

High order symplectic integrators based on continuous-stage Runge-Kutta-Nyström methods

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Abstract

On the basis of the previous work by Tang & Zhang (Appl. Math. Comput. 323, 2018, p. 204–219), in this paper we present a more effective way to construct high-order symplectic integrators for solving second order Hamiltonian equations. Instead of analyzing order conditions step by step as shown in the previous work, the new technique of this paper is using Legendre expansions to deal with the simplifying assumptions for order conditions. With the new technique, high-order symplectic integrators can be conveniently devised by truncating an orthogonal series.

Keywords: Continuous-stage Runge-Kutta-Nyström methods; Hamiltonian systems; Symplectic integrators; Legendre polynomial expansion; Simplifying assumptions.

1. Introduction

In the last few decades, geometric integrators for the numerical solution of various differential systems have attracted much attention in the field of scientific and engineering computations [3, 10, 13, 14, 17, 21, 26]. Such type of integrators are related with the terminology “geometric” because they are applied to systems with geometric features. Strictly speaking, they must preserve at least one of geometric properties of the given system. The most significant advantage of employing such integrators is that they can not only correctly capture the qualitative behaviors of the exact flow of the system in phase space, but also give rise to a more accurate long-time integration than general-purpose methods [2, 17, 27, 38].

As is well known, traditional numerical methods such as Runge-Kutta (RK) methods, partitioned Runge-Kutta (PRK) methods and Runge-Kutta-Nyström (RKN) methods play a prominent role in the numerical discretization of ordinary differential equations (ODEs) [8, 15, 16]. Many geometric integrators can be established from these numerical methods [20, 25, 28, 29, 30, 31], and they are preferable for practical use due to their elegant formulations and standardized implementations [17, 26]. Recently, as a generalized form of these classical methods, numerical schemes with

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continuous stage (which implies infinitely-many stages) have been proposed and developed in the literature [7, 8, 18, 22, 23, 32, 33, 34, 35, 37]. The construction of such “continuous” integrators seems much easier than traditional methods with finite stages, as the Butcher coefficients are taken as continuous functions and they are allowed for orthogonal expansions [5, 34, 35, 37, 39]. It turned out that with the help of continuous-stage approach we can construct many classical integrators of arbitrarily-high order, without needing to solve the tedious nonlinear algebraic equations, usually associated with the order conditions of the numerical methods, in terms of many unknown coefficients. Moreover, some important geometric integrators can be readily derived with this new approach, and the prototype integrators amongst them are: symplectic methods for Hamiltonian systems, symmetric methods for reversible systems, and energy-preserving methods for Hamiltonian (even Poisson) systems [4, 9, 11, 22, 23, 24, 34, 35, 37].

It is worth mentioning that by using continuous-stage approach one may get some interesting results. A significant instance is that no RK methods are energy-preserving for general non-polynomial Hamiltonian systems [9], but energy-preserving csRK methods obviously exist [4, 6, 18, 22, 23, 24, 33, 32, 34]. It is shown in [32, 36] that some Galerkin variational methods can be closely connected to continuous-stage (P)RK methods. In addition, continuous-stage approaches may promote the investigation of conjugate symplecticity of energy-preserving methods [18, 19, 34].

Recently, the present author et al. [37] have investigated the construction of symplectic RKN-type integrators on the basis of continuous-stage methods. It is shown in [37] that by analyzing order conditions one by one with Legendre expansions, symplectic integrators of any order can be constructed step by step. However, when the same approaches are used for deriving higher-order integrators, one has to perform much more complicated analyses and tedious calculations, as more and more order conditions have to be considered. To address this difficulty, in this paper we propose a more effective way to construct high-order integrators by considering the simplifying assumptions for order conditions. Actually, a similar technique has been previously developed in [34] for constructing RK-type methods.

The paper is organized as follows: In Section 2, we introduce the definition of RKN-type methods for solving second-order differential equations; In Section 3, the order theory will be discussed; In Section 4, we expound our approach for constructing high-order symplectic integrators; Finally, a few conclusions are drawn in Section 5.

2. Runge-Kutta-Nyström-type methods

Consider the following initial value problem in the form of second-order system,

$$q'' = f(t, q), \quad q(t_0) = q_0, \quad q'(t_0) = q'_0, \quad (1)$$

where $f : \mathbb{R} \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a sufficiently smooth vector-valued function. The most popular numerical methods for solving (1) are Runge-Kutta-Nyström methods, which can be defined as follows.

Definition 2.1. [17] A Runge-Kutta-Nyström (RKN) method for solving (1) is defined by

$$Q_i = q_0 + hc_i q'_0 + h^2 \sum_{j=1}^s \bar{a}_{ij} f(t_0 + c_j h, Q_j), \quad i = 1, \dots, s, \quad (2a)$$

$$q_1 = q_0 + hq'_0 + h^2 \sum_{i=1}^s \bar{b}_i f(t_0 + c_i h, Q_i), \quad (2b)$$

$$q'_1 = q'_0 + h \sum_{i=1}^s b_i f(t_0 + c_i h, Q_i), \quad (2c)$$

which can be characterized by the following Butcher tableau

$$\begin{array}{c|c} c & \bar{A} \\ \hline & \bar{b} \\ \hline & b \end{array}$$

where $\bar{A} = (\bar{a}_{ij})_{s \times s}$, $\bar{b} = (\bar{b}_1, \dots, \bar{b}_s)$, $b = (b_1, \dots, b_s)$, $c = (c_1, \dots, c_s)$.

In a similar manner, one defines continuous-stage Runge-Kutta-Nyström methods.

Definition 2.2. [37] Let $\bar{A}_{\tau, \sigma}$ be a function of variables $\tau, \sigma \in [0, 1]$ and $\bar{B}_\tau, B_\tau, C_\tau$ be functions of $\tau \in [0, 1]$. A continuous-stage Runge-Kutta-Nyström (csRKN) method for solving (1) is given by

$$Q_\tau = q_0 + hC_\tau q'_0 + h^2 \int_0^1 \bar{A}_{\tau, \sigma} f(t_0 + C_\sigma h, Q_\sigma) d\sigma, \quad \tau \in [0, 1], \quad (3a)$$

$$q_1 = q_0 + hq'_0 + h^2 \int_0^1 \bar{B}_\tau f(t_0 + C_\tau h, Q_\tau) d\tau, \quad (3b)$$

$$q'_1 = q'_0 + h \int_0^1 B_\tau f(t_0 + C_\tau h, Q_\tau) d\tau, \quad (3c)$$

which can be characterized by the following Butcher tableau

$$\begin{array}{c|c} C_\tau & \bar{A}_{\tau, \sigma} \\ \hline & \bar{B}_\tau \\ \hline & B_\tau \end{array}$$

We shall refer to the methods in Definition 2.1 and 2.2 as ‘‘RKN-type methods’’.

3. Order theory for RKN-type methods

Definition 3.1. [15] A RKN-type method has order p , if for any sufficiently regular problem (1), as $h \rightarrow 0$, its local error satisfies

$$q_1 - q(t_0 + h) = \mathcal{O}(h^{p+1}), \quad q'_1 - q'(t_0 + h) = \mathcal{O}(h^{p+1}).$$

A ‘‘modern’’ order theory for RKN methods can be found in [15, 17, 26] and references therein. However, in this section we do not plan to review all aspects of the order theory, but the elegant parts in terms of simplifying assumptions for order conditions will be picked up and then extended for csRKN methods.

3.1. Order theory for RKN methods

In order to reduce the difficulty of analyzing the order accuracy, the following simplifying assumptions for order conditions were proposed [15, 17]

$$\begin{aligned} B(\xi) : \sum_{i=1}^s b_i c_i^{\kappa-1} &= \frac{1}{\kappa}, \quad 1 \leq \kappa \leq \xi, \\ CN(\eta) : \sum_{j=1}^s \bar{a}_{ij} c_j^{\kappa-1} &= \frac{c_i^{\kappa+1}}{\kappa(\kappa+1)}, \quad 1 \leq i \leq s, 1 \leq \kappa \leq \eta-1, \\ DN(\zeta) : \sum_{i=1}^s b_i c_i^{\kappa-1} \bar{a}_{ij} &= \frac{b_j c_j^{\kappa+1}}{\kappa(\kappa+1)} - \frac{b_j c_j}{\kappa} + \frac{b_j}{\kappa+1}, \quad 1 \leq j \leq s, 1 \leq \kappa \leq \zeta-1. \end{aligned}$$

Theorem 3.2. [15] *If the coefficients of the RKN method (2a)-(2c) satisfy the simplifying assumptions $B(p)$, $CN(\eta)$, $DN(\zeta)$, and if $\bar{b}_i = b_i(1 - c_i)$, for all $i = 1, \dots, s$, then the method has order at least $\min\{p, 2\eta + 2, \eta + \zeta\}$.*

3.2. Order theory for csRKN methods

Similarly to the classical case, we propose the following simplifying assumptions:

$$\begin{aligned} \mathcal{B}(\xi) : \int_0^1 B_\tau C_\tau^{\kappa-1} d\tau &= \frac{1}{\kappa}, \quad 1 \leq \kappa \leq \xi, \\ \mathcal{CN}(\eta) : \int_0^1 \bar{A}_{\tau,\sigma} C_\sigma^{\kappa-1} d\sigma &= \frac{C_\tau^{\kappa+1}}{\kappa(\kappa+1)}, \quad 1 \leq \kappa \leq \eta-1, \\ \mathcal{DN}(\zeta) : \int_0^1 B_\tau C_\tau^{\kappa-1} \bar{A}_{\tau,\sigma} d\tau &= \frac{B_\sigma C_\sigma^{\kappa+1}}{\kappa(\kappa+1)} - \frac{B_\sigma C_\sigma}{\kappa} + \frac{B_\sigma}{\kappa+1}, \quad 1 \leq \kappa \leq \zeta-1, \end{aligned}$$

where $\tau, \sigma \in [0, 1]$.

Theorem 3.3. *If the coefficients of the csRKN method (3a)-(3c) satisfy the simplifying assumptions $\mathcal{B}(p)$, $\mathcal{CN}(\eta)$, $\mathcal{DN}(\zeta)$, and if $\bar{B}_\tau = B_\tau(1 - C_\tau)$, for $\tau \in [0, 1]$, then the method has order at least $\min\{p, 2\eta + 2, \eta + \zeta\}$.*

Proof. This result can be proved similarly to the classical result [15]. □

We firstly introduce the ι -degree normalized shifted Legendre polynomial $P_\iota(t)$ by using the Rodrigues' formula

$$P_0(t) = 1, \quad P_\iota(t) = \frac{\sqrt{2\iota+1}}{\iota!} \frac{d^\iota}{dt^\iota} \left(t^\iota (t-1)^\iota \right), \quad \iota = 1, 2, 3, \dots$$

A well-known property of Legendre polynomials is that they are orthogonal to each other with respect to the $L^2([0, 1])$ inner product

$$\int_0^1 P_\iota(t) P_\kappa(t) dt = \delta_{\iota\kappa}, \quad \iota, \kappa = 0, 1, 2, \dots,$$

and they satisfy the following integration formulas

$$\begin{aligned}
\int_0^x P_0(t) dt &= \xi_1 P_1(x) + \frac{1}{2} P_0(x), \\
\int_0^x P_\iota(t) dt &= \xi_{\iota+1} P_{\iota+1}(x) - \xi_\iota P_{\iota-1}(x), \quad \iota = 1, 2, 3, \dots, \\
\int_x^1 P_\iota(t) dt &= \delta_{\iota 0} - \int_0^x P_\iota(t) dt, \quad \iota = 0, 1, 2, \dots,
\end{aligned} \tag{4}$$

where $\xi_\iota = \frac{1}{2\sqrt{4\iota^2-1}}$ and $\delta_{\iota\kappa}$ is the Kronecker delta. Hereafter we assume $B_\tau = 1, C_\tau = \tau$ [34, 35]. Consequently, the first assumption $\mathcal{B}(\xi)$ can be reduced to

$$\int_0^1 \tau^{\kappa-1} d\tau = \frac{1}{\kappa}, \quad \kappa = 1, \dots, \xi,$$

which is obviously satisfied for any positive integer ξ . For convenience, we denote this fact by $\mathcal{B}(\infty)$. In addition, by taking the derivative with respect to τ and σ respectively, it follows from $\mathcal{CN}(\eta)$ and $\mathcal{DN}(\zeta)$

$$\begin{aligned}
\mathcal{CN}'(\eta) : \quad & \int_0^1 \frac{d}{d\tau} \bar{A}_{\tau, \sigma} \sigma^{\kappa-1} d\sigma = \frac{\tau^\kappa}{\kappa} = \int_0^\tau \sigma^{\kappa-1} d\sigma, \quad 1 \leq \kappa \leq \eta - 1, \\
\mathcal{DN}'(\zeta) : \quad & \int_0^1 \tau^{\kappa-1} \frac{d}{d\sigma} \bar{A}_{\tau, \sigma} d\tau = \frac{\sigma^\kappa}{\kappa} - \frac{1}{\kappa} = - \int_\sigma^1 \tau^{\kappa-1} d\tau, \quad 1 \leq \kappa \leq \zeta - 1.
\end{aligned} \tag{5}$$

Note that (5) do not imply $\mathcal{CN}(\eta)$ and $\mathcal{DN}(\zeta)$, hence we additionally assume

$$\int_0^1 \bar{A}_{0, \sigma} \sigma^{\kappa-1} d\sigma = 0, \quad 1 \leq \kappa \leq \eta - 1, \tag{6}$$

and

$$\int_0^1 \tau^{\kappa-1} \bar{A}_{\tau, 0} d\tau = \frac{1}{\kappa+1} = \int_0^1 \tau^\kappa d\tau, \quad 1 \leq \kappa \leq \zeta - 1,$$

which in turn gives rise to

$$\int_0^1 \tau^{\kappa-1} (\bar{A}_{\tau, 0} - \tau) d\tau = 0, \quad 1 \leq \kappa \leq \zeta - 1. \tag{7}$$

Since the Legendre polynomial sequence $\{P_\iota(t)\}$ forms a complete orthogonal set in $L^2([0, 1])$, it allows us to consider the following expansions (with τ and σ being fixed respectively)

$$\frac{d}{d\tau} \bar{A}_{\tau, \sigma} = \sum_{\iota \geq 0} \gamma_\iota(\tau) P_\iota(\sigma), \quad \frac{d}{d\sigma} \bar{A}_{\tau, \sigma} = \sum_{\iota \geq 0} \lambda_\iota(\sigma) P_\iota(\tau), \tag{8}$$

where $\gamma_\iota(\tau), \lambda_\iota(\sigma)$ are unknown coefficient functions. Observe that (5) imply

$$\begin{aligned}
\mathcal{CN}'(\eta) : \quad & \int_0^1 \frac{d}{d\tau} \bar{A}_{\tau, \sigma} P_{\kappa-1}(\sigma) d\sigma = \int_0^\tau P_{\kappa-1}(\sigma) d\sigma, \quad 1 \leq \kappa \leq \eta - 1, \\
\mathcal{DN}'(\zeta) : \quad & \int_0^1 P_{\kappa-1}(\tau) \frac{d}{d\sigma} \bar{A}_{\tau, \sigma} d\tau = - \int_\sigma^1 P_{\kappa-1}(\tau) d\tau, \quad 1 \leq \kappa \leq \zeta - 1,
\end{aligned} \tag{9}$$

which leads to

$$\begin{aligned}\gamma_\iota(\tau) &= \int_0^\tau P_\iota(\sigma) d\sigma, \quad 0 \leq \iota \leq \eta - 2, \\ \lambda_\iota(\sigma) &= - \int_\sigma^1 P_\iota(\tau) d\tau, \quad 0 \leq \iota \leq \zeta - 2.\end{aligned}\tag{10}$$

Substituting (10) into (8) and using (4) gives

$$\begin{aligned}\frac{d}{d\tau} \bar{A}_{\tau, \sigma} &= \sum_{\iota=0}^{\eta-2} \int_0^\tau P_\iota(x) dx P_\iota(\sigma) + \sum_{\iota \geq \eta-1} \gamma_\iota(\tau) P_\iota(\sigma) \\ &= \frac{1}{2} + \sum_{\iota=0}^{\eta-2} \xi_{\iota+1} P_{\iota+1}(\tau) P_\iota(\sigma) - \sum_{\iota=0}^{\eta-3} \xi_{\iota+1} P_{\iota+1}(\sigma) P_\iota(\tau) + \sum_{\iota \geq \eta-1} \gamma_\iota(\tau) P_\iota(\sigma),\end{aligned}\tag{11}$$

$$\begin{aligned}\frac{d}{d\sigma} \bar{A}_{\tau, \sigma} &= - \sum_{\iota=0}^{\zeta-2} \int_\sigma^1 P_\iota(x) dx P_\iota(\tau) + \sum_{\iota \geq \zeta-1} \lambda_\iota(\sigma) P_\iota(\tau) \\ &= -\frac{1}{2} - \sum_{\iota=0}^{\zeta-3} \xi_{\iota+1} P_{\iota+1}(\tau) P_\iota(\sigma) + \sum_{\iota=0}^{\zeta-2} \xi_{\iota+1} P_{\iota+1}(\sigma) P_\iota(\tau) + \sum_{\iota \geq \zeta-1} \lambda_\iota(\sigma) P_\iota(\tau).\end{aligned}\tag{12}$$

Integrating (11) with respect to τ and (12) with respect to σ , yields

$$\begin{aligned}\bar{A}_{\tau, \sigma} - \bar{A}_{0, \sigma} &= \frac{1}{2} \tau + \sum_{\iota=0}^{\eta-2} \xi_{\iota+1} \int_0^\tau P_{\iota+1}(x) dx P_\iota(\sigma) \\ &\quad - \sum_{\iota=0}^{\eta-3} \xi_{\iota+1} P_{\iota+1}(\sigma) \int_0^\tau P_\iota(x) dx + \sum_{\iota \geq \eta-1} \int_0^\tau \gamma_\iota(x) dx P_\iota(\sigma), \\ \bar{A}_{\tau, \sigma} - \bar{A}_{\tau, 0} &= -\frac{1}{2} \sigma - \sum_{\iota=0}^{\zeta-3} \xi_{\iota+1} P_{\iota+1}(\tau) \int_0^\sigma P_\iota(x) dx \\ &\quad + \sum_{\iota=0}^{\zeta-2} \xi_{\iota+1} \int_0^\sigma P_{\iota+1}(x) dx P_\iota(\tau) + \sum_{\iota \geq \zeta-1} \int_0^\sigma \lambda_\iota(x) dx P_\iota(\tau).\end{aligned}\tag{13}$$

Taking into account (6) and (7), implies

$$\begin{aligned}\int_0^1 \bar{A}_{0, \sigma} P_{\kappa-1}(\sigma) d\sigma &= 0, \quad 1 \leq \kappa \leq \eta - 1, \\ \int_0^1 P_{\kappa-1}(\tau) (\bar{A}_{\tau, 0} - \tau) d\tau &= 0, \quad 1 \leq \kappa \leq \zeta - 1.\end{aligned}\tag{14}$$

We then consider the following orthogonal expansions

$$\bar{A}_{0, \sigma} = \sum_{\iota \geq 0} \alpha_\iota P_\iota(\sigma), \quad \bar{A}_{\tau, 0} - \tau = \sum_{\iota \geq 0} \beta_\iota P_\iota(\tau),\tag{15}$$

where $\alpha_\iota, \beta_\iota$ are real numbers. By inserting (15) into (14) we get

$$\alpha_\iota = 0, \quad 0 \leq \iota \leq \eta - 2; \quad \beta_\iota = 0, \quad 0 \leq \iota \leq \zeta - 2.\tag{16}$$

Then, it follows

$$\bar{A}_{0,\sigma} = \sum_{\iota \geq \eta-1} \alpha_\iota P_\iota(\sigma), \quad \bar{A}_{\tau,0} = \tau + \sum_{\iota \geq \zeta-1} \beta_\iota P_\iota(\tau). \quad (17)$$

Using the known equality $\tau = \frac{1}{2}P_0(\tau) + \xi_1 P_1(\tau)$ and inserting (17) into (13), gives

$$\begin{aligned} \bar{A}_{\tau,\sigma} &= \frac{1}{4}P_0(\tau) + \frac{1}{2}\xi_1 P_1(\tau) + \sum_{\iota=0}^{\eta-2} \xi_{\iota+1} \int_0^\tau P_{\iota+1}(x) dx P_\iota(\sigma) \\ &\quad - \sum_{\iota=0}^{\eta-3} \xi_{\iota+1} P_{\iota+1}(\sigma) \int_0^\tau P_\iota(x) dx + \sum_{\iota \geq \eta-1} (\alpha_\iota + \int_0^\tau \gamma_\iota(x) dx) P_\iota(\sigma), \\ \bar{A}_{\tau,\sigma} &= \frac{1}{4}P_0(\tau) + \xi_1 P_1(\tau) - \frac{1}{2}\xi_1 P_1(\sigma) - \sum_{\iota=0}^{\zeta-3} \xi_{\iota+1} P_{\iota+1}(\tau) \int_0^\sigma P_\iota(x) dx \\ &\quad + \sum_{\iota=0}^{\zeta-2} \xi_{\iota+1} \int_0^\sigma P_{\iota+1}(x) dx P_\iota(\tau) + \sum_{\iota \geq \zeta-1} (\beta_\iota + \int_0^\sigma \lambda_\iota(x) dx) P_\iota(\tau). \end{aligned}$$

By exploiting (4) once again, it ends up with

$$\begin{aligned} \bar{A}_{\tau,\sigma} &= \frac{1}{6} - \frac{1}{2}\xi_1 P_1(\sigma) + \frac{1}{2}\xi_1 P_1(\tau) + \sum_{\iota=1}^{\eta-3} \xi_\iota \xi_{\iota+1} P_{\iota-1}(\tau) P_{\iota+1}(\sigma) \\ &\quad - \sum_{\iota=1}^{\eta-2} (\xi_\iota^2 + \xi_{\iota+1}^2) P_\iota(\tau) P_\iota(\sigma) + \sum_{\iota=1}^{\eta-1} \xi_\iota \xi_{\iota+1} P_{\iota+1}(\tau) P_{\iota-1}(\sigma) \\ &\quad + \sum_{\iota \geq \eta-1} \phi_\iota(\tau) P_\iota(\sigma), \\ \bar{A}_{\tau,\sigma} &= \frac{1}{6} - \frac{1}{2}\xi_1 P_1(\sigma) + \frac{1}{2}\xi_1 P_1(\tau) + \sum_{\iota=1}^{\zeta-1} \xi_\iota \xi_{\iota+1} P_{\iota-1}(\tau) P_{\iota+1}(\sigma) \\ &\quad - \sum_{\iota=1}^{\zeta-2} (\xi_\iota^2 + \xi_{\iota+1}^2) P_\iota(\tau) P_\iota(\sigma) + \sum_{\iota=1}^{\zeta-3} \xi_\iota \xi_{\iota+1} P_{\iota+1}(\tau) P_{\iota-1}(\sigma) \\ &\quad + \sum_{\iota \geq \zeta-1} \psi_\iota(\sigma) P_\iota(\tau), \end{aligned}$$

where

$$\begin{aligned} \phi_\iota(\tau) &= \alpha_\iota + \int_0^\tau \gamma_\iota(x) dx, \quad \iota \geq \eta-1, \\ \psi_\iota(\sigma) &= \beta_\iota + \int_0^\sigma \lambda_\iota(x) dx \quad \iota \geq \zeta-1. \end{aligned}$$

We summarize the results above in the following lemma.

Lemma 3.4. *For the csRKN method (3a)-(3c) denoted by $(\bar{A}_{\tau,\sigma}, \bar{B}_\tau, B_\tau, C_\tau)$ with the assumption $B_\tau = 1, C_\tau = \tau$, we have the following statements:*

(I)

$$\begin{aligned}
\mathcal{CN}(\eta) \iff \bar{A}_{\tau,\sigma} = & \frac{1}{6} - \frac{1}{2}\xi_1 P_1(\sigma) + \frac{1}{2}\xi_1 P_1(\tau) + \sum_{\iota=1}^{\eta-3} \xi_\iota \xi_{\iota+1} P_{\iota-1}(\tau) P_{\iota+1}(\sigma) \\
& - \sum_{\iota=1}^{\eta-2} (\xi_\iota^2 + \xi_{\iota+1}^2) P_\iota(\tau) P_\iota(\sigma) + \sum_{\iota=1}^{\eta-1} \xi_\iota \xi_{\iota+1} P_{\iota+1}(\tau) P_{\iota-1}(\sigma) \\
& + \sum_{\iota \geq \eta-1} \phi_\iota(\tau) P_\iota(\sigma),
\end{aligned} \tag{18}$$

where $\xi_\iota = \frac{1}{2\sqrt{4\iota^2-1}}$ ($\iota \geq 1$) and $\phi_\iota(\tau)$ ($\iota \geq \eta - 1$) are arbitrary L^2 -integrable functions;

(II)

$$\begin{aligned}
\mathcal{DN}(\zeta) \iff \bar{A}_{\tau,\sigma} = & \frac{1}{6} - \frac{1}{2}\xi_1 P_1(\sigma) + \frac{1}{2}\xi_1 P_1(\tau) + \sum_{\iota=1}^{\zeta-1} \xi_\iota \xi_{\iota+1} P_{\iota-1}(\tau) P_{\iota+1}(\sigma) \\
& - \sum_{\iota=1}^{\zeta-2} (\xi_\iota^2 + \xi_{\iota+1}^2) P_\iota(\tau) P_\iota(\sigma) + \sum_{\iota=1}^{\zeta-3} \xi_\iota \xi_{\iota+1} P_{\iota+1}(\tau) P_{\iota-1}(\sigma) \\
& + \sum_{\iota \geq \zeta-1} \psi_\iota(\sigma) P_\iota(\tau),
\end{aligned} \tag{19}$$

where ξ_ι is defined as above, and $\psi_\iota(\sigma)$ ($\iota \geq \zeta - 1$) are arbitrary L^2 -integrable functions.

Theorem 3.5. For the csRKN method (3a)-(3c) denoted by $(\bar{A}_{\tau,\sigma}, \bar{B}_\tau, B_\tau, C_\tau)$ with the assumption $B_\tau = 1, C_\tau = \tau$, the following two statements are equivalent to each other:

(I) Both $\mathcal{CN}(\eta)$ and $\mathcal{DN}(\zeta)$ hold;(II) The coefficient $\bar{A}_{\tau,\sigma}$ admits the following expansion:

$$\begin{aligned}
\bar{A}_{\tau,\sigma} = & \frac{1}{6} - \frac{1}{2}\xi_1 P_1(\sigma) + \frac{1}{2}\xi_1 P_1(\tau) + \sum_{\iota=1}^{N_1} \xi_\iota \xi_{\iota+1} P_{\iota-1}(\tau) P_{\iota+1}(\sigma) \\
& - \sum_{\iota=1}^{N_2} (\xi_\iota^2 + \xi_{\iota+1}^2) P_\iota(\tau) P_\iota(\sigma) + \sum_{\iota=1}^{N_3} \xi_\iota \xi_{\iota+1} P_{\iota+1}(\tau) P_{\iota-1}(\sigma) \\
& + \sum_{\substack{i \geq \zeta-1 \\ j \geq \eta-1}} \omega_{(i,j)} P_i(\tau) P_j(\sigma),
\end{aligned} \tag{20}$$

where $N_1 = \max\{\eta - 3, \zeta - 1\}$, $N_2 = \max\{\eta - 2, \zeta - 2\}$, $N_3 = \max\{\eta - 1, \zeta - 3\}$, $\xi_\iota = \frac{1}{2\sqrt{4\iota^2-1}}$ and $\omega_{(i,j)}$ are arbitrary real numbers.

Proof. This theorem can be proved by using Lemma 3.4. Let us consider the expansions of $\phi_\iota(\tau)$ and $\psi_\iota(\sigma)$

$$\begin{aligned}
\phi_\iota(\tau) &= \sum_{i \geq 0} \mu_i^\iota P_i(\tau), \quad \iota \geq \eta - 1, \\
\psi_\iota(\sigma) &= \sum_{j \geq 0} \nu_j^\iota P_j(\sigma), \quad \iota \geq \zeta - 1,
\end{aligned}$$

where μ_i^l, ν_j^l are real numbers. Considering that

$$P_i(\tau)P_j(\sigma), \quad i, j = 0, 1, 2, \dots$$

form a complete orthogonal set in $L^2([0, 1] \times [0, 1])$, and substituting the two expansions above into (18) and (19) respectively, we then get the final result by comparing similar terms. \square

Since $\mathcal{B}(\infty)$ holds true for a csRKN method, Theorem 3.3 and 3.5 allow to readily derive its order as $\min\{\infty, 2\eta + 2, \eta + \zeta\} = \min\{2\eta + 2, \eta + \zeta\}$.

Remark 3.6. For the sake of obtaining a practical csRKN method, we have to define a finite form for $\bar{A}_{\tau, \sigma}$. A natural and simple way is to truncate the series (20). As a consequence, the Butcher coefficient $\bar{A}_{\tau, \sigma}$ becomes a bivariate polynomial in terms of τ and σ .

3.3. RKN methods by using quadrature formulas

As for the practical implementation of the csRKN method (3a)-(3c), one has to approximate the integrals by quadratures. Using a quadrature formula denoted by $(b_i, c_i)_{i=1}^s$ yields an s -stage RKN method

$$Q_i = q_0 + hC_i q'_0 + h^2 \sum_{j=1}^s b_j \bar{A}_{ij} f(t_0 + C_j h, Q_j), \quad i = 1, \dots, s, \quad (21a)$$

$$q_1 = q_0 + hq'_0 + h^2 \sum_{i=1}^s b_i \bar{B}_i f(t_0 + C_i h, Q_i), \quad (21b)$$

$$q'_1 = q'_0 + h \sum_{i=1}^s b_i B_i f(t_0 + C_i h, Q_i), \quad (21c)$$

where $\bar{A}_{ij} = \bar{A}_{c_i, c_j}, \bar{B}_i = \bar{B}_{c_i}, B_i = B_{c_i}, C_i = C_{c_i}$, which can be characterized by the following Butcher tableau

$$\begin{array}{c|ccc} C_1 & b_1 \bar{A}_{11} & \cdots & b_s \bar{A}_{1s} \\ \vdots & \vdots & & \vdots \\ C_s & b_1 \bar{A}_{s1} & \cdots & b_s \bar{A}_{ss} \\ \hline & b_1 \bar{B}_1 & \cdots & b_s \bar{B}_s \\ \hline & b_1 B_1 & \cdots & b_s B_s \end{array} \quad (22)$$

Particularly, if we assume $\bar{B}_\tau = B_\tau(1 - C_\tau), B_\tau = 1, C_\tau = \tau$ for $\tau \in [0, 1]$, then it gives an s -stage classical RKN method with tableau

$$\begin{array}{c|ccc} c_1 & b_1 \bar{A}_{11} & \cdots & b_s \bar{A}_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & b_1 \bar{A}_{s1} & \cdots & b_s \bar{A}_{ss} \\ \hline & \bar{b}_1 & \cdots & \bar{b}_s \\ \hline & b_1 & \cdots & b_s \end{array} \quad (23)$$

where $\bar{b}_i = b_i(1 - c_i), i = 1, \dots, s$. For the sake of analyzing the order of the RKN method (23), linked with Remark 3.6, we have the following result.

Theorem 3.7. Assume $\bar{A}_{\tau,\sigma}$ is a bivariate polynomial of degree π^τ in τ and degree π^σ in σ , and the quadrature formula $(b_i, c_i)_{i=1}^s$ is of order p . If a csRKN method (3a)-(3c) denoted by $(\bar{A}_{\tau,\sigma}, \bar{B}_\tau, B_\tau, C_\tau)$ with $\bar{B}_\tau = B_\tau(1 - C_\tau)$, $B_\tau = 1$, $C_\tau = \tau$, $\tau \in [0, 1]$ and both $\mathcal{CN}(\eta)$, $\mathcal{DN}(\zeta)$ hold, then the RKN method (23) is at least of order

$$\min\{p, 2\alpha + 2, \alpha + \beta\},$$

where $\alpha = \min\{\eta, p - \pi^\sigma + 1\}$ and $\beta = \min\{\zeta, p - \pi^\tau + 1\}$.

Proof. Since $\int_0^1 g(x) dx = \sum_{i=1}^s b_i g(c_i)$ holds for any polynomial $g(x)$ of degree up to $p-1$, by using the quadrature formula $(b_i, c_i)_{i=1}^s$ to compute the integrals of $\mathcal{B}(\xi)$, $\mathcal{CN}(\eta)$, $\mathcal{DN}(\zeta)$ one obtains:

$$\begin{aligned} \sum_{i=1}^s b_i c_i^{\kappa-1} &= \frac{1}{\kappa}, \quad \kappa = 1, \dots, p, \\ \sum_{j=1}^s (b_j \bar{A}_{ij}) c_j^{\kappa-1} &= \frac{c_i^{\kappa+1}}{\kappa(\kappa+1)}, \quad i = 1, \dots, s, \quad \kappa = 1, \dots, \alpha - 1, \\ \sum_{i=1}^s b_i c_i^{\kappa-1} (b_j \bar{A}_{ij}) &= \frac{b_j c_j^{\kappa+1}}{\kappa(\kappa+1)} - \frac{b_j c_j}{\kappa} + \frac{b_j}{\kappa+1}, \quad j = 1, \dots, s, \quad \kappa = 1, \dots, \beta - 1. \end{aligned}$$

where $\alpha = \min\{\eta, p - \pi^\sigma + 1\}$ and $\beta = \min\{\zeta, p - \pi^\tau + 1\}$. These formulas imply that the RKN method (23) satisfies $B(p)$, $CN(\alpha)$ and $DN(\beta)$, and it is observed that $\bar{b}_i = b_i(1 - c_i)$ is naturally satisfied for each $i = 1, \dots, s$. Consequently, the statement follows from Theorem 3.2. \square

4. Construction of high-order symplectic integrators

Hamiltonian systems constitute a very important subclass of dynamical systems in the field of classical and non-classical mechanics [1, 10, 12, 17, 26, 13, 14]. Such type of systems can be written as

$$z' = J^{-1} \nabla_z H(z), \quad z(t_0) = z_0 \in \mathbb{R}^{2d}, \quad z = \begin{pmatrix} p \\ q \end{pmatrix}, \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}. \quad (24)$$

Symplectic integrators are of great interest for solving such systems [2, 12, 13, 14, 21, 26, 17], as they usually reproduce excellent qualitative behaviors of the exact flow [10, 27] and exhibit bounded energy errors for exponentially-long time [17].

In what follows, we restrict our attention to a special type of Hamiltonian systems with the Hamiltonian function

$$H(z) = \frac{1}{2} p^T M p + V(q),$$

where M is a constant symmetric matrix, and $V(q)$ is a scalar function. Such systems are usually called separable Hamiltonian systems, which reads

$$\begin{cases} p' = -\nabla_q V(q), \\ q' = M p. \end{cases} \quad (25)$$

Substituting the second equation into the first equation gives

$$q'' = -M \nabla_q V(q). \quad (26)$$

Denote $f(q) = -M\nabla_q V(q)$ and $g(q) = -\nabla_q V(q)$, for solving the equation (26), we propose the following csRKN method

$$Q_\tau = q_0 + hC_\tau Mp_0 + h^2 \int_0^1 \bar{A}_{\tau,\sigma} f(Q_\sigma) d\sigma, \quad \tau \in [0, 1], \quad (27a)$$

$$q_1 = q_0 + hMp_0 + h^2 \int_0^1 \bar{B}_\tau f(Q_\tau) d\tau, \quad (27b)$$

$$p_1 = p_0 + h \int_0^1 B_\tau g(Q_\tau) d\tau, \quad (27c)$$

which is derived by replacing the variable q' with Mp in Definition 2.2 but with M eliminated in the last formula. In [37], the authors have proved the following results.

Theorem 4.1. [37] *The csRKN method denoted by $(\bar{A}_{\tau,\sigma}, \bar{B}_\tau, B_\tau, C_\tau)$ with $B_\tau = 1, C_\tau = \tau$ is symplectic, if $\bar{A}_{\tau,\sigma}$ and \bar{B}_τ possess the following forms in terms of Legendre polynomials*

$$\begin{aligned} \bar{B}_\tau &= 1 - \tau = \frac{1}{2}P_0(\tau) - \xi_1 P_1(\tau), \quad \tau \in [0, 1], \\ \bar{A}_{\tau,\sigma} &= \alpha_{(0,0)} + \alpha_{(0,1)}P_1(\sigma) + \alpha_{(1,0)}P_1(\tau) + \sum_{i+j>1} \alpha_{(i,j)}P_i(\tau)P_j(\sigma), \quad \tau, \sigma \in [0, 1], \end{aligned} \quad (28)$$

where $\alpha_{(0,0)}$ is an arbitrary real number, $\alpha_{(0,1)} - \alpha_{(1,0)} = -\xi_1 = -\frac{\sqrt{3}}{6}$, and $\alpha_{(i,j)} = \alpha_{(j,i)}$, $\forall i+j > 1$.

Theorem 4.2. [37] *If the csRKN method denoted by $(\bar{A}_{\tau,\sigma}, \bar{B}_\tau, B_\tau, C_\tau)$ satisfies the symplecticity conditions*

$$\bar{B}_\tau = B_\tau(1 - C_\tau), \quad \tau \in [0, 1], \quad (29a)$$

$$B_\tau(\bar{B}_\sigma - \bar{A}_{\tau,\sigma}) = B_\sigma(\bar{B}_\tau - \bar{A}_{\sigma,\tau}), \quad \tau, \sigma \in [0, 1], \quad (29b)$$

then the associated RKN method (22) derived by using a quadrature formula $(b_i, c_i)_{i=1}^s$ is symplectic.

Instead of constructing symplectic integrators step by step with each step getting one higher order as in [37], now we can directly use Theorem 3.5. One just needs to compare the two series in terms of Legendre polynomials as shown in (20) and (28), and then devise symplectic csRKN integrators by a suitable truncation of the series. Theorem 4.2 implies that one can use quadrature formulas to get standard symplectic RKN methods from symplectic csRKN methods, and the order of the resulting methods can be analyzed by Theorem 3.7. It turns out that all the symplectic integrators presented in [37] can be recovered by using this new technique. Moreover, new symplectic integrators can be established in a more convenient way, for instance, if we take $\bar{B}_\tau = 1 - \tau$, $B_\tau = 1$, $C_\tau = \tau$ and

$$\begin{aligned} \bar{A}_{\tau,\sigma} &= \frac{1}{6} - \frac{1}{2}\xi_1 P_1(\sigma) + \frac{1}{2}\xi_1 P_1(\tau) + \sum_{\iota=1}^2 \xi_\iota \xi_{\iota+1} P_{\iota-1}(\tau) P_{\iota+1}(\sigma) \\ &\quad - (\xi_1^2 + \xi_2^2) P_1(\tau) P_1(\sigma) + \sum_{\iota=1}^2 \xi_\iota \xi_{\iota+1} P_{\iota+1}(\tau) P_{\iota-1}(\sigma) + \theta P_2(\tau) P_2(\sigma), \end{aligned} \quad (30)$$

where $\xi_i = \frac{1}{2\sqrt{4i^2-1}}$ and θ is an arbitrary real parameter, then, the use of the 3-point Gaussian quadrature, produces a family of 3-stage 6-order symplectic RKN methods, having Butcher tableau

$\frac{5-\sqrt{15}}{10}$	$\frac{2+30\theta}{135}$	$\frac{19-6\sqrt{15}-120\theta}{270}$	$\frac{62-15\sqrt{15}+120\theta}{540}$
$\frac{1}{2}$	$\frac{19+6\sqrt{15}-120\theta}{432}$	$\frac{1+15\theta}{27}$	$\frac{19-6\sqrt{15}-120\theta}{432}$
$\frac{5+\sqrt{15}}{10}$	$\frac{62+15\sqrt{15}+120\theta}{540}$	$\frac{19+6\sqrt{15}-120\theta}{270}$	$\frac{2+30\theta}{135}$
	$\frac{5+\sqrt{15}}{36}$	$\frac{2}{9}$	$\frac{5-\sqrt{15}}{36}$
	$\frac{5}{18}$	$\frac{4}{9}$	$\frac{5}{18}$

5. Concluding remarks

In this paper, we present a new technique to construct high-order symplectic integrators via analyzing the simplifying assumptions for order conditions by means of orthogonal expansions. The new technique shows that high-order integrators can be devised by truncating an orthogonal series. Besides, one could introduce some free parameters in the formulation of Butcher coefficients — an underlying application for this is that one may get explicit or semi-explicit integrators with suitable choices of these parameters (see [37]).

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