extremals or integrating a Hamiltonian equation is reduced to the integration of a first-order partial differential equation, the so-called Hamilton-Jacobi equation. Despite the fact that the integration of partial differential equations is usually more difficult than solving ordinary differential equations, Hamilton-Jacobi theory has been proved to be a powerful tool not only in the study of problems of optics, mechanics and geometry, but also in the numerical computation. In this section, we give the simple description of Hamilton-Jacobi equations and recall some results on the generating functions for symplectic PRK methods. The readers can refer to [3] and references therein for the more details.

Hamilton-Jacobi equation is the following first-order PDE

$$\frac{\partial S}{\partial t} + H(\frac{\partial S}{\partial q}, q) = 0 \tag{1}$$

with function $H = H(p_1, \cdots, p_n, q_1, \cdots, q_n)$. Its solution $S(t, q)$ is called generating function.

To calculate the solution of Hamilton-Jacobi equation (1), we differentiate (1) w.r.t q and denote $p = \frac{\partial S}{\partial q}(t, q)$, then it leads to the following first-order quasi-linear PDE for p

$$\frac{\partial p}{\partial t} + (\frac{\partial p}{\partial q})^T H_p(p, q) = -H_q(p, q) \tag{2}$$

with $H_q = (H_{q_1}, \cdots H_{q_n})^T$, $H_p = (H_{p_1}, \cdots, H_{p_n})^T$. It is easy to know

$$\frac{dt}{ds} = 1, \qquad \frac{dq}{ds} = H_p \tag{3}$$

is the characteristic equation of (2). Along the characteristic line, (2) becomes

$$\frac{\partial p}{\partial t}\frac{dt}{ds} + (\frac{\partial p}{\partial q})^T \frac{dq}{ds} = \frac{dp}{ds}(t, q) = -H_q(p, q). \tag{4}$$

Combining (3) and (4), we conclude that Hamiltonian system is the characteristic equation of Hamilton-Jacobi equation. Finding the solution of Hamilton-Jacobi equations is related closely to solving the Hamiltonian systems.

Since the equivalence between Hamiltonian equations and Euler-Lagrange equations by Legendre transformation $p = L_{\dot{q}}$, the solution S of Hamilton-Jacobi equations is also related to Lagrangian function L. Using (1), we have

$$\frac{dS}{dt}(t, q) = \frac{\partial S}{\partial t} + (\frac{\partial S}{\partial q})^T \dot{q} = -H(\frac{\partial S}{\partial q}, q) + (\frac{\partial S}{\partial q})^T \dot{q} = L(q, \dot{q}) \tag{5}$$

with Lagrangian function $L = p\dot{q} - H(p, q)$. Taking the integral of (5), we obtain

$$S(t, q) = \int_0^t L(q(\tau), \dot{q}(\tau)) d\tau, \tag{6}$$

which is the action functional for Lagrangian function L. For the solution $q(t)$ of Euler-Lagrange equation $\frac{d}{dt}L_{\dot{q}} = L_q$ with fixed boundary value $q(0) = q_0, q(t) = q_1$, S is also taken as the function of q_0, q_1 denoted by S^1

$$S^1(q_0, q_1) = \int_0^t L(q(\tau), \dot{q}(\tau)) d\tau. \tag{7}$$

Denote $p_1 = p(t) = L_{\dot{q}}(q(t), \dot{q}(t)), p_0 = p(0) = L_{\dot{q}}(q(0), \dot{q}(0))$. Differentiating (7) w.r.t. q_1, q_0, it is easy to derive

$$\frac{\partial S^1}{\partial q_1} = p_1, \qquad \frac{\partial S^1}{\partial q_0} = -p_0. \tag{8}$$

And the relation

$$dp_1 \wedge dq_1 - dp_0 \wedge dq_0 = d(p_1^T dq_1 - p_0^T dq_0) = d((\frac{\partial S^1}{\partial q_1})^T dq_1 + (\frac{\partial S^1}{\partial q_0})^T dq_0) = d^2 S^1 = 0$$

shows that mapping $(q_0, p_0) \longrightarrow (q_1, p_1)$ defined by (8) is symplectic. The function $S^1(q_0, q_1)$ related to the symplectic map is called the generating function of first kind. By the different choice of independent coordinate variables, this symplectic map can be reconstructed by different relations ([3]).

What follows, we turn our attention to the relation between symplectic PRK methods and Hamilton-Jacobi equations. Consider the following discrete version of (6)

$$\mathbb{S}^1(q_k, q_{k+1}, \Delta t) = \Delta t \sum_{i=1}^{s} b_i L(Q_i^k, \dot{Q}_i^k) \tag{9}$$

presented in [9], where

$$q_{k+1} = q_k + \Delta t \sum_{i=1}^{s} b_i \dot{Q}_i^k, \tag{10}$$

$$Q_i^k = q_k + \Delta t \sum_{j=1}^{s} a_{ij} \dot{Q}_j^k. \tag{11}$$

Based on discrete Euler-Lagrange equation

$$0 = D_1 \mathbb{S}^1(q_k, q_{k+1}, \Delta t) + D_2 \mathbb{S}^1(q_{k-1}, q_k, \Delta t),$$

we obtain

$$\begin{aligned} 0 &= \Delta t \sum_{i=1}^{s} b_i((\frac{\partial Q_i^k}{\partial q_k})^T L_q^k + (\frac{\partial Q_i^{k-1}}{\partial q_k})^T L_q^{k-1} + (\frac{\partial \dot{Q}_i^k}{\partial q_k})^T L_{\dot{q}}^k + (\frac{\partial \dot{Q}_i^{k-1}}{\partial q_k})^T L_{\dot{q}}^{k-1}) \\ &= \Delta t^2 \sum_{i,j=1}^{s} (-b_j \hat{a}_{ji})(\frac{\partial \dot{Q}_j^k}{\partial q_k})^T L_q^k + \Delta t^2 \sum_{i,j=1}^{s} b_i a_{ij}(\frac{\partial \dot{Q}_j^{k-1}}{\partial q_k})^T L_q^{k-1} + \Delta t \sum_{i=1}^{s} b_i((\frac{\partial \dot{Q}_i^k}{\partial q_k})^T L_{\dot{q}}^k + (\frac{\partial \dot{Q}_i^{k-1}}{\partial q_k})^T L_{\dot{q}}^{k-1}) \end{aligned}$$

with $L^k = L(Q_i^k, \dot{Q}_i^k), \hat{a}_{ji} = b_i - \frac{b_i a_{ij}}{b_j}$. In the above equality, relations $-I = \Delta t \sum\limits_{i=1}^{s} b_i \frac{\partial \dot{Q}_i^k}{\partial q_k}$, $\frac{\partial Q_i^k}{\partial q_k} = I + \Delta t \sum\limits_{j=1}^{s} a_{ij} \frac{\partial \dot{Q}_j^k}{\partial q_k}$, $\frac{\partial Q_i^{k-1}}{\partial q_k} = \Delta t \sum\limits_{j=1}^{s} a_{ij} \frac{\partial \dot{Q}_j^{k-1}}{\partial q_k}$ have been applied. Denote $\bar{a}_{ik} = \sum\limits_{j=1}^{s} b_j \hat{a}_{ji} (\frac{\partial \dot{Q}_j^k}{\partial q_k})^T, \bar{b}_{ik} =$

$-\sum_{j=1}^{s} b_i a_{ij} (\frac{\partial \dot{Q}_j^{k-1}}{\partial q_k})^T, \bar{c}_{ik} = b_i (\frac{\partial \dot{Q}_i^k}{\partial q_k})^T, \bar{d}_{ik} = b_i (\frac{\partial \dot{Q}_i^{k-1}}{\partial q_k})^T$, it follows from the above equality that

$$\begin{aligned}
&\Delta t \sum_{i=1}^{s} \bar{a}_{ik} L_q(Q_i^k, \dot{Q}_i^k) + \Delta t \sum_{i=1}^{s} \bar{b}_{ik} L_q(Q_i^{k-1}, \dot{Q}_i^{k-1}) \\
&= \sum_{i=1}^{s} \bar{c}_{ik} L_{\dot{q}}(Q_i^k, \dot{Q}_i^k) + \sum_{i=1}^{s} \bar{d}_{ik} L_{\dot{q}}(Q_i^{k-1}, \dot{Q}_i^{k-1})
\end{aligned}$$

with $\Delta t \sum_{i=1}^{s} (\bar{a}_{ik} + \bar{b}_{ik}) = -I - \Delta t \sum_{i,j=1}^{s} b_i a_{ij} (\frac{\partial \dot{Q}_j^{k-1}}{\partial q_k} + \frac{\partial \dot{Q}_j^k}{\partial q_k})$, $\sum_{i=1}^{s} \bar{c}_{ik} = -I/\Delta t$, $\sum_{i=1}^{s} \bar{d}_{ik} = I/\Delta t$, which is the discrete version of Euler-Lagrange equation.

(9) is related to a symplectic PRK method ([3])

$$p_{k+1} = p_k - \Delta t \sum_{i=1}^{s} b_i \dot{P}_i^k, \qquad P_i^k = p_k - \Delta t \sum_{j=1}^{s} \hat{a}_{ij} \dot{P}_j^k, \tag{12}$$

$$q_{k+1} = q_k + \Delta t \sum_{i=1}^{s} b_i \dot{Q}_i^k, \qquad Q_i^k = q_k + \Delta t \sum_{j=1}^{s} a_{ij} \dot{Q}_j^k, \tag{13}$$

$$\dot{P}_i^k = H_q(P_i^k, Q_i^k), \qquad \dot{Q}_i^k = H_p(P_i^k, Q_i^k) \tag{14}$$

by the relations

$$p_{k+1} = \frac{\partial \mathbb{S}^1}{\partial q_{k+1}} \qquad \text{and} \qquad p_k = -\frac{\partial \mathbb{S}^1}{\partial q_k},$$

where the symplectic conditions $b_i b_j - b_i a_{ij} - b_j \hat{a}_{ji} = 0$, $i, j = 1, \cdots, s$ are satisfied.

In fact, with $\mathbb{S}^1$ in the form of (9), it is easy to know

$$p_{k+1} = \frac{\partial \mathbb{S}^1}{\partial q_{k+1}} = \Delta t \sum_{i=1}^{s} b_i ((\frac{\partial Q_i^k}{\partial q_{k+1}})^T L_q^k + (\frac{\partial \dot{Q}_i^k}{\partial q_{k+1}})^T L_{\dot{q}}^k), \tag{15}$$

$$-p_k = \frac{\partial \mathbb{S}^1}{\partial q_k} = \Delta t \sum_{i=1}^{s} b_i ((\frac{\partial Q_i^k}{\partial q_k})^T L_q^k + (\frac{\partial \dot{Q}_i^k}{\partial q_k})^T L_{\dot{q}}^k). \tag{16}$$

From (13), it follows that

$$0 = I - \Delta t \sum_{i=1}^{s} b_i \frac{\partial \dot{Q}_i^k}{\partial q_{k+1}}, \qquad 0 = I + \Delta t \sum_{i=1}^{s} b_i \frac{\partial \dot{Q}_i^k}{\partial q_k}, \tag{17}$$

$$\frac{\partial Q_i^k}{\partial q_{k+1}} = \Delta t \sum_{j=1}^{s} a_{ij} \frac{\partial \dot{Q}_j^k}{\partial q_{k+1}}, \qquad \frac{\partial Q_i^k}{\partial q_k} = I + \Delta t \sum_{j=1}^{s} a_{ij} \frac{\partial \dot{Q}_j^k}{\partial q_k}. \tag{18}$$

Multiplying (15) and (16) by $\Delta t \sum_{i=1}^{s} b_i \frac{\partial \dot{Q}_i^k}{\partial q_{k+1}} = I$ and $-\Delta t \sum_{i=1}^{s} b_i \frac{\partial \dot{Q}_i^k}{\partial q_k} = I$ respectively, it reads

$$\Delta t \sum_{i=1}^{s} b_i (\frac{\partial \dot{Q}_i^k}{\partial q_{k+1}})^T p_{k+1} = \Delta t^2 \sum_{i,j=1}^{s} b_j a_{ji} (\frac{\partial \dot{Q}_i^k}{\partial q_{k+1}})^T L_q(Q_j^k, \dot{Q}_j^k) + \Delta t \sum_{i=1}^{s} b_i (\frac{\partial \dot{Q}_i^k}{\partial q_{k+1}})^T L_{\dot{q}}(Q_i^k, \dot{Q}_i^k),$$

$$\Delta t \sum_{i=1}^{s} b_i (\frac{\partial \dot{Q}_i^k}{\partial q_k})^T p_k = -\Delta t^2 \sum_{i=1}^{s} (b_i b_j - b_j a_{ji}) (\frac{\partial \dot{Q}_i^k}{\partial q_k})^T L_q(Q_j^k, \dot{Q}_j^k) + \Delta t \sum_{i=1}^{s} b_i (\frac{\partial \dot{Q}_i^k}{\partial q_k})^T L_{\dot{q}}(Q_i^k, \dot{Q}_i^k).$$

When $b_i \neq 0$, which provides

$$p_{k+1} = \Delta t \sum_{j=1}^{s} \frac{b_j a_{ji}}{b_i} L_q(Q_j^k, \dot{Q}_j^k) + L_{\dot{q}}(Q_i^k, \dot{Q}_i^k), \tag{19}$$

$$p_k = -\Delta t \sum_{j=1}^{s} \frac{b_i b_j - b_j a_{ji}}{b_i} L_q(Q_j^k, \dot{Q}_j^k) + L_{\dot{q}}(Q_i^k, \dot{Q}_i^k). \tag{20}$$

Substituting (19) into (20) leads to

$$p_k = -\Delta t \sum_{j=1}^{s} b_j L_q(Q_j^k, \dot{Q}_j^k) + p_{k+1},$$

$$L_{\dot{q}}(Q_i^k, \dot{Q}_i^k) = p_k + \Delta t \sum_{j=1}^{s} \hat{a}_{ij} L_q(Q_j^k, \dot{Q}_j^k)$$

with $\hat{a}_{ij} = b_j - \frac{b_j a_{ji}}{b_i}$. Let $P_i^k = L_{\dot{q}}(Q_i^k, \dot{Q}_i^k), \dot{P}_i^k = L_q(Q_i^k, \dot{Q}_i^k)$, $H(P_i^k, Q_i^k) = P_i^k \dot{Q}_i^k - L(Q_i^k, \dot{Q}_i^k)$, then

$$H_p(P_i^k, Q_i^k) = \dot{Q}_i^k, \qquad H_q(P_i^k, Q_i^k) = -\dot{P}_i^k.$$

PRK method (12)-(14) can be reformulated with

$$\mathbb{S}^2(p_{k+1}, q_k, \Delta t) = \Delta t \sum_{i=1}^{s} b_i H(P_i^k, Q_i^k) - \Delta t^2 \sum_{i,j=1}^{s} H_q^T(P_i^k, Q_i^k) H_p(P_j^k, Q_j^k)$$

by the relations ([3])

$$q_{k+1} - q_k = \frac{\partial \mathbb{S}^2}{\partial p_{k+1}}, \qquad p_{k+1} - p_k = -\frac{\partial \mathbb{S}^2}{\partial q_k}.$$

Remark 2.1. The difference between $\mathbb{S}^1$ and $\mathbb{S}^2$ is

$$p_{k+1}^T (q_{k+1} - q_k) - \mathbb{S}^2(p_{k+1}, q_k, \Delta t) = \mathbb{S}^1(q_k, q_{k+1}, \Delta t).$$

Remark 2.2. The generating function

$$\mathbb{S}^3(\frac{p_{k+1} + p_k}{2}, \frac{q_{k+1} + q_k}{2}, \Delta t) = \Delta t \sum_{i=1}^{s} b_i H(P_i^k, Q_i^k) + \frac{\Delta t^2}{2} \sum_{i,j=1}^{s} (b_j \hat{a}_{ji} - b_i a_{ij}) {H_q}^T(P_i^k, Q_i^k) H_p(P_j^k, Q_j^k)$$

can generate PRK method (12)-(14) with the relations

$$p_{k+1} - p_k = -\frac{\partial \mathbb{S}^3}{\partial q}(\frac{p_{k+1} + p_k}{2}, \frac{q_{k+1} + q_k}{2}),$$

$$q_{k+1} - q_k = \frac{\partial \mathbb{S}^3}{\partial p}(\frac{p_{k+1} + p_k}{2}, \frac{q_{k+1} + q_k}{2}).$$

Introducing new variables $u = \frac{p_{k+1}+p_k}{2}, v = \frac{q_{k+1}+q_k}{2}$, and differentiating (12) and (13) w.r.t v leads to

$$\frac{\partial P_i^k}{\partial v} = \frac{\partial p_k}{\partial v} - \Delta t \sum_{j=1}^{s} \hat{a}_{ij}(H_{qp}(P_j^k, Q_j^k)\frac{\partial P_j^k}{\partial v} + H_{qq}(P_j^k, Q_j^k)\frac{\partial Q_j^k}{\partial v}), \tag{21}$$

$$\frac{\partial Q_i^k}{\partial v} = \frac{\partial q_k}{\partial v} + \Delta t \sum_{j=1}^{s} a_{ij}(H_{pp}(P_j^k, Q_j^k)\frac{\partial P_j^k}{\partial v} + H_{pq}(P_j^k, Q_j^k)\frac{\partial Q_j^k}{\partial v}), \tag{22}$$

$$\frac{\partial p_{k+1}}{\partial v} = \frac{\partial p_k}{\partial v} - \Delta t \sum_{i=1}^{s} b_i(H_{qp}(P_i^k, Q_i^k)\frac{\partial P_i^k}{\partial v} + H_{qq}(P_i^k, Q_i^k)\frac{\partial Q_i^k}{\partial v}), \tag{23}$$

$$\frac{\partial q_{k+1}}{\partial v} = \frac{\partial q_k}{\partial v} + \Delta t \sum_{i=1}^{s} b_i(H_{pp}(P_i^k, Q_i^k)\frac{\partial P_i^k}{\partial v} + H_{pq}(P_i^k, Q_i^k)\frac{\partial Q_i^k}{\partial v}). \tag{24}$$

Calculating the derivative of $\mathbb{S}^3$

$$\begin{aligned}
\frac{\partial \mathbb{S}^3}{\partial v} &= \Delta t \sum_{i=1}^{s} b_i((\frac{\partial P_i^k}{\partial v})^T H_p^i + (\frac{\partial Q_i^k}{\partial v})^T H_q^i) + \frac{\Delta t^2}{2}\sum_{i,j=1}^{s}(b_j \hat{a}_{ji} - b_i a_{ij})((((\frac{\partial P_j^k}{\partial v})^T (H_{pp}^j)^T \\
&+ (\frac{\partial Q_j^k}{\partial v})^T (H_{pq}^j)^T) H_q^i + ((\frac{\partial P_i^k}{\partial v})^T (H_{qp}^i)^T + (\frac{\partial Q_i^k}{\partial v})^T (H_{qq}^i)^T) H_p^j) \\
&= \Delta t^2 \sum_{i,j=1}^{s} (-\frac{b_i b_j}{2} + \frac{b_j \hat{a}_{ji} - b_i a_{ij}}{2} + b_i a_{ij})((\frac{\partial P_j^k}{\partial v})^T (H_{pp}^j)^T + (\frac{\partial Q_j^k}{\partial v})^T (H_{pq}^j)^T) H_q^i \\
&+ \Delta t^2 \sum_{i,j=1}^{s} (\frac{b_i b_j}{2} + \frac{-b_j a_{ji} + b_i \hat{a}_{ij}}{2} - b_i \hat{a}_{ij})((\frac{\partial P_j^k}{\partial v})^T (H_{qp}^j)^T + (\frac{\partial Q_j^k}{\partial v})^T (H_{qq}^j)^T) H_p^i + \Delta t \sum_{i=1}^{s} b_i H_q^i
\end{aligned}$$

with $H_q^i = H_q(P_i^k, Q_i^k), H_{qp}^i = H_{qp}(P_i^k, Q_i^k)$. Here, (21)-(24) and $\frac{1}{2}(\frac{\partial p_{k+1}}{\partial v} + \frac{\partial p_k}{\partial v}) = 0$, $\frac{1}{2}(\frac{\partial q_{k+1}}{\partial v} + \frac{\partial q_k}{\partial v}) = 1$ are used. Under condition $b_i b_j - b_i a_{ij} - b_j \hat{a}_{ji} = 0, i, j = 1, \cdots, s$, it yields

$$\frac{\partial \mathbb{S}^3}{\partial v} = \Delta t \sum_{i=1}^{s} b_i H_q(P_i^k, Q_i^k).$$

Similarly,

$$\begin{aligned}
\frac{\partial \mathbb{S}^3}{\partial u} &= \Delta t \sum_{i=1}^{s} b_i((\frac{\partial P_i^k}{\partial u})^T H_p^i + (\frac{\partial Q_i^k}{\partial u})^T H_q^i) + \frac{\Delta t^2}{2}\sum_{i,j=1}^{s}(b_j \hat{a}_{ji} - b_i a_{ij})((((\frac{\partial P_j^k}{\partial u})^T (H_{pp}^j)^T \\
&+ (\frac{\partial Q_j^k}{\partial u})^T (H_{pq}^j)^T) H_q^i + ((\frac{\partial P_i^k}{\partial u})^T (H_{qp}^i)^T + (\frac{\partial Q_i^k}{\partial u})^T (H_{qq}^i)^T) H_p^j) \\
&= \Delta t \sum_{i=1}^{s} b_i H_p(P_i^k, Q_i^k).
\end{aligned}$$

Remark 2.3. PRK method (12) -(14) can be expressed by the relations

$$p_{k+1} - p_k = -\frac{\partial \mathbb{S}^2}{\partial q_{k+1}}(p_k, q_{k+1}), \qquad q_{k+1} - q_k = \frac{\partial \mathbb{S}^2}{\partial p_k}(p_k, q_{k+1})$$

with $\mathbb{S}^2$ in the following formulation

$$\mathbb{S}^2(p_k, q_{k+1}, \Delta t) = \Delta t \sum_{i=1}^{s} b_i H(P_i^k, Q_i^k) + \Delta t^2 \sum_{i,j=1}^{s} b_j \hat{a}_{ji} H_q^T(P_i^k, Q_i^k) H_p(P_j^k, Q_j^k).$$

Obviously,

$$\begin{aligned}
\frac{\partial \mathbb{S}^2}{\partial p_k} &= \Delta t \sum_{i=1}^{s} b_i((\frac{\partial P_i^k}{\partial p_k})^T H_p^i + (\frac{\partial Q_i^k}{\partial p_k})^T H_q^i) + \Delta t^2 \sum_{i,j=1}^{s} b_j \hat{a}_{ji}(((\frac{\partial P_j^k}{\partial p_k})^T (H_{pp}^j)^T + (\frac{\partial Q_j^k}{\partial p_k})^T (H_{pq}^j)^T) H_q^i \\
&\quad + ((\frac{\partial P_i^k}{\partial p_k})^T (H_{qp}^i)^T + (\frac{\partial Q_i^k}{\partial p_k})^T (H_{qq}^i)^T) H_p^j) \\
&= \Delta t \sum_{i=1}^{s} b_i H_p(P_i^k, Q_i^k),
\end{aligned}$$

$$\begin{aligned}
\frac{\partial \mathbb{S}^2}{\partial q_{k+1}} &= \Delta t \sum_{i=1}^{s} b_i((\frac{\partial P_i^k}{\partial q_{k+1}})^T H_p^i + (\frac{\partial Q_i^k}{\partial q_{k+1}})^T H_q^i) + \Delta t^2 \sum_{i,j=1}^{s} b_j \hat{a}_{ji}((\frac{\partial P_j^k}{\partial q_{k+1}})^T (H_{pp}^j)^T + (\frac{\partial Q_j^k}{\partial q_{k+1}})^T (H_{pq}^j)^T) H_q^i \\
&\quad + ((\frac{\partial P_i^k}{\partial q_{k+1}})^T (H_{qp}^i)^T + (\frac{\partial Q_i^k}{\partial q_{k+1}})^T (H_{qq}^i)^T) H_p^j) \\
&= \Delta t \sum_{i=1}^{s} b_i H_q(P_i^k, Q_i^k).
\end{aligned}$$

3 DW Hamilton-Jacobi equation

Similar to Hamilton-Jacobi theory in Hamiltonian ODEs, for Hamiltonian PDEs the DW Hamilton-Jacobi equation plays the important role. In this section, we introduce the equation and investigate its characteristics.

Consider the following first order PDE

$$\frac{\partial S^t}{\partial t} + \sum_{i=1}^{m} \frac{\partial S^{x_i}}{\partial x_i} + H(u, \frac{\partial S^t}{\partial u}, \frac{\partial S^x}{\partial u}) = 0, \tag{25}$$

where S^t is the function of t and u, S^{x_i} is the function of x_i and u, $u = (u^1, \cdots, u^n), x = (x_1, \cdots, x_m)$. It is the DW Hamilton-Jacobi equation and is related to Lagrangian function and Hamiltonian function with following theorems.

Theorem 3.1. *Multi-symplectic Hamiltonian system*

$$\begin{aligned}
&u_t^j = H_{p_j^t}, \qquad u_{x_i}^j = H_{p_j^{x_i}}, \\
&\frac{\partial p_j^t}{\partial t} + \frac{\partial p_j^{x_i}}{\partial x_i} = -H_{u^j}, \quad i = 1, \cdots, m, j = 1, \cdots, n
\end{aligned} \tag{26}$$

is the characteristic equation of DW Hamilton-Jacobi equation (25).

Proof. Differentiating (25) w.r.t u, we have

$$\frac{\partial^2 S^t}{\partial t \partial u^k} + \sum_{i=1}^{m} \frac{\partial^2 S^{x_i}}{\partial x_i \partial u^k} + H_{u^k} + \sum_{j=1}^{n} \frac{\partial^2 S^t}{\partial u^k \partial u^j} H_{\frac{\partial S^t}{\partial u^j}} + \sum_{i=1}^{m}\sum_{j=1}^{n} \frac{\partial^2 S^{x_i}}{\partial u^k \partial u^j} H_{\frac{\partial S^{x_i}}{\partial u^j}} = 0, k = 1, \cdots, n. \quad (27)$$

Let $p_k^t = \frac{\partial S^t}{\partial u^k}, p_k^{x_i} = \frac{\partial S^{x_i}}{\partial u^k}$. Noticing that p_k^t depends only on t and u, $p_j^{x_i}$ depends only on x_i and u, (27) can be rewritten as the following first order PDEs for $p = (p^t, p^x)^T$

$$\frac{\partial p_k^t}{\partial t} + \sum_{i=1}^{m} \frac{\partial p_k^{x_i}}{\partial x_i} + H_{u^k} + \sum_{j=1}^{n} H_{p_j^t} \frac{\partial p_k^t}{\partial u^j} + \sum_{i=1}^{m}\sum_{j=1}^{n} H_{p_i^{x_i}} \frac{\partial p_k^{x_i}}{\partial u^j} = 0, \quad (28)$$

$$\frac{\partial p_k^t}{\partial x_i} + \frac{\partial p_k^{x_i}}{\partial t} + \sum_{j \neq i} \frac{\partial p_k^{x_i}}{\partial x_j} = 0, \qquad i = 1, \cdots, m, k = 1, \cdots, n \quad (29)$$

with $p^t = (p_1^t, \cdots, p_n^t)^T$, $p^x = (p_1^{x_1} \cdots, p_n^{x_1}, \cdots, p_1^{x_m}, \cdots, p_n^{x_m})^T$. The characteristic equation of first order PDEs (28) and (29)

$$\det \begin{pmatrix} (\gamma_1 + \sum_{j=1}^{n} H_{p_j^t}\gamma_3^{(j)}) I_{n\times n} & (\gamma_2^{(1)} + \sum_{j=1}^{n} H_{p_j^{x_1}}\gamma_3^{(j)}) I_{n\times n} & \cdots & (\gamma_2^{(m)} + \sum_{j=1}^{n} H_{p_j^{x_m}}\gamma_3^{(j)}) I_{n\times n} \\ \gamma_2^{(1)} I_{n\times n} & (\gamma_1 + \sum_{i\neq 1}\gamma_2^{(i)}) I_{n\times n} & & \mathbf{0} \\ \cdots & & & \\ & \mathbf{0} & \ddots & \\ \gamma_2^{(m)} I_{n\times n} & & & (\gamma_1 + \sum_{i \neq m}\gamma_2^{(i)}) I_{n\times n} \end{pmatrix} = 0$$

is a homogenenous polynomial of degree $n(m+1)$ in variables $\gamma_1, \gamma_2^{(i)}, \gamma_3^{(j)}, i = 1, \cdots, m, j = 1, \cdots, n$. $(0, 1, \cdots, -1/H_{p_j^{x_i}}, \cdots)$ and $(1, 0, \cdots, -1/H_{p_j^t}, \cdots)$, $i = 1, \cdots, m$, $j = 1, \cdots, n$ are its solutions.

Along the characteristic lines

$$\frac{du^j}{H_{p_j^t}} = \frac{dt}{1}, \qquad \frac{du^j}{H_{p_j^{x_i}}} = \frac{dx_i}{1}, \quad i = 1, \cdots, m, j = 1, \cdots, n, \quad (30)$$

(28) gives us

$$H_{u^k} + \frac{\partial p_k^t}{\partial t} + \sum_{i=1}^{m} \frac{\partial p_k^{x_i}}{\partial x_i} + \sum_{j=1}^{n} u_t^j \frac{\partial p_k^t}{\partial u^j} + \sum_{i=1}^{m}\sum_{j=1}^{n} u_{x_i}^j \frac{\partial p_k^{x_i}}{\partial u^j} = 0.$$

It implies that

$$D_t p_k^t(t, u(x,t)) + \sum_{i=1}^{m} D_{x_i} p_k^{x_i}(x_i, u(x,t)) = -H_{u^k}(u, p^t, p^x), k = 1, \cdots, n, \quad (31)$$

where D_t denotes the total derivative, $D_t p_k^t(t, u(x,t)) = \frac{\partial p_k^t}{\partial t} + \sum_{j=1}^{n} \frac{\partial u^j}{\partial t}\frac{\partial p_k^t}{\partial u^j}$. Regarding p_j^t and $p_j^{x_i}$ as the function of x, t, multi-symplectic Hamiltonian system (26) is the combination of (30) and (31). The proof is finished. □

Theorem 3.2. *DW Hamilton-Jacobi equation (25) is equivalent to the action functional of Lagrangian function L by transformations*

$$p_j^t = \frac{\partial S^t}{\partial u^j}, \quad p_j^{x_i} = \frac{\partial S^{x_i}}{\partial u^j}, \quad i = 1, \cdots, m, j = 1, \cdots, n. \tag{32}$$

Proof. Integrating DW Hamilton-Jacobi equation (25) over region $\Omega \in \mathbf{R}^{m+1}$, we derive

$$\int_\Omega \frac{\partial S^t}{\partial t} dxdt + \sum_{i=1}^m \int_\Omega \frac{\partial S^{x_i}}{\partial x_i} dxdt = -\int_\Omega H(u, \frac{\partial S^t}{\partial u}, \frac{\partial S^x}{\partial u}) dxdt.$$

Under transformations (32), we obtain

$$\begin{aligned}
\int_\Omega D_t S^t dxdt + \sum_{i=1}^m \int_\Omega D_{x_i} S^{x_i} dxdt &= \int_\Omega (\frac{\partial S^t}{\partial t} + (\frac{\partial S^t}{\partial u})^T u_t + \sum_{i=1}^m \frac{\partial S^{x_i}}{\partial x_i} + \sum_{i=1}^m \sum_{j=1}^n \frac{\partial S^{x_i}}{\partial u^j} u_{x_i}^j) dxdt \\
&= \int_\Omega ((\frac{\partial S^t}{\partial u})^T u_t + \sum_{i=1}^m \sum_{j=1}^n \frac{\partial S^{x_i}}{\partial u^j} u_{x_i}^j - H(u, \frac{\partial S^t}{\partial u}, \frac{\partial S^x}{\partial u})) dxdt \\
&= \int_\Omega ((p^t)^T u_t + \sum_{i=1}^m \sum_{j=1}^n p_j^{x_i} u_{x_i}^j - H(u, p^t, p^x)) dxdt \\
&= \int_\Omega L(u, u_t, u_x) dxdt
\end{aligned}$$

with $L(u, u_t, u_x) = {p^t}^T u_t + \sum_{i=1}^m \sum_{j=1}^n p_j^{x_i} u_{x_i}^j - H(u, p^t, p^x)$, $D_t, D_{x_i}, i = 1, \cdots, m$ being the total derivatives. This implies that

$$(-1)^m \int_{\partial\Omega} S^t(t, u) dx + \sum_{i=1}^m (-1)^{i-1} \int_{\partial\Omega} S^{x_i}(x, u) d\hat{x}_i dt = \int_\Omega L(u, u_t, u_x) dxdt,$$

where $\partial\Omega$ is the boundary of Ω, $dx = dx_1 \cdots dx_m$, $d\hat{x_i} = dx_1 \cdots dx_{i-1} dx_{i+1} \cdots dx_m, i = 1, 2 \cdots, m$. This completes the proof. □

Based on Euler-Lagrange equations, the general principle relating variational symmetry groups to conservations laws is first revealed by Noether Theorem in very general form ([8, 10]). For the study of conservation laws in Hamiltonian systems, it is valuable to notice the role played by the Hamilton-Jacobi equations. For convenience, we provide the definitions of conservation laws and generalized vector fields ([10]) as follows.

Definition 3.3. For a system of differential equations $\Delta(t, x, j^n(u)) = 0$, if

$$D_t F^t + \sum_{i=1}^m D_{x_i} E^{x_i} = 0$$

vanishes for all solutions of the given system, then it is called a conservation law of the system. Here, D_t, D_{x_i} are the total derivatives, $j^n(u) = (u^1, \cdots, u^n, \frac{\partial u^1}{\partial x_i}, \cdots, \frac{\partial u^n}{\partial x_i}, \cdots, \frac{\partial^n u^1}{\partial x_i^n}, \cdots, \frac{\partial^n u^n}{\partial x_i^n})$, F^t, $E_i^{x_i}$ are the functions of $t, x, j^n(u)$, $i = 0, \cdots, m$.

Definition 3.4. A generalized vector field is expressed formally in the form

$$V = \xi(t,x,u,u_t,u_x,\cdots)\frac{\partial}{\partial t} + \sum_{i=1}^{m} \eta_i(t,x,u,u_t,u_x,\cdots)\frac{\partial}{\partial x_i} + \sum_{j=1}^{n} \varphi_j(t,x,u,u_t,u_x,\cdots)\frac{\partial}{\partial u^j}.$$

Definition 3.5. A generalized vector field V is a generalized infinitesimal symmetry of a system of n-order differential equations

$$\Delta[u] = \Delta(t,x,j^n(u))$$

if and only if

$$j(V)(\Delta) = 0$$

for every smooth function $u(t,x)$.

In the above definition, $j(V)$ denotes the infinite prolongation of vector field V, and is calculated by the prolongation formula

$$j(V) = V + \sum_{j=1}^{n}\sum_{J}(D_J(\varphi_j - \xi u_t^j - \sum_{i=1}^{m}\eta_i u_{x_i}^j) + \xi u_{J,t}^j + \sum_{i=1}^{m}\eta_i u_{J,x_i}^j)\frac{\partial}{\partial u_J^j}$$

with $u_{x_i}^j = \frac{\partial u^j}{\partial x_i}, u_{J,x_i}^j = \frac{\partial u_{x_i}^j}{\partial x_J}$, $J = j_1\cdots j_k, k \geq 1$ and $D_J = D_{j_1}\cdots D_{j_k}$ is the J-th total derivative.

The relation between conservation laws of multi-symplectic Hamiltonian systems and generalized symmetries of DW Hamilton-Jacobi equations is revealed in the following theorem.

Theorem 3.6. *$V = A^t(t,x,u,\frac{\partial S^t}{\partial u})\frac{\partial}{\partial S^t} + \sum_{i=1}^{m} A^{x_i}(t,x,u,\frac{\partial S^x}{\partial u})\frac{\partial}{\partial S^{x_i}}$ is a generalized symmetry of DW Hamilton-Jacobi equation (25) if and only if*

$$D_t A^t + \sum_{i=1}^{m} D_{x_i} A^{x_i} = 0$$

is a conservation law of multi-symplectic Hamiltonian system (25).

Proof Let $V = A^t\frac{\partial}{\partial S^t} + \sum_{i=1}^{m} A^{x_i}\frac{\partial}{\partial S^{x_i}}$ is the generalized symmetry of DW Hamilton-Jacobi system

$$\Delta(u,\frac{\partial S^t}{\partial t},\frac{\partial S^x}{\partial x},\frac{\partial S^t}{\partial u},\frac{\partial S^x}{\partial u}) = \frac{\partial S^t}{\partial t} + \sum_{i=1}^{m}\frac{\partial S^{x_i}}{\partial x_i} + H(u,\frac{\partial S^t}{\partial u},\frac{\partial S^x}{\partial u}),$$

then according to Definition 3.5, we have

$$0 = j(V)(\Delta) = j^1(V)(\Delta) = D_t A^t + \sum_{i=1}^{m} D_{x_i} A^{x_i} + \sum_{j=1}^{n} D_{u^j} A^t \frac{\partial H}{\partial \frac{\partial S^t}{\partial u^j}} + \sum_{i=1}^{m}\sum_{j=1}^{n} D_{u^j} A^{x_i}\frac{\partial H}{\partial \frac{\partial S^{x_i}}{\partial u^j}}$$

with $j^1(V) = V + D_t A^t \frac{\partial}{\partial \frac{\partial S^t}{\partial t}} + \sum_{j=1}^{n} D_{u^j} A^t \frac{\partial}{\partial \frac{\partial S^t}{\partial u^j}} + \sum_{i=1}^{m} D_{x_i} A^{x_i} \frac{\partial}{\partial \frac{\partial S^{x_i}}{\partial x_i}} + \sum_{i=1}^{m}\sum_{j=1}^{n} D_{u^j} A^{x_i} \frac{\partial}{\partial \frac{\partial S^{x_i}}{\partial u^j}}$ and total derivative $D_t A^t = \frac{\partial A^t}{\partial t} + \sum_{j=1}^{n} \frac{\partial A^t}{\partial \frac{\partial S^t}{\partial u^j}} \frac{\partial^2 S^t}{\partial u^j \partial t}$. From the above equality, we derive

$$\begin{aligned}0 = &\frac{\partial A^t}{\partial t} + \sum_{j=1}^{n} \frac{\partial A^t}{\partial u^j} \frac{\partial H}{\partial \frac{\partial S^t}{\partial u^j}} + \sum_{j=1}^{n} \frac{\partial A^t}{\partial \frac{\partial S^t}{\partial u^j}} (\frac{\partial^2 S^t}{\partial u^j \partial t} + \sum_{i=1}^{n} \frac{\partial^2 S^t}{\partial u^i \partial u^j} \frac{\partial H}{\partial \frac{\partial S^t}{\partial u^i}}) \\ &+ \sum_{i=1}^{m} \frac{\partial A^{x_i}}{\partial x_i} + \sum_{i=1}^{m}\sum_{j=1}^{n} \frac{\partial A^{x_i}}{\partial u^j} \frac{\partial H}{\partial \frac{\partial S^{x_i}}{\partial u^j}} + \sum_{i,l=1}^{m}\sum_{k=1}^{n} \frac{\partial A^{x_i}}{\partial \frac{\partial S^{x_l}}{\partial u^k}} (\frac{\partial^2 S^{x_l}}{\partial u^k \partial x_i} + \sum_{j=1}^{n} \frac{\partial^2 S^{x_l}}{\partial u^k \partial u^j} \frac{\partial H}{\partial \frac{\partial S^{x_i}}{\partial u^j}}).\end{aligned} \tag{33}$$

Denote $p_j^{x_i} = \frac{\partial S^{x_i}}{\partial u^j}$, $p_i^t = \frac{\partial S^t}{\partial u^i}$. For the solution u of (26), it follows from (33) that

$$\begin{aligned}&\frac{\partial A^t}{\partial t} + \sum_{j=1}^{n} \frac{\partial A^t}{\partial u^j} \frac{\partial H}{\partial p_j^t} + \sum_{j=1}^{n} \frac{\partial A^t}{\partial p_j^t} (\frac{\partial p_j^t}{\partial t} + \sum_{i=1}^{n} \frac{\partial p_j^t}{\partial u^i} u_t^i) \\ &+ \sum_{i=1}^{m} \frac{\partial A^{x_i}}{\partial x_i} + \sum_{i=1}^{m}\sum_{j=1}^{n} \frac{\partial A^{x_i}}{\partial u^j} \frac{\partial H}{\partial p_j^{x_i}} + \sum_{i,l=1}^{m}\sum_{k=1}^{n} \frac{\partial A^{x_i}}{\partial p_k^{x_l}} (\frac{\partial p_k^{x_l}}{\partial x_i} + \sum_{j=1}^{n} \frac{\partial p_k^{x_l}}{\partial u^j} u_{x_i}^j) = 0.\end{aligned} \tag{34}$$

Using $D_t p_j^t = \frac{\partial p_j^t}{\partial t} + \sum_{i=1}^{n} \frac{\partial p_j^t}{\partial u^i} u_t^i$ and $D_{x_i} p_k^{x_l} = \frac{\partial p_k^{x_l}}{\partial x_i} + \sum_{j=1}^{n} \frac{\partial p_k^{x_l}}{\partial u^j} u_{x_i}^j$, (34) gives us that

$$D_t A^t + \sum_{i=1}^{m} D_{x_i} A^{x_i} = 0 \tag{35}$$

holds for any solution of (26) with two functions $A^t(t, x, u(t,x), p^t(t,x))$ and $A^{x_i}(t, x_i, u(t,x), p^x(t,x))$. On the other hand, if (35) is a conservation law of (26), then (33) holds, which provides that V is the generalized symmetry of DW Hamilton-Jacobi equation (25).

4 Generating functions for multi-symplectic PRK methods

In this section, we present the generating functions for multi-symplectic PRK methods based on DW Hamilton-Jacobi equations.

For numerical discretization, we make use of an uniform meshgrid on the plane of (x,t) with temporal step Δt and spatial step Δx. Denote $u_i^0 \approx u(c_i\Delta x, 0), u_0^m \approx u(0, \tilde{c}_m \Delta t)$, $U_{i,m} \approx u(c_i \Delta x, \tilde{c}_m \Delta t)$, $\partial_t U_{i,m} \approx u_t(c_i \Delta x, \tilde{c}_m \Delta t)$, $\partial_x U_{i,m} \approx u_x(c_i \Delta x, \tilde{c}_m \Delta t)$, $c_i = \sum_{j=1}^{s} a_{ij}$ and $\tilde{c}_m = \sum_{n=1}^{m} \tilde{a}_{mn}$.

Applying PRK method ([4, 5]) to (26) both in time direction and space direction, we derive

$$u_i^1 - u_i^0 = \Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t U_{i,m}, \qquad U_{i,m} - u_i^0 = \Delta t \sum_{n=1}^{r} \tilde{a}_{mn} \partial_t U_{i,n}, \tag{36}$$

$$(p^t)_i^1 - (p^t)_i^0 = \Delta t \sum_{m=1}^{r} \tilde{B}_m \partial_t P_{i,m}^t, \qquad P_{i,m}^t - (p^t)_i^0 = \Delta t \sum_{n=1}^{r} \tilde{A}_{mn} \partial_t P_{i,n}^t, \tag{37}$$

$$u_1^m - u_0^m = \Delta x \sum_{i=1}^{s} b_i \partial_x U_{i,m}, \qquad U_{i,m} - u_0^m = \Delta x \sum_{j=1}^{s} a_{ij} \partial_x U_{j,m}, \tag{38}$$

$$(p^x)_1^m - (p^x)_0^m = \Delta x \sum_{i=1}^{s} B_i \partial_x P_{i,m}^x, \qquad P_{i,m}^x - (p^x)_0^m = \Delta x \sum_{j=1}^{s} A_{ij} \partial_x P_{j,m}^x, \tag{39}$$

$$\partial_t U_{i,m} = H_{p^t}(U_{i,m}, P_{i,m}^t, P_{i,m}^x), \qquad \partial_x U_{i,m} = H_{p^x}(U_{i,m}, P_{i,m}^t, P_{i,m}^x), \tag{40}$$

$$\partial_t P_{i,m}^t + \partial_x P_{i,m}^x = -H_u(U_{i,m}, P_{i,m}^t, P_{i,m}^x). \tag{41}$$

Theorem 4.1. *Suppose the coefficients of PRK method (36)-(41) satisfy*

$$b_i A_{ij} + B_j a_{ji} - b_i B_j = 0, \tag{42}$$

$$\tilde{b}_m \tilde{A}_{mn} + \tilde{B}_n \tilde{a}_{nm} - \tilde{b}_m \tilde{B}_n = 0, \tag{43}$$

$$b_i = B_i,\ \tilde{b}_m = \tilde{B}_m \quad i, j = 1, \cdots, s, m, n = 1, \cdots, r. \tag{44}$$

Then its generating functions are

$$\mathbb{S}_t^1(\Delta t, u_i^1, u_i^0) = \Delta t \sum_{m=1}^{r} \tilde{B}_m (L(U_{i,m}, \partial_t U_{i,m}, \partial_x U_{i,m}) - \frac{\partial S^x}{\partial x}(x_i, U_{i,m}) - (\frac{\partial S^x}{\partial u}(x_i, U_{i,m}))^T \partial_x U_{i,m}), \tag{45}$$

$$\mathbb{S}_x^1(\Delta x, u_1^m, u_0^m) = \Delta x \sum_{i=1}^{s} B_i (L(U_{i,m}, \partial_t U_{i,m}, \partial_x U_{i,m}) - \frac{\partial S^t}{\partial t}(t_m, U_{i,m}) - (\frac{\partial S^t}{\partial u}(t_m, U_{i,m}))^T \partial_t U_{i,m}) \tag{46}$$

with relations

$$\frac{\partial \mathbb{S}_t^1}{\partial u_i^0} = -(p^t)_i^0, \qquad \frac{\partial \mathbb{S}_t^1}{\partial u_i^1} = (p^t)_i^1, \tag{47}$$

$$\frac{\partial \mathbb{S}_x^1}{\partial u_0^m} = -(p^x)_0^m, \qquad \frac{\partial \mathbb{S}_x^1}{\partial u_1^m} = (p^x)_1^m. \tag{48}$$

Proof. Consider conditional extremum problem: finding the value $\partial_t U_{i,m}$ which minimizes $\mathbb{S}_t^1$ with $U_{i,m} - u_i^0 = \Delta t \sum_{n=1}^{r} \tilde{a}_{mn} \partial_t U_{i,n}$ under constraint $u_i^1 = u_i^0 + \Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t U_{i,m}$.

Let $\bar{\mathbb{S}}_t^1 = \mathbb{S}_t^1 + \lambda(u_i^1 - u_i^0 - \Delta t \sum\limits_{m=1}^{r} \tilde{b}_m \partial_t U_{i,m})$, we derive

$$\begin{aligned}\frac{\partial \bar{\mathbb{S}}_t^1}{\partial \partial_t U_{i,n}} = \Delta t \sum_{m=1}^{r} \tilde{B}_m ((\frac{\partial U_{i,m}}{\partial \partial_t U_{i,n}})^T L_u + (\frac{\partial \partial_t U_{i,m}}{\partial \partial_t U_{i,n}})^T L_{u_t} - (\frac{\partial U_{i,m}}{\partial \partial_t U_{i,n}})^T \frac{\partial^2 S^x}{\partial x \partial u} \\ - (\frac{\partial U_{i,m}}{\partial \partial_t U_{i,n}})^T \frac{\partial^2 S^x}{\partial u^2} \partial_x U_{i,m}) - \Delta t \lambda \tilde{b}_n = 0,\end{aligned} \tag{49}$$

$$\begin{aligned}\frac{\partial \mathbb{S}_t^1}{\partial u_i^0} = \Delta t \sum_{m=1}^{r} \tilde{B}_m ((\frac{\partial U_{i,m}}{\partial u_i^0})^T (L_u - \frac{\partial^2 S^x}{\partial u \partial x}) + (\frac{\partial \partial_t U_{i,m}}{\partial u_i^0})^T L_{u_t} + (\frac{\partial \partial_x U_{i,m}}{\partial u_i^0})^T (L_{u_x} - \frac{\partial S^x}{\partial u}) \\ - (\frac{\partial U_{i,m}}{\partial u_i^0})^T \frac{\partial^2 S^x}{\partial u^2} \partial_x U_{i,m}),\end{aligned} \tag{50}$$

$$\begin{aligned}\frac{\partial \mathbb{S}_t^1}{\partial u_i^1} = \Delta t \sum_{m=1}^{r} \tilde{B}_m ((\frac{\partial U_{i,m}}{\partial u_i^1})^T (L_u - \frac{\partial^2 S^x}{\partial u \partial x}) + (\frac{\partial \partial_t U_{i,m}}{\partial u_i^1})^T L_{u_t} + (\frac{\partial \partial_x U_{i,m}}{\partial u_i^1})^T (L_{u_x} - \frac{\partial S^x}{\partial u}) \\ - (\frac{\partial U_{i,m}}{\partial u_i^1})^T \frac{\partial^2 S^x}{\partial u^2} \partial_x U_{i,m}).\end{aligned} \tag{51}$$

(36) provides us

$$\frac{\partial U_{i,m}}{\partial \partial_t U_{i,n}} = \Delta t \tilde{a}_{mn}, \tag{52}$$

$$\frac{\partial U_{i,m}}{\partial u_i^0} = I + \Delta t \sum_{n=1}^{r} \tilde{a}_{mn} \frac{\partial \partial_t U_{i,n}}{\partial u_i^0}, \qquad \frac{\partial U_{i,m}}{\partial u_i^1} = \Delta t \sum_{n=1}^{r} \tilde{a}_{mn} \frac{\partial \partial_t U_{i,n}}{\partial u_i^1}, \tag{53}$$

$$0 = I - \Delta t \sum_{m=1}^{r} \tilde{b}_m \frac{\partial \partial_t U_{i,m}}{\partial u_i^1}, \qquad 0 = I + \Delta t \sum_{m=1}^{r} \tilde{b}_m \frac{\partial \partial_t U_{i,m}}{\partial u_i^0}. \tag{54}$$

Substituting (52) and (54) into (49), we obtain

$$-\lambda = \Delta t^2 \sum_{m,n=1}^{r} \tilde{B}_m \tilde{a}_{mn} (\frac{\partial \partial_t U_{i,n}}{\partial u_i^0})^T (L_u - \frac{\partial^2 S^x}{\partial x \partial u} - \frac{\partial^2 S^x}{\partial u^2} \partial_x U_{i,m}) + \Delta t \sum_{n=1}^{r} \tilde{B}_n (\frac{\partial \partial_t U_{i,n}}{\partial u_i^0})^T L_{u_t}, \tag{55}$$

$$\lambda = \Delta t^2 \sum_{m,n=1}^{r} \tilde{B}_m \tilde{a}_{mn} (\frac{\partial \partial_t U_{i,n}}{\partial u_i^1})^T (L_u - \frac{\partial^2 S^x}{\partial x \partial u} - \frac{\partial^2 S^x}{\partial u^2} \partial_x U_{i,m}) + \Delta t \sum_{n=1}^{r} \tilde{B}_n (\frac{\partial \partial_t U_{i,n}}{\partial u_i^1})^T L_{u_t}. \tag{56}$$

With (53),(55) and (56) it follows from (50) and (51) that

$$\frac{\partial \mathbb{S}_t^1}{\partial u_i^0} = \Delta t \sum_{m=1}^{r} \tilde{B}_m (L_u - \frac{\partial^2 S^x}{\partial u^2} \partial_x U_{i,m} - \frac{\partial^2 S^x}{\partial x \partial u}) - \lambda, \tag{57}$$

$$\frac{\partial \mathbb{S}_t^1}{\partial u_i^1} = \lambda, \tag{58}$$

where the relation $L_{u_x}(U_{i,m},\partial_t U_{i,m},\partial_x U_{i,m}) = \frac{\partial S^x}{\partial u}(x_i,U_{i,m})$ is used. By (47), (57) and (58), we obtain

$$(p^t)_i^1 - (p^t)_i^0 = \Delta t \sum_{m=1}^{r} \tilde{B}_m (L_u - \frac{\partial S^x}{\partial u^2}\partial_x U_{i,m} - \frac{\partial^2 S^x}{\partial x \partial u}) = \Delta t \sum_{m=1}^{r} \tilde{B}_m \partial_t P^t_{i,m} \tag{59}$$

with $\partial_t P^t_{i,m} = L_u - \frac{\partial^2 S^x}{\partial u^2}\partial_x U_{i,m} - \frac{\partial^2 S^x}{\partial x \partial u}$. Denote $P^t_{i,m} = L_{u_t}(U_{i,m},\partial_t U_{i,m},\partial_x U_{i,m})$, from (49) and (57), we obtain

$$\begin{aligned}
-(p^t)_i^0 = \frac{\partial \mathbb{S}_t^1}{\partial u_i^0} &= \Delta t \sum_{m=1}^{r} \tilde{B}_m \partial_t P^t_{i,m} - \Delta t \sum_{m=1}^{r} \frac{\tilde{B}_m \tilde{a}_{mn}}{\tilde{b}_n}\partial_t P^t_{i,m} - \frac{\tilde{B}_n}{\tilde{b}_n} L_{u_t} \\
&= \Delta t \sum_{m=1}^{r} (\tilde{B}_m - \frac{\tilde{B}_m \tilde{a}_{mn}}{\tilde{b}_n})\partial_t P^t_{i,m} - \frac{\tilde{B}_n}{\tilde{b}_n} L_{u_t} \\
&= \Delta t \sum_{m=1}^{r} \tilde{A}_{nm} \partial_t P^t_{i,m} - P^t_{i,n}
\end{aligned} \tag{60}$$

with $\tilde{b}_m = \tilde{B}_m$ and $-\tilde{A}_{nm} = \frac{\tilde{B}_m \tilde{a}_{mn} - \tilde{b}_n \tilde{B}_m}{\tilde{b}_n}$. Combining (59) and (60), (37) is obtained. Similarly, consider the conditional extremum problem for the x direction: finding the value $\partial_x U_{i,m}$ which minimizes $\mathbb{S}_x^1$ with $U_{i,m} - u_0^m = \Delta x \sum_{j=1}^{s} a_{ij}\partial_x U_{j,m}$ under constraint $u_1^m = u_0^m + \Delta x \sum_{i=1}^{s} b_i \partial_x U_{i,m}$. Let $\bar{\mathbb{S}}_x^1 = \mathbb{S}_x^1 + \mu(u_1^m - u_0^m - \Delta x \sum_{i=1}^{s} b_i \partial_x U_{i,m})$, we gain

$$\begin{aligned}
\frac{\partial \bar{\mathbb{S}}_x^1}{\partial \partial_x U_{j,m}} &= \Delta x \sum_{i=1}^{s} B_i ((\frac{\partial U_{i,m}}{\partial \partial_x U_{j,m}})^T L_u + (\frac{\partial \partial_x U_{i,m}}{\partial \partial_x U_{j,m}})^T L_{u_x} - (\frac{\partial U_{i,m}}{\partial \partial_x U_{j,m}})^T \frac{\partial^2 S^t}{\partial t \partial u} \\
&\quad - (\frac{\partial U_{i,m}}{\partial \partial_x U_{j,m}})^T \frac{\partial^2 S^t}{\partial u^2}\partial_t U_{i,m}) - \Delta x \mu b_j = 0,
\end{aligned} \tag{61}$$

$$\frac{\partial \mathbb{S}_x^1}{\partial u_0^m} = \Delta x \sum_{i=1}^{s} B_i ((\frac{\partial U_{i,m}}{\partial u_0^m})^T (L_u - \frac{\partial^2 S^t}{\partial t \partial u} - \frac{\partial^2 S^t}{\partial u^2}\partial_t U_{i,m}) + (\frac{\partial \partial_t U_{i,m}}{\partial u_0^m})^T (L_{u_t} - \frac{\partial S^t}{\partial u}) + (\frac{\partial \partial_x U_{i,m}}{\partial u_0^m})^T L_{u_x}) \tag{62}$$

$$\frac{\partial \mathbb{S}_x^1}{\partial u_1^m} = \Delta x \sum_{i=1}^{s} B_i ((\frac{\partial U_{i,m}}{\partial u_1^m})^T (L_u - \frac{\partial^2 S^t}{\partial t \partial u} - \frac{\partial^2 S^t}{\partial u^2}\partial_t U_{i,m}) + (\frac{\partial \partial_t U_{i,m}}{\partial u_1^m})^T (L_{u_t} - \frac{\partial S^t}{\partial u}) + (\frac{\partial \partial_x U_{i,m}}{\partial u_1^m})^T L_{u_x}). \tag{63}$$

(38) and (61)-(63) imply that

$$\frac{\partial \mathbb{S}_x^1}{\partial u_0^m} = \Delta x \sum_{i=1}^{s} B_i (L_u - \frac{\partial^2 S^t}{\partial u^2}\partial_t U_{i,m} - \frac{\partial^2 S^t}{\partial t \partial u}) - \mu = -(p^x)_0^m, \tag{64}$$

$$\frac{\partial \mathbb{S}_x^1}{\partial u_1^m} = \mu = (p^x)_1^m. \tag{65}$$

Let $\partial_x P^x_{i,m} = L_u - \frac{\partial^2 S^t}{\partial u^2}\partial_t U_{i,m} - \frac{\partial^2 S^t}{\partial t \partial u}$, $P^x_{i,m} = L_{u_x}$. Then

$$(p^x)^m_1 - (p^x)^m_0 = \Delta x \sum_{i=1}^{s} B_i (L_u - \frac{\partial^2 S^t}{\partial u^2}\partial_t U_{i,m} - \frac{\partial^2 S^t}{\partial t \partial u}) = \Delta x \sum_{i=1}^{s} B_i \partial_x P^x_{i,m}.$$

The combination of (61) and (64) leads to

$$\sum_{i=1}^{s} \frac{B_i a_{ij} - B_i b_j}{b_j} \partial_x P^x_{i,m} = (p^x)^m_0 - L_{u_x},$$

$$\sum_{i=1}^{s} A_{ji} \partial_x P^x_{i,m} + (p^x)^m_0 = P^x_{j,m}.$$

And

$$\partial_t P^t_{i,m} + \partial_x P^x_{i,m} = H_u(U_{i,m}, P^t_{i,m}, P^x_{i,m})$$

with $H(U_{i,m}, P^t_{i,m}, P^x_{i,m}) = (P^t_{i,m})^T \partial_t U_{i,m} + (P^x_{i,m})^T \partial_x U_{i,m} - L(U_{i,m}, \partial_t U_{i,m}, \partial_x U_{i,m})$, $-A_{ji} = \frac{B_i a_{ij} - b_j B_i}{b_j}$, $b_i = B_i$. The proof is finished. □

Theorem 4.2. *Under the conditions of above theorem, (36)-(41) is obtained by generating functions*

$$\mathbb{S}^2_t(\Delta t, (p^t)^1_i, u^0_i) = \Delta t^2 \sum_{m,n=1}^{r} \tilde{b}_n \tilde{a}_{nm} (\partial_t P^t_{i,n})^T \partial_t U_{i,m} - \Delta t \sum_{m=1}^{r} \tilde{b}_m \frac{\partial S^t}{\partial t}(t_m, U_{i,m}), \tag{66}$$

$$\mathbb{S}^2_x(\Delta x, (p^x)^m_1, u^m_0) = \Delta x^2 \sum_{i,j=1}^{s} b_j a_{ji} (\partial_x P^x_{j,m})^T \partial_x U_{i,m} - \Delta x \sum_{i=1}^{s} b_i \frac{\partial S^x}{\partial x}(x_i, U_{i,m}) \tag{67}$$

with relations

$$\frac{\partial \mathbb{S}^2_t}{\partial (p^t)^1_i} = u^1_i - u^0_i, \qquad \frac{\partial \mathbb{S}^2_x}{\partial (p^x)^m_1} = u^m_1 - u^m_0,$$
$$\frac{\partial \mathbb{S}^2_t}{\partial u^0_i} = (p^t)^0_i - (p^t)^1_i, \qquad \frac{\partial \mathbb{S}^2_x}{\partial u^m_0} = (p^x)^m_0 - (p^x)^m_1.$$

Proof. It follows from (37) that

$$\frac{\partial P^t_{i,m}}{\partial u^0_i} = \Delta t \sum_{n=1}^{r} \tilde{A}_{mn} \frac{\partial \partial_t P^t_{i,n}}{\partial u^0_i} - \Delta t \sum_{m=1}^{r} \tilde{B}_m \frac{\partial \partial_t P^t_{i,m}}{\partial u^0_i}, \tag{68}$$

$$\frac{\partial P^t_{i,m}}{\partial (p^t)^1_i} - I = \Delta t \sum_{n=1}^{r} \tilde{A}_{mn} \frac{\partial \partial_t P^t_{i,n}}{\partial (p^t)^1_i} - \Delta t \sum_{m=1}^{r} \tilde{B}_m \frac{\partial \partial_t P^t_{i,m}}{\partial (p^t)^0_i}. \tag{69}$$

By (53), (68) and (69), we gain

$$\begin{aligned}\frac{\partial \mathbb{S}_t^2}{\partial u_i^0} &= \Delta t^2 \sum_{m,n=1}^{r} \tilde{b}_n \tilde{a}_{nm} ((\frac{\partial \partial_t P_{i,n}^t}{\partial u_i^0})^T \partial_t U_{i,m} + (\frac{\partial \partial_t U_{i,m}}{\partial u_i^0})^T \partial_t P_{i,n}^t) - \Delta t \sum_{m=1}^{r} \tilde{b}_m (\frac{\partial U_{i,m}}{\partial u_i^0})^T \frac{\partial^2 S^t}{\partial t \partial u} \\
&= -\Delta t \sum_{m=1}^{r} \tilde{b}_m (\frac{\partial U_{i,m}}{\partial u_i^0})^T (\partial_t P_{i,m}^t - \frac{\partial^2 S^t}{\partial u^2} \partial_t U_{i,m}) + \Delta t^2 \sum_{m,n=1}^{r} \tilde{b}_n \tilde{a}_{nm} ((\frac{\partial \partial_t P_{i,n}^t}{\partial u_i^0})^T \partial_t U_{i,m} \\
&\quad + (\frac{\partial \partial_t U_{i,m}}{\partial u_i^0})^T \partial_t P_{i,n}^t) \\
&= -\Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t P_{i,m}^t - \Delta t^2 \sum_{m,n=1}^{r} \tilde{b}_m \tilde{a}_{mn} (\frac{\partial \partial_t U_{i,n}}{\partial u_i^0})^T \partial_t P_{i,m}^t + \Delta t^2 \sum_{m,n=1}^{r} \tilde{b}_m \tilde{a}_{mn} (\frac{\partial \partial_t U_{i,n}}{\partial u_i^0})^T \partial_t P_{i,m}^t \\
&\quad + \Delta t \sum_{m=1}^{r} (\tilde{b}_m \tilde{A}_{mn} - \tilde{b}_m \tilde{B}_n + \tilde{b}_n \tilde{a}_{nm}) (\frac{\partial \partial_t P_{i,n}^t}{\partial u_i^0})^T \partial_t U_{i,m} \\
&= -\Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t P_{i,m}^t\end{aligned}$$

with $\partial_t P_{i,m}^t = \frac{\partial^2 S^t}{\partial t \partial u}(t_m, U_{i,m}) + \frac{\partial^2 S^t}{\partial u^2}(t_m, U_{i,m}) \partial_t U_{i,m}$. In the above equality, $(\frac{\partial U_{i,m}}{\partial u_i^0})^T \frac{\partial^2 S^t}{\partial u^2} = (\frac{\partial P_{i,m}^t}{\partial u_i^0})^T$ and the conditions of multi-symplecticity (43), (44) are utilized. Similarly,

$$\begin{aligned}\frac{\partial \mathbb{S}_t^2}{\partial (p^t)_i^1} &= \Delta t^2 \sum_{m,n=1}^{r} \tilde{b}_n \tilde{a}_{nm} ((\frac{\partial \partial_t P_{i,n}^t}{\partial (p^t)_i^1})^T \partial_t U_{i,m} + (\frac{\partial \partial_t U_{i,m}}{\partial (p^t)_i^1})^T \partial_t P_{i,n}^t) - \Delta t \sum_{m=1}^{r} \tilde{b}_m (\frac{\partial U_{i,m}}{\partial (p^t)_i^1})^T \frac{\partial^2 S^t}{\partial t \partial u} \\
&= -\Delta t \sum_{m=1}^{r} \tilde{b}_m (\frac{\partial U_{i,m}}{\partial (p^t)_i^1})^T (\partial_t P_{i,m}^t - \frac{\partial^2 S^t}{\partial u^2} \partial_t U_{i,m}) + \Delta t^2 \sum_{m,n=1}^{r} \tilde{b}_n \tilde{a}_{nm} (\frac{\partial \partial_t P_{i,n}^t}{\partial (p^t)_i^1})^T \partial_t U_{i,m} \\
&\quad + (\frac{\partial \partial_t U_{i,m}}{\partial (p^t)_i^1})^T \partial_t P_{i,n}^t) \\
&= \Delta t \sum_{m=1}^{r} \tilde{b}_m \partial_t U_{i,m},\end{aligned}$$

where we make use of equalities $\frac{\partial U_{i,m}}{\partial (p^t)_i^1} = \Delta t \sum_{m=1}^{r} \tilde{a}_{mn} \frac{\partial \partial_t U_{i,n}}{\partial (p^t)_i^1}$, $(\frac{\partial U_{i,m}}{\partial (p^t)_i^1})^T \frac{\partial^2 S^t}{\partial u^2} = (\frac{\partial P_{i,m}^t}{\partial (p^t)_i^1})^T$ and (69). The another half of this theorem can be proved in the same way as above. This completes the proof. □

Consider wave equation in multi-symplectic Hamiltonian formulation

$$\begin{aligned} u_t = v, \qquad u_x = w, \\ v_t - w_x = -V'(u). \end{aligned}$$

The multi-symplectic PRK method for wave equation is

$$u_i^1 - u_i^0 = \Delta t \sum_{m=1}^{r} \tilde{b}_m V_{i,m}, \qquad U_{i,m} - u_i^0 = \Delta t \sum_{n=1}^{r} \tilde{a}_{mn} V_{i,n}, \tag{70}$$

$$v_i^1 - v_i^0 = \Delta t \sum_{m=1}^{r} \tilde{B}_m \partial_t V_{i,m}, \qquad V_{i,m} - v_i^0 = \Delta t \sum_{n=1}^{r} \tilde{A}_{mn} \partial_t V_{i,n}, \tag{71}$$

$$u_1^m - u_0^m = \Delta x \sum_{i=1}^{s} b_i W_{i,m}, \qquad U_{i,m} - u_0^m = \Delta x \sum_{j=1}^{s} a_{ij} W_{j,m}, \tag{72}$$

$$w_1^m - w_0^m = \Delta x \sum_{i=1}^{s} B_i (V'(U_{i,m}) + \partial_t V_{i,m}), \quad W_{i,m} - w_0^m = \Delta x \sum_{j=1}^{s} A_{ij} (V'(U_{j,m}) + \partial_t V_{j,m}). \tag{73}$$

Substituting (71) and (73) into (70) and (72), it is reduced to multi-symplectic Runge-Kutta-Nyström (RKN) method ([5])

$$u_i^1 - u_i^0 = \Delta t v_i^0 + \Delta t^2 \sum_{n=1}^{r} \tilde{\beta}_n \partial_t V_{i,n}, \qquad u_1^m - u_0^m = \Delta x w_0^m + \Delta x^2 \sum_{j=1}^{s} \beta_j (V'(U_{j,m}) + \partial_t V_{j,m}), \tag{74}$$

$$w_1^m - w_0^m = \Delta x \sum_{i=1}^{s} B_i (V'(U_{i,m}) + \partial_t V_{i,m}), \qquad U_{i,m} - u_i^0 = \Delta t \tilde{c}_m v_i^0 + \Delta t^2 \sum_{k=1}^{r} \tilde{\alpha}_{mk} \partial_t V_{i,k}, \tag{75}$$

$$U_{i,m} - u_0^m = \Delta x c_i w_0^m + \Delta x^2 \sum_{k=1}^{s} \alpha_{ik} (V'(U_{k,m}) + \partial_t V_{k,m}), \qquad v_i^1 - v_i^0 = \Delta t \sum_{m=1}^{r} \tilde{B}_m \partial_t V_{i,m}, \tag{76}$$

where $\tilde{\alpha}_{mk} = \sum_{n=1}^{r} \tilde{a}_{mn} \tilde{A}_{nk}$, $\tilde{\beta}_n = \sum_{m=1}^{r} \tilde{b}_m \tilde{A}_{mn}$, $\beta_j = \sum_{i=1}^{s} b_i A_{ij}, \alpha_{ik} = \sum_{j=1}^{s} a_{ij} A_{jk}$. Applying theorem 5.4, the generating function for (70)-(73) is

$$\mathbb{S}_t^2(\Delta t, v_i^1, u_i^0) = \Delta t^2 \sum_{m,n=1}^{r} \tilde{b}_n \tilde{a}_{nm} (\partial_t V_{i,n})^T V_{i,m} - \Delta t \sum_{m=1}^{r} \tilde{b}_m \frac{\partial S^t}{\partial t}(t_m, U_{i,m}),$$
$$\mathbb{S}_x^2(\Delta x, w_1^m, u_0^m) = \Delta x^2 \sum_{i,j=1}^{s} b_j a_{ji} (\partial_x W_{j,m})^T W_{i,m} - \Delta x \sum_{i=1}^{s} b_i \frac{\partial S^x}{\partial x}(x_i, U_{i,m}),$$

thus the generating function for (74)-(76) is

$$\mathbb{S}_t^2(\Delta t, v_i^1, u_i^0) = \Delta t^2 \sum_{n=1}^{r} \tilde{b}_n \tilde{c}_n (\partial_t V_{i,n})^T v_i^0 + \Delta t^3 \sum_{n,k=1}^{r} \tilde{b}_n \tilde{\alpha}_{nk} \partial_t V_{i,k} - \Delta t \sum_{m=1}^{r} \tilde{b}_m \frac{\partial S^t}{\partial t}(t_m, U_{i,m}),$$

$$\mathbb{S}_x^2(\Delta x, w_1^m, u_0^m) = \Delta x^2 \sum_{j=1}^{s} b_j c_j (\partial_x W_{j,m})^T w_0^m + \Delta x^3 \sum_{j,k=1}^{s} b_j \alpha_{jk} (V'(U_{k,m}) + \partial t V_{k,m}) - \Delta x \sum_{i=1}^{s} b_i \frac{\partial S^x}{\partial x}(x_i, U_{i,m})$$

with the coefficients satisfying $\beta_i = B_i(1 - c_i), \tilde{\beta}_m = \tilde{B}_m(1 - \tilde{c}_m)$, $\beta_i B_j - B_j \alpha_{ji} = \beta_j B_i - B_i \alpha_{ij}$, $\tilde{\beta}_m \tilde{B}_n - \tilde{B}_n \tilde{\alpha}_{nm} = \tilde{\beta}_n \tilde{B}_m - \tilde{B}_m \tilde{\alpha}_{mn}$.

5 Conclusions

The multi-symplectic PRK method is important in numerical computing multi-symplectic Hamiltonian systems. In this paper, we present its generating functions based on DW Hamilton-Jacobi theory and provide the generating functions for multi-symplectic RKN methods for wave equations. For Hamiltonian PDEs, DW Hamilton-Jacobi equation is the generalization of Hamilton-Jacobi equation in the case of Hamiltonian ODEs. It plays the main role in the relation between generating functions and multi-symplectic PRK methods. The more applications of DW Hamilton-Jacobi equations to the numerical computation in Hamiltonian PDEs will be in our future work.

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