Continuous-stage Runge-Kutta-Nyström methods

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Abstract

We develop continuous-stage Runge-Kutta-Nyström (csRKN) methods in this paper. By leading weight function into the formalism of csRKN methods and modifying the original pattern of continuous-stage methods, we establish a new and larger framework for csRKN methods and it enables us to derive more effective RKN-type methods. Particularly, a variety of classical weighted orthogonal polynomials can be used in the construction of RKN-type methods. As an important application, new families of symmetric and symplectic integrators can be easily acquired in such framework. Numerical experiments have verified the effectiveness of the new integrators presented in this paper.

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

1. Introduction

The seminal idea of continuous-stage methods was introduced by Butcher (1972) in \cite{Butcher1972} (see also \cite{Butcher1974, Butcher1975} for a more detailed description), which suggests a “continuous” extension of Runge-Kutta (RK) methods by allowing the number of stages to be infinite so that the discrete index set \{1, 2, \ldots, s\} becomes the interval [0, 1]. Unfortunately, this creative idea has been completely ignored in a very long period of time. Such situation was continued until the year 2010, Hairer activated the idea by using it to interpret his energy-preserving collocation methods \cite{Hairer2010} and then an elegant mathematical formalism for continuous-stage Runge-Kutta methods was created by him. Since then, there has been a revival of interest in the study of continuous-stage methods, and some researchers consciously or unconsciously conduct their studies closely related with such a subject. The first related work after Hairer’s was given by Tang & Sun \cite{Tang2016}, stating that there is an interesting connection between Galerkin variational methods and continuous-stage methods, and it was shown in \cite{Tang2016} that energy-preserving methods such as \(s\)-stage trapezoidal methods \cite{Hairer1989}, average vector field methods \cite{Hairer1991}, and infinite Hamiltonian boundary value methods \cite{Hairer1992} (as well as Hairer’s energy-preserving collocation methods \cite{Hairer2010}) can be unified in the framework of continuous-stage methods. In recent years, there are a series of papers intensively studying in such subject \cite{Hairer2010, Tang2016, Tang2017, Tang2018, Tang2019, Tang2020, Tang2021, Tang2022}.

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So far, the available methods with continuous stage can be grouped into the following three classes: continuous-stage Runge-Kutta (csRK) methods [37, 38, 43, 44], continuous-stage partitioned Runge-Kutta (csPRK) methods [40], and continuous-stage Runge-Kutta-Nyström (csRKN) methods [39, 42]. It turns out that with the idea of continuous-stage methods we can easily construct many effective integrators of arbitrarily-high order, without needing to solve the tedious nonlinear algebraic equations (usually associated with the order conditions) in terms of many unknown coefficients. Particularly, a crucial technique for constructing continuous-stage methods with arbitrary order is developed in [38, 39, 40, 42, 44], which is mainly based on the orthogonal polynomial expansion.

Compared with standard RK & RK-like discretizations, the continuous-stage approaches may provide us a new insight in many aspects of numerical solution of differential equations, seeing that the Butcher coefficients (as functions) are assumed to be “continuous” or “smooth” which potentially allows us to use some analytical tools such as Taylor expansion, inner product, limit operation, orthogonal expansion, differentiation, integration, etc [22, 38, 39, 40, 42, 44]. Owing to this point, sometimes it may lead to surprising applications. A good case in point is that no RK methods are energy-preserving for general non-polynomial Hamiltonian systems [8], whereas energy-preserving csRK methods can be easily constructed [4, 17, 23, 24, 26, 37, 36, 38]. Another example is given by Tang & Sun [36], which states that some Galerkin variational methods can be interpreted as continuous-stage (P)RK methods, but they can not be completely understood in the classical (P)RK framework.

Over the last few decades, geometric integration for the numerical solution of differential equations has attracted much attention (see, for example, [2, 9, 11, 12, 13, 16, 20, 21, 27, 28, 29, 33, 34, 52]), for the reason that numerical discretization respecting the geometric properties of the exact flow are very important for long-time integration [2, 16, 30, 51]. In recent years, continuous-stage methods have found their interesting applications in geometric integration. For example, symplectic and multi-symplectic integrators can be derived by using Galerkin variational approaches, and these integrators can be interpreted and analyzed in the framework of continuous-stage methods [36, 41, 48]; some newly-developed energy-preserving methods can be closely related to continuous-stage methods [4, 8, 10, 17, 22, 23, 24, 26, 36, 40]; new families of symplectic and symmetric methods can be constructed by using the idea of continuous-stage methods [37, 38, 42, 43, 44, 45, 46, 47, 50]; the study of conjugate symplecticity of energy-preserving methods may be promoted in the context of continuous-stage methods [17, 18], etc. Undoubtedly, other new applications of continuous-stage methods in geometric integration are actively under development.

More recently, the present author et al. [42, 39] have developed symplectic RKN-type integrators by virtue of continuous-stage methods. In this paper, we are going to enlarge the primitive framework of csRKN methods to a new one which enables us to treat more complicated cases. For this sake, by using the similar idea presented in [47], we will lead weight function into the formalism of csRKN methods and define the continuous-stage methods in a general interval $I$ (finite or infinite). By doing this, a variety of classical weighted orthogonal polynomials can be used in the construction of RKN-type methods. As an important application, new symmetric and symplectic integrators can be easily derived in this new framework.

This paper will be organized as follows. In Section 2, we introduce the new definition of csRKN methods for solving second-order differential equations. This is followed by Section 3, where the order theory by using simplifying assumptions will be given. Section 4 is devoted to present our
2. Continuous-stage Runge-Kutta-Nyström methods

We are concerned with the initial value problem governed by a second-order system

\[ q'' = f(t, q), \quad q(t_0) = q_0, \quad q'(t_0) = q'_0, \]  

(2.1)

where \( f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d \) is assumed to be a smooth vector-valued function.

**Definition 2.1.** A non-negative function \( w(x) \) is called a weight function on the interval \( I \), if it satisfies the following two conditions:

(a) The \( k \)-th moment \( \int_I x^k w(x) \, dx \), \( k \in \mathbb{N} \) exists;

(b) For any non-negative function \( u(x) \), \( \int_I u(x) w(x) \, dx = 0 \) implies \( u(x) \equiv 0 \).

Based on the notion of weight function, we introduce the following definition of continuous-stage Runge-Kutta-Nyström methods which is an extended version of that given in [39, 42].

**Definition 2.2.** Let \( w(x) \) be a weight function defined on \( I \) (finite or infinite), \( \bar{A}_{\tau,\sigma} \) be a function of variables \( \tau, \sigma \in I \) and \( \bar{B}_\tau, B_\tau, C_\tau \) be functions of \( \tau \in I \). The continuous-stage Runge-Kutta-Nyström (csRKN) method for solving (2.1) is given by

\[
Q_\tau = q_0 + hC_\tau q'_0 + h^2 \int_I \bar{A}_{\tau,\sigma} w(\sigma) f(t_0 + C_\sigma h, Q_\sigma) d\sigma, \quad \tau \in I, \\
q_1 = q_0 + hq'_0 + h^2 \int_I \bar{B}_\tau w(\tau) f(t_0 + C_\tau h, Q_\tau) d\tau, \\
q'_1 = q'_0 + h \int_I B_\tau w(\tau) f(t_0 + C_\tau h, Q_\tau) d\tau,
\]

(2.2a, 2.2b, 2.2c)

which can be characterized by the following Butcher tableau

\[
\begin{array}{c|cc}
C_\tau & \bar{A}_{\tau,\sigma} w(\sigma) \\
\hline & \bar{B}_\tau w(\tau) \\
& B_\tau w(\tau)
\end{array}
\]

**Remark 2.3.** For the case when \( I \) is an infinite interval, we assume that the improper integrals of (2.2a, 2.2c) satisfy some conditions (in terms of uniform convergence) such that differentiation under the integral sign with respect to parameter \( h \) (step size) is legal.

**Remark 2.4.** If we let \( I = [0, 1] \) and \( w(x) = 1 \), then it results in the methods developed in [39, 42]. However, remark that the primitive framework of csRKN methods given in [39, 42] can not be applicable for more complicated cases, e.g., the case for weighting on a infinite interval \(( -\infty, +\infty)\) or any other general interval \( I \).
3. Discussions on the order theory

**Definition 3.1.** [14] A csRKN method is called order \( p \), if for all sufficiently regular problem (2.1), as \( h \to 0 \), its local error satisfies

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

**3.1. The order of csRKN methods**

Following the idea of classical cases [14] [16], we propose the following simplifying assumptions

\[
\mathcal{B}(\xi) : \int_I B_\tau w(\tau) C_{\tau}^{\kappa - 1} d\tau = \frac{1}{\kappa}, \quad 1 \leq \kappa \leq \xi,
\]

\[
\mathcal{C}\mathcal{N}(\eta) : \int_I \bar{A}_{\tau, \sigma} w(\sigma) C_{\sigma}^{\kappa - 1} d\sigma = \frac{C_{\eta}^{\kappa + 1}}{\kappa(\kappa + 1)}, \quad 1 \leq \kappa \leq \eta - 1,
\]

\[
\mathcal{D}\mathcal{N}(\zeta) : \int_I B_\tau w(\tau) C_{\tau}^{\kappa - 1} \bar{A}_{\tau, \sigma} d\tau = \frac{B_\sigma C_{\sigma}^{\kappa + 1}}{\kappa(\kappa + 1)} + \frac{B_\sigma}{\kappa + 1}, \quad 1 \leq \kappa \leq \zeta - 1,
\]

where \( \tau, \sigma \in I \).

**Theorem 3.2.** If the csRKN method (2.2a)-(2.2c) with its coefficients satisfying the simplifying assumptions \( \mathcal{B}(p), \mathcal{C}\mathcal{N}(\eta), \mathcal{D}\mathcal{N}(\zeta) \), and if \( B_\tau = B_\tau(1 - C_\tau) \) is always fulfilled, then the method is of order at least \( \min\{p, 2\eta + 2, \eta + \zeta\} \).

**Proof.** This is a straightforward result of Theorem 3.3 in [39].

In what follows, we will use the hypothesis \( C_\tau = \tau \) (and thus \( \bar{B}_\tau = B_\tau(1 - \tau) \)) throughout this paper. Let us establish a lemma in the first place.

**Lemma 3.3.** With the hypothesis \( C_\tau = \tau \), the simplifying assumptions \( \mathcal{B}(\xi), \mathcal{C}\mathcal{N}(\eta) \) and \( \mathcal{D}\mathcal{N}(\zeta) \) are equivalent to, respectively,

\[
\mathcal{B}(\xi) : \int_I B_\tau w(\tau) \phi(\tau) d\tau = \int_0^1 \phi(x) dx, \quad \forall \phi \text{ with } \deg(\phi) \leq \xi - 1,
\]

\[
\mathcal{C}\mathcal{N}(\eta) : \int_I \bar{A}_{\tau, \sigma} w(\sigma) \phi(\sigma) d\sigma = \int_0^\alpha \phi(x) dx da, \quad \forall \phi \text{ with } \deg(\phi) \leq \eta - 2,
\]

\[
\mathcal{D}\mathcal{N}(\zeta) : \int_I B_\tau \bar{A}_{\tau, \sigma} w(\tau) \phi(\tau) d\tau = B_\sigma \left( \int_0^\alpha \phi(x) dx da + \int_0^1 x\phi(x) dx \right), \quad \forall \phi \text{ with } \deg(\phi) \leq \zeta - 2,
\]

where \( \deg(\phi) \) stands for the degree of polynomial function \( \phi \).

**Proof.** With the hypothesis \( C_\tau = \tau \), we can rewrite \( \mathcal{B}(\xi), \mathcal{C}\mathcal{N}(\eta) \) and \( \mathcal{D}\mathcal{N}(\zeta) \) as

\[
\mathcal{B}(\xi) : \int_I B_\tau w(\tau) \tau^{\kappa - 1} d\tau = \int_0^1 x^{\kappa - 1} dx, \quad 1 \leq \kappa \leq \xi,
\]

\[
\mathcal{C}\mathcal{N}(\eta) : \int_I \bar{A}_{\tau, \sigma} w(\sigma) \sigma^{\kappa - 1} d\sigma = \int_0^\alpha \int_0^\alpha x^{\kappa - 1} dx da, \quad 1 \leq \kappa \leq \eta - 1,
\]

\[
\mathcal{D}\mathcal{N}(\zeta) : \int_I B_\tau w(\tau) \tau^{\kappa - 1} \bar{A}_{\tau, \sigma} d\tau = B_\sigma \left( \int_0^\alpha \int_0^\alpha x^{\kappa - 1} dx da + \int_0^1 x \cdot x^{\kappa - 1} dx \right), \quad 1 \leq \kappa \leq \zeta - 1,
\]

\footnote{It should be noticed that in \( \mathcal{D}\mathcal{N}(\zeta) \) we have removed “\( w(\sigma) \)” from both sides of the formula.}
Therefore, these formulae are satisfied for all monomials like $x^\iota$ with degree $\iota$ no larger than $\xi - 1, \eta - 2$ and $\zeta - 2$ respectively. Consequently, the final result follows from the fact that any polynomial function $\phi$ can be expressed as a linear combination of monomials.

It is known that for a given weight function $w(x)$, there exists a sequence of orthogonal polynomials in the weighted function space (Hilbert space) \[ L^2_w(I) = \{ u \text{ is measurable on } I : \int_I |u(x)|^2 w(x) \, dx < +\infty \} \]
which is linked with the inner product
\[
\langle u, v \rangle_w = \int_I u(x)v(x) w(x) \, dx. \tag{3.4}
\]

To proceed with our discussions, we denote a sequence of weighted orthogonal polynomials by \( \{ P_n(x) \}_{n=0}^\infty \), which consists of a complete set in the Hilbert space \( L^2_w(I) \). It is known that \( P_n(x) \) has exactly \( n \) real simple zeros in the interval \( I \). For convenience, in what follows we always assume the orthogonal polynomials are normalized, i.e., satisfying
\[
\langle P_i, P_j \rangle_w = \delta_{ij}, \quad i, j = 0, 1, 2, \ldots.
\]

**Theorem 3.4.** Let \( C_\tau = \tau \) and suppose \( B_\tau, \tilde{A}_{\tau, \sigma}, (B_\tau \tilde{A}_{\tau, \sigma}) \in L^2_w(I) \), then we have

(a) \( B(\xi) \) holds \( \iff \) \( B_\tau \) has the following form in terms of the normalized orthogonal polynomials in \( L^2_w(I) \):
\[
B_\tau = \sum_{j=0}^{\xi-1} \int_0^1 P_j(x) \, dx P_j(\tau) + \sum_{j \geq \xi} \lambda_j P_j(\tau), \tag{3.5}
\]
where \( \lambda_j \) are any real parameters;

(b) \( CN(\eta) \) holds \( \iff \) \( \tilde{A}_{\tau, \sigma} \) has the following form in terms of the normalized orthogonal polynomials in \( L^2_w(I) \):
\[
\tilde{A}_{\tau, \sigma} = \sum_{j=0}^{\eta-2} \int_0^\sigma \int_0^\tau P_j(x) \, dx \, d\alpha P_j(\sigma) + \sum_{j \geq \eta-1} \phi_j(\tau) P_j(\sigma), \tag{3.6}
\]
where \( \phi_j(\tau) \) are any \( L^2_w \)-integrable real functions;

(c) \( DN(\zeta) \) holds \( \iff \) \( B_\tau \tilde{A}_{\tau, \sigma} \) has the following form in terms of the normalized orthogonal polynomials in \( L^2_w(I) \):
\[
B_\tau \tilde{A}_{\tau, \sigma} = \sum_{j=0}^{\zeta-2} B_j \left( \int_\sigma^1 \int_0^\alpha P_j(x) \, dx \, d\alpha + \int_0^1 xP_j(x) \, dx \right) P_j(\tau) + \sum_{j \geq \zeta-1} \psi_j(\sigma) P_j(\tau), \tag{3.7}
\]
where \( \psi_j(\sigma) \) are any \( L^2_w \)-integrable real functions.

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The notation \( \tilde{A}_{\tau, \sigma} \) stands for the one-variable function in terms of \( \sigma \), and \( \tilde{A}_{\tau, \sigma} \) can be understood likewise.
Proof. This theorem can be proved in the same manner as Theorem 2.3 of [44]. For part (a), consider the following orthogonal polynomial expansion in $L^2_w(I)$

$$B_\tau = \sum_{j \geq 0} \lambda_j P_j(\tau), \quad \lambda_j \in \mathbb{R},$$

and substitute the formula above into (3.1) (with $\phi$ replaced by $P_j$) in Lemma 3.3, then it follows

$$\lambda_j = \int_0^1 P_j(x) \, dx, \quad j = 0, \cdots, \xi - 1,$$

which gives (3.5). For part (b) and (c), consider the following orthogonal expansions of $\tilde{A}_{\tau,\sigma}$ with respect to $\sigma$ and $B_\tau \tilde{A}_{\tau,\sigma}$ with respect to $\tau$ in $L^2_w(I)$, respectively,

$$\tilde{A}_{\tau,\sigma} = \sum_{j \geq 0} \phi_j(\tau) P_j(\sigma), \quad \phi_j(\tau) \in L^2_w(I),$$

$$B_\tau \tilde{A}_{\tau,\sigma} = \sum_{j \geq 0} \psi_j(\sigma) P_j(\tau), \quad \psi_j(\sigma) \in L^2_w(I),$$

and then substitute them into (3.2) and (3.3), which then leads to the final results.

\[ \square \]

Remark 3.5. For the sake of obtaining a practical csRKN method, we have to define a finite form for $B_\tau$ and $\tilde{A}_{\tau,\sigma}$. A natural and simple way is to truncate the series (3.5) and (3.6). As a consequence, $B_\tau$ and $\tilde{A}_{\tau,\sigma}$ become polynomial functions.

3.2. The order of RKN methods by using quadrature formulas

In the practical implementation, generally we have to approximate the integrals of the csRKN method by numerical quadrature formulas. For this sake, we introduce the following $s$-point weighted interpolatory quadrature formula

$$\int_I \Phi(\tau) w(\tau) \, d\tau \approx \sum_{i=1}^{s} b_i \Phi(c_i), \quad c_i \in I,$$

(3.8)

where

$$b_i = \int_I \ell_i(\tau) w(\tau) \, d\tau, \quad \ell_i(\tau) = \prod_{j=1,j\neq i}^{s} \frac{\tau - c_j}{c_i - c_j}, \quad i = 1, \cdots, s.$$

After applying the quadrature formula to (2.2a)-(2.2c), it gives rise to an $s$-stage RKN method

$$Q_i = q_0 + hC_i q_0' + h^2 \sum_{j=1}^{s} b_j A_{ij} f(t_0 + C_j h, Q_j), \quad i = 1, \cdots, s,$$

(3.9a)

$$q_1 = q_0 + hq_0' + h^2 \sum_{i=1}^{s} b_i B_i f(t_0 + C_i h, Q_i),$$

(3.9b)

$$q_1' = q_0' + h \sum_{i=1}^{s} b_i B_i f(t_0 + C_i h, Q_i).$$

(3.9c)
where $Q_i := Q_{c_i}, \tilde{A}_{ij} := \tilde{A}_{c_i,c_j}, \tilde{B}_i := \tilde{B}_{c_i}, B_i := B_{c_i}, C_i := C_{c_i} = c_i$ (recall that $C_\tau = \tau$), which can be characterized by

\[
\begin{array}{c|ccc}
  c_1 & b_1 A_{11} & \cdots & b_s A_{1s} \\
  \vdots & \vdots & & \vdots \\
  c_s & b_1 A_{s1} & \cdots & b_s A_{ss} \\
\hline
  b_1 B_1 & \cdots & b_s B_s \\
\end{array}
\]  

(3.10)

In order to analyze the order of the RKN method (3.10), we propose the following result which is closely related with Remark 3.5.

Theorem 3.6. Assume the underlying quadrature formula (3.8) is of order $p$, and $\tilde{A}_{\tau, \sigma}$ is of degree $\pi^\tau_A$ with respect to $\tau$ and of degree $\pi^\sigma_A$ with respect to $\sigma$, and $B_\tau$ is of degree $\pi^\tau_B$. If we assume $C_\tau = \tau, B_\tau = B_\tau(1 - \tau)$, and all the simplifying assumptions $B(\xi), C N(\eta), D N(\zeta)$ are fulfilled, then the RKN method (3.10) is at least of order

\[
\min\{\rho, 2\alpha + 2, \alpha + \beta\},
\]

where $\rho = \min\{\xi, p - \pi^\tau_B\}, \alpha = \min\{\eta, p - \pi^\sigma_A + 1\}$ and $\beta = \min\{\zeta, p - \pi^\tau_A - \pi^\tau_B + 1\}$.

Proof. Since the quadrature formula (3.8) holds for any polynomial $\Phi(x)$ of degree up to $p - 1$, by using it to compute the integrals of $B(\xi), C N(\eta), D N(\zeta)$ it gives

\[
\begin{align*}
\sum_{i=1}^s (b_i B_i) c_i^{\kappa-1} &= \frac{1}{\kappa}, \quad \kappa = 1, \ldots, \rho, \\
\sum_{j=1}^s (b_j \tilde{A}_{ij}) c_j^{\kappa-1} &= \frac{c_j^{\kappa+1}}{\kappa(\kappa + 1)}, \quad i = 1, \ldots, s, \quad \kappa = 1, \ldots, \alpha - 1, \\
\sum_{i=1}^s (b_i B_i) c_i^{\kappa-1}(b_j \tilde{A}_{ij}) &= \frac{(b_j B_j) c_j^{\kappa+1}}{\kappa(\kappa + 1)} - \frac{b_j B_j c_j}{\kappa} + \frac{b_j B_j}{\kappa + 1}, \quad j = 1, \ldots, s, \quad \kappa = 1, \ldots, \beta - 1.
\end{align*}
\]

where $\rho = \min\{\xi, p - \pi^\tau_B\}, \alpha = \min\{\eta, p - \pi^\sigma_A + 1\}$ and $\beta = \min\{\zeta, p - \pi^\tau_A - \pi^\tau_B + 1\}$. These formulas imply that the RKN method with coefficients given by (3.10) satisfies the classical simplifying assumptions $B(\rho), C N(\alpha)$ and $D N(\beta)$ (see [16]), and it is observed that we also have $b_i B_i = b_i B_i(1 - c_i)$ for each $i = 1, \ldots, s$. Consequently, it gives rise to the order of the method by the classical result [16] [14].

4. Geometric integration by csRKN methods

In this section, we discuss the geometric integration by csRKN methods. As pointed out in [16], symplectic integrators for Hamiltonian systems and symmetric integrators for reversible systems play a central role in the geometric integration of differential equations, for the reason that they possess excellent numerical behaviors in long-time integration. So far, there are many literatures concentrating on the theoretical analysis and empirical study of these integrators, see [2] [11] [12] [13] [16] [21] [29] and references therein.
4.1. Symplectic integrators

A very important subclass of dynamical systems in classical and non-classical mechanics are the so-called Hamiltonian systems [1], which read

\[ z' = J^{-1} \nabla_z H(z), \quad z(t_0) = z_0 \in \mathbb{R}^{2d}, \quad z = \begin{pmatrix} p \\ q \end{pmatrix}, \quad J = \begin{pmatrix} 0 & I_{d \times d} \\ -I_{d \times d} & 0 \end{pmatrix}, \tag{4.1} \]

where \( q \in \mathbb{R}^d \) represents the position coordinates, \( p \in \mathbb{R}^d \) the momentum coordinates, and \( H \) the Hamiltonian function (generally represents the total energy). Such system possesses a symplectic structure (a characteristic property of the system [16]), which means the phase flow \( \varphi_t \) satisfies

\[ d \varphi_t(z_0) \wedge J d \varphi_t(z_0) = d z_0 \wedge J d z_0, \quad \forall z_0 \in D, \]

where \( \wedge \) represents the wedge product, and \( D \) is an open subset in the phase space. For the sake of respecting such geometric structure in numerical discretization, symplectic integrators are suggested by some earlier scientists (see [11, 27, 52] and references therein), the definition of which can be stated as follows.

**Definition 4.1.** A one-step method \( \phi_h : z_0 = (p_0, q_0) \mapsto (p_1, q_1) = z_1 \) is called symplectic if and only if

\[ d \phi_h(z_0) \wedge J d \phi_h(z_0) = d z_0 \wedge J d z_0, \quad \forall z_0 \in D, \]

whenever the method is applied to a smooth Hamiltonian system.

A class of Hamiltonian systems frequently encountered in practice is the following

\[ p' = -\nabla_q V(q), \quad q' = Mp, \tag{4.2} \]

with the Hamiltonian

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

where \( M \) is a constant symmetric matrix, and \( V(q) \) is a scalar function. This equations can also be rewritten as a second-order system

\[ q'' = -M \nabla_q V(q). \tag{4.3} \]

By using the notations \( f(q) = -M \nabla_q V(q) \) and \( g(q) = -\nabla_q V(q) \), we propose the following csRKN method for solving (4.3)

\[ Q_\tau = q_0 + hC_\tau M p_0 + h^2 \int_I \bar{A}_{\tau, \sigma} w(\sigma) f(Q_\sigma) d\sigma, \quad \tau \in I, \tag{4.4a} \]
\[ q_1 = q_0 + hM p_0 + h^2 \int_I B_\tau w(\tau) f(Q_\tau) d\tau, \tag{4.4b} \]
\[ p_1 = p_0 + h \int_I B_\tau w(\tau) g(Q_\tau) d\tau. \tag{4.4c} \]

Remark that here we have removed the constant matrix \( M \) from both sides of 4.4c which will not affect the order of the method. The following theorems have extended the corresponding results previously presented in [39].
Theorem 4.2. If the coefficients of a csRKN method \((4.4a-4.4c)\) satisfy

\[
\begin{align*}
\bar{B}_\tau &= B_\tau(1 - C_\tau), \quad \tau \in I, \\
B_\tau(\bar{B}_\sigma - \bar{A}_{\tau,\sigma}) &= B_\sigma(\bar{B}_\tau - \bar{A}_{\sigma,\tau}), \quad \tau, \sigma \in I,
\end{align*}
\]

then the method is symplectic for solving the system \((4.3)\).

Proof. The proof is very the same as that of Theorem 4.2 in \([39]\) with the range of integration replaced by a general interval \(I\).

Remark 4.3. Theorem 4.2 implies that the symplecticity of the csRKN methods is independent of its weight function.

Theorem 4.4. Suppose that \(C_\tau = \tau\) and \(\bar{A}_{\tau,\sigma}/B_\sigma \in L_w(I \times I)\), then the symplectic condition given in Theorem 4.2 is equivalent to the fact that \(\bar{B}_\tau\) and \(\bar{A}_{\tau,\sigma}\) have the following form in terms of the normalized orthogonal polynomials \(P_n(x)\) in \(L_w^2(I)\)

\[
\begin{align*}
\bar{B}_\tau &= B_\tau(1 - \tau), \quad \tau \in I, \\
\bar{A}_{\tau,\sigma} &= B_\sigma \left(\alpha_{(0,0)} + \alpha_{(0,1)} P_1(\sigma) + \alpha_{(1,0)} P_1(\tau) + \sum_{i+j>1} \alpha_{(i,j)} P_i(\tau) P_j(\sigma)\right), \quad \tau, \sigma \in I,
\end{align*}
\]

where \(\alpha_{(0,0)}\) is an arbitrary real number, \(\alpha_{(0,1)} - \alpha_{(1,0)} = -\langle x, P_1(x) \rangle_w\) \((\text{see } (3.4))\), and the parameters \(\alpha_{(i,j)}\) are symmetric, i.e., \(\alpha_{(i,j)} = \alpha_{(j,i)}\) for \(\forall i + j > 1\).

Proof. On account of \(C_\tau = \tau\), we have

\[
\bar{B}_\tau = B_\tau(1 - \tau),
\]

inserting it into \((4.5b)\), then it yields

\[
B_\tau \bar{A}_{\tau,\sigma} - B_\sigma \bar{A}_{\sigma,\tau} = B_\tau B_\sigma(\tau - \sigma),
\]

which leads to

\[
\frac{\bar{A}_{\tau,\sigma}}{B_\sigma} - \frac{\bar{A}_{\sigma,\tau}}{B_\tau} = \tau - \sigma.
\]

Here we assume \(B_\tau \neq 0\), otherwise the csRKN method will be not practical for possessing no order accuracy. With the help of \(\tau = \sum_{i=0}^{1} \langle x, P_i(x) \rangle_w P_i(\tau)\) and notice that \(P_0(\tau) = P_0(\sigma) = \text{constant}\), \((4.8)\) becomes

\[
\begin{align*}
\frac{\bar{A}_{\tau,\sigma}}{B_\sigma} - \frac{\bar{A}_{\sigma,\tau}}{B_\tau} &= \sum_{i=0}^{1} \langle x, P_i(x) \rangle_w P_i(\tau) - \sum_{i=0}^{1} \langle x, P_i(x) \rangle_w P_i(\sigma), \\
&= \langle x, P_1(x) \rangle_w \left( P_1(\tau) - P_1(\sigma) \right).
\end{align*}
\]

Next, consider the expansion of \(\bar{A}_{\tau,\sigma}/B_\sigma\) along the normalized orthogonal basis \(\{P_i(\tau)P_j(\sigma)\}_{i,j=0}^{\infty}\) of \(L_w^2(I \times I)\)

\[
\frac{\bar{A}_{\tau,\sigma}}{B_\sigma} = \alpha_{(0,0)} + \alpha_{(0,1)} P_1(\sigma) + \alpha_{(1,0)} P_1(\tau) + \sum_{i+j>1} \alpha_{(i,j)} P_i(\tau) P_j(\sigma), \quad \alpha_{(i,j)} \in \mathbb{R}.
\]
By exchanging $\tau$ and $\sigma$ it gives
\[ \tilde{A}_{\sigma,\tau}/B_\tau = \alpha_{(0,0)} + \alpha_{(0,1)}P_1(\tau) + \alpha_{(1,0)}P_1(\sigma) + \sum_{i+j>1} \alpha_{(i,j)}P_1(\sigma)P_i(\tau), \]
where we have interchanged the indexes $i$ and $j$. By substituting the above two expressions into (4.9), it yields
\[ \alpha_{(0,0)} \in \mathbb{R}, \quad \alpha_{(0,1)} = -\langle x, P_1(x) \rangle_w, \quad \alpha_{(1,j)} = \alpha_{(j,i)}, \quad \forall i+j > 1, \]
which completes the proof by using (4.10).

**Theorem 4.5.** If the coefficients of a csRKN method (4.4a-4.4c) satisfies the symplectic conditions (4.5a-4.5b), then the RKN method (3.10) derived by using the quadrature formula (3.8) is always symplectic.

**Proof.** Please refer to Theorem 4.1 of [42] for a similar proof.

**Theorem 4.6.** With the hypothesis $C_\tau = \tau$, for a symplectic csRKN method with coefficients satisfying (4.5a-4.5b), we have the following statements:

(a) $B(\xi)$ and $C_N(\eta) \Rightarrow D_N(\zeta)$, where $\zeta = \min\{\xi, \eta\}$;
(b) $B(\xi)$ and $D_N(\zeta) \Rightarrow C_N(\eta)$, where $\eta = \min\{\xi, \zeta\}$.

**Proof.** Here we only provide the proof of (a), as (b) can be proved in a similar manner. From the proof of Theorem 4.4, we have get the formula (4.7) using the hypothesis $C_\tau = \tau$. Based on this, by multiplying $\sigma^{\kappa-1}$ from both sides of (4.7) and taking integral it gives
\[ B_\tau \int_I \tilde{A}_{\tau,\sigma} \sigma^{\kappa-1} d\sigma - \int_I B_\sigma \sigma^{\kappa-1} \tilde{A}_{\sigma,\tau} d\sigma = B_\tau \int_I B_\sigma \sigma^{\kappa-1}(\tau - \sigma) d\sigma, \quad \kappa = 1, 2, \ldots, \zeta - 1. \]  
(4.12)

Now let $\zeta = \min\{\xi, \eta\}$, and then $B(\xi)$ and $CN(\zeta)$ can be used for calculating the integrals of (4.12). As a result, we have
\[ B_\tau \frac{\tau^{\kappa+1}}{\kappa(\kappa + 1)} - \int_I B_\sigma \sigma^{\kappa-1} \tilde{A}_{\sigma,\tau} d\sigma = \frac{B_\tau \tau}{\kappa + 1}, \quad \kappa = 1, 2, \ldots, \zeta - 1. \]
Recall that $C_\tau = \tau$, it gives rise to
\[ \int_I B_\sigma \sigma^{\kappa-1} \tilde{A}_{\sigma,\tau} d\sigma = \frac{B_\tau C_\tau^{\kappa+1}}{\kappa(\kappa + 1)} - \frac{B_\tau C_\tau}{\kappa} + \frac{B_\tau}{\kappa + 1}, \quad \kappa = 1, 2, \ldots, \zeta - 1. \]
Finally, by exchanging $\tau \leftrightarrow \sigma$ in the formula above, it gives $D_N(\zeta)$ with $\zeta = \min\{\xi, \eta\}$.

**Remark 4.7.** A counterpart result for classical symplectic RKN methods can be similarly obtained.

On the basis of these preliminaries, following the same idea of [46], we introduce an operational procedure for deriving symplectic RKN-type integrators:

**Step 1.** Let $C_\tau = \tau$, $B_\tau = B_\tau(1 - C_\tau)$ and make an ansatz for $B_\tau$ by using (3.5) so as to satisfy
\(B(\xi)\). Note that a finite number of parameters, say \(\lambda_i\), could be kept as free parameters;

**Step 2.** Suppose \(\bar{\tt A}_{\tau, \sigma}\) is in the form (by Theorem 4.4, a truncation is needed)

\[
\bar{\tt A}_{\tau, \sigma} = B_\sigma \left( \alpha_{(0,0)} + \alpha_{(0,1)} P_1(\sigma) + \alpha_{(1,0)} P_1(\tau) + \sum_{i+j>1} \alpha_{(i,j)} P_i(\tau) P_j(\sigma) \right),
\]

(4.13)

where the parameters \(\alpha_{(i,j)}\) satisfy (4.11), and then substitute \(\bar{\tt A}_{\tau, \sigma}\) into \(\mathcal{CN}(\eta)\) (usually let \(\eta < \xi\)) for determining \(\alpha_{(i,j)}\):

\[
\int_{\bar{I}} \bar{\tt A}_{\tau, \sigma} w(\sigma) \phi_k(\sigma) \, d\sigma = \int_0^\tau \int_0^\tau \phi_k(x) \, dx \, d\alpha, \quad k = 0, 1, \ldots, n - 2,
\]

Here, \(\phi_k(x)\) stands for any polynomial of degree \(k\), which performs very similarly as the “test function” used in general finite element analysis;

**Step 3.** Write down \(B_\tau, \bar{\tt B}_\tau\) and \(\bar{\tt A}_{\tau, \sigma}\) (satisfy \(B(\xi)\) and \(\mathcal{CN}(\eta)\) automatically), which results in a symplectic csRKN method of order at least \(\min\{\xi, 2\eta + 2, \eta + \zeta\} = \min\{\xi, \eta + \zeta\}\) with \(\zeta = \min\{\xi, \eta\}\) by Theorem 3.2 and 4.6. If needed, we then acquire symplectic RKN methods by using quadrature rules (see Theorem 4.5).

The procedure above gives a general framework for deriving symplectic integrators. In view of Theorem 3.6 and 4.6, it is suggested to design Butcher coefficients with low-degree \(\bar{\tt A}_{\tau, \sigma}\) and \(\tt B_\tau\), and \(\eta\) is better to take as \(\eta \approx \frac{1}{2} \xi\). Besides, for the sake of conveniently computing those integrals of \(\mathcal{CN}(\eta)\) in the second step, the following ansatz may be advisable (let \(\rho \geq \eta\) and \(\xi \geq 2\eta - 1\))

\[
\begin{align*}
&\tt C_\tau = \tau, \quad B_\tau = \sum_{j=0}^{\xi-1} \int_0^1 P_j(x) \, dx P_j(\tau), \quad \tt \bar{B}_\tau = \tt B_\tau(1 - \tau), \\
&\bar{\tt A}_{\tau, \sigma} = B_\sigma \left( \alpha_{(0,0)} + \alpha_{(0,1)} P_1(\sigma) + \alpha_{(1,0)} P_1(\tau) + \sum_{1<i+j\leq \xi, \rho \leq \xi - \eta + 1} \alpha_{(i,j)} P_i(\tau) P_j(\sigma) \right),
\end{align*}
\]

(4.14)

where \(\alpha_{(0,1)} - \alpha_{(1,0)} = -\langle x, P_1(x) \rangle w\), \(\alpha_{(i,j)} = \alpha_{(j,i)}\), \(i + j > 1\). Because of the index \(j\) restricted by \(j \leq \xi - \eta + 1\) in (4.14), we can use \(B(\xi)\) to arrive at (please c.f. (3.1))

\[
\begin{align*}
&\int_{\bar{I}} \bar{\tt A}_{\tau, \sigma} w(\sigma) \phi_k(\sigma) \, d\sigma \\
&= \int_{\bar{I}} B_\sigma \left( \alpha_{(0,0)} + \alpha_{(0,1)} P_1(\sigma) + \alpha_{(1,0)} P_1(\tau) + \sum_{1<i+j\leq \xi, \rho \leq \xi - \eta + 1} \alpha_{(i,j)} P_i(\tau) P_j(\sigma) \right) w(\sigma) \phi_k(\sigma) \, d\sigma \\
&= \left( \alpha_{(0,0)} + \alpha_{(1,0)} P_1(\tau) \right) \int_0^1 \phi_k(x) \, dx + \alpha_{(0,1)} \int_0^1 P_1(x) \phi_k(x) \, dx \\
&\quad + \sum_{1<i+j\leq \xi, \rho \leq \xi - \eta + 1} \alpha_{(i,j)} P_i(\tau) \int_0^1 P_j(x) \phi_k(x) \, dx, \quad 0 \leq k \leq \eta - 2.
\end{align*}
\]

An alternative technique is to consider using \(\mathcal{DN}(\zeta)\). 

---

\(1\) An alternative technique is to consider using \(\mathcal{DN}(\zeta)\).
Therefore, \( \mathcal{CN}(\eta) \) implies that

\[
(\alpha(0,0) + \alpha(1,0)P_1(\tau)) \int_0^1 \phi_k(x) \, dx + \alpha(0,1) \int_0^1 P_1(x)\phi_k(x) \, dx \\
+ \sum_{1 < i+j \leq 2 \atop i \leq \rho_1 \leq j \leq \xi - \eta + 1} \alpha(i,j)P_i(\tau) \int_0^1 P_j(x)\phi_k(x) \, dx = \int_0^\alpha \phi_k(x) \, dx \, d\alpha, \quad 0 \leq k \leq \eta - 2.
\]

(4.15)

where \( \alpha(0,1) - \alpha(1,0) = -\langle x, P_1(x) \rangle_w \), \( \alpha(i,j) = \alpha(j,i) \), \( i + j > 1 \). Finally, it needs to settle \( \alpha(i,j) \) by transposing, comparing or merging similar items of (4.15) after the polynomial on right-hand side of (4.15) being represented by the basis \( \{P_j(\tau)\}_{j=0}^\infty \). In view of the symmetry of \( \alpha(i,j) \), if we let \( r = \min\{\rho, \xi - \eta + 1\} \), then actually the number of degrees of freedom of these parameters is \((r + 1)(r + 2)/2\), by noticing that

\[ \alpha(i,j) = 0, \quad \text{for } i > r \text{ or } j > r. \]

### 4.2. Symmetric integrators

Theoretical analyses and a large number of numerical tests indicate that symmetric integrators applied to (near-)integrable reversible systems share similar properties to symplectic integrators applied to (near-)integrable Hamiltonian systems: linear error growth, near-conservation of first integrals, existence of invariant tori [16]. The good long-time behavior of symmetric integrators motivates us to find more new integrators.

**Definition 4.8. [16]** A numerical one-step method \( \phi_h \) is called symmetric (or time-reversible) if it satisfies

\[ \phi^*_h = \phi^{-1}_h \]

where \( \phi^*_h = \phi^{-1}_h \) is referred to as the adjoint method of \( \phi_h \).

**Remark 4.9.** Symmetry implies that the original method and the adjoint method give identical numerical results. A well-known property of symmetric integrators is that they possess an even order [16]. By the definition, a one-step method \( z_1 = \phi_h(z_0; t_0, t_1) \) is symmetric if exchanging \( h \leftrightarrow -h \), \( z_0 \leftrightarrow z_1 \) and \( t_0 \leftrightarrow t_1 \) leaves the original method unaltered.

In order to derive symmetric integrators, we assume the interval \( I \) to be the following two cases:

(i) \( I = [a, b] \) (finite interval) with \( a + b = 1 \);

(ii) \( I = (-\infty, +\infty) \) (infinite interval).

In what follows, we first establish the adjoint method of a given csRKN method. From (2.2a, 2.2c), by interchanging \( t_0, q_0, q'_0, h \) with \( t_1, q_1, q'_1, -h \), respectively, we have

\[
Q_{\tau} = q_1 - hC_\tau q'_1 + h^2 \int_I \bar{A}_{\tau,\sigma} w(\sigma)f(t_1 - C_\sigma h, Q_\sigma) \, d\sigma, \quad \tau \in I, \quad (4.16a)
\]

\[
q_0 = q_1 - hq'_1 + h^2 \int_I \bar{B}_\tau w(\tau)f(t_1 - C_\tau h, Q_{\tau}) \, d\tau, \quad (4.16b)
\]

\[
q'_0 = q'_1 - h \int_I B_{\tau} w(\tau)f(t_1 - C_\tau h, Q_{\tau}) \, d\tau. \quad (4.16c)
\]
Note that \( t_1 - C_\tau h = t_0 + (1 - C_\tau)h \), (4.16) becomes
\[
q_1' = q_0' + h \int_I B_\tau w(\tau)f(t_0 + (1 - C_\tau)h, Q_\tau)d\tau,
\]
substituting it into (4.16b) then we get
\[
q_1 = q_0 + hq_0' + h^2 \int_I (B_\tau - B_\tau^*)w(\tau)f(t_0 + (1 - C_\tau)h, Q_\tau)d\tau.
\] (4.18)
Next, inserting (4.17) and (4.18) into (4.16a), it follows that
\[
Q_\tau = q_0 + h(1 - C_\tau)q_0' + h^2 \int_I \left( B_{\sigma}(1 - C_\tau) - B_\sigma + \tilde{A}_{\tau,\sigma} \right) w(\sigma)f(t_0 + (1 - C_\sigma)h, Q_\sigma)d\sigma.
\]
By a change of variables (replacing \( \tau \) and \( \sigma \) with \( 1 - \tau \) and \( 1 - \sigma \) respectively), (4.19), (4.18) and (4.17) can be recast as
\[
Q^*_\tau = q_0 + hC^*_\tau q_0' + h^2 \int_I \tilde{A}^*_{\tau,\sigma} w(1 - \sigma)f(t_0 + C^*_\sigma h, Q^*_\sigma)d\sigma, \quad \tau \in I,
\]
\[
q_1 = q_0 + hq_0' + h^2 \int_I \tilde{B}^*_\tau w(1 - \tau)f(t_0 + C^*_\tau h, Q^*_\tau)d\tau,
\] (4.20)
\[
q_1' = q_0' + h \int_I \tilde{B}^*_\tau w(1 - \tau)f(t_0 + C^*_\tau h, Q^*_\tau)d\tau,
\]
where \( Q^*_\tau = Q_{1-\tau}, \tau \in I \) and
\[
C^*_\tau = 1 - C_{1-\tau},
\]
\[
\tilde{A}^*_{\tau,\sigma} = B_{1-\sigma}(1 - C_{1-\tau}) - B_{1-\sigma} + \tilde{A}_{1-\tau,1-\sigma},
\]
\[
\tilde{B}^*_\tau = B_{1-\tau} - \tilde{B}_{1-\tau},
\]
\[
\tilde{B}^*_\tau = B_{1-\tau},
\]
for \( \tau, \sigma \in I \). Consequently, we get the adjoint method given by (4.20)-(4.21). Hence if we require
\[
C_\tau = C^*_\tau, \quad \tilde{A}_{\tau,\sigma}w(\sigma) = \tilde{A}^*_{\tau,\sigma} w(1 - \sigma), \quad \tilde{B}_\tau w(\tau) = \tilde{B}^*_\tau w(1 - \tau), \quad B_\tau w(\tau) = B^*_\tau w(1 - \tau),
\]
then the original csRKN method is symmetric. We summarize the results above in the following theorem.

**Theorem 4.10.** If a csRKN method (2.2a-2.2c) satisfies
\[
C_\tau = 1 - C_{1-\tau},
\]
\[
\tilde{A}_{\tau,\sigma}w(\sigma) = \left( B_{1-\sigma}(1 - C_{1-\tau}) - B_{1-\sigma} + \tilde{A}_{1-\tau,1-\sigma} \right) w(1 - \sigma),
\] (4.22)
\[
\tilde{B}_\tau w(\tau) = (B_{1-\tau} - \tilde{B}_{1-\tau}) w(1 - \tau),
\]
\[
B_\tau w(\tau) = B_{1-\tau} w(1 - \tau),
\]
for \( \forall \tau, \sigma \in I \), then the method is symmetric. Particularly, if the weight function \( w(x) \) satisfies \( w(x) \equiv w(1 - x) \), then the symmetric condition (4.22) becomes
\[
C_\tau = 1 - C_{1-\tau},
\]
\[
\tilde{A}_{\tau,\sigma} = B_{1-\sigma}(1 - C_{1-\tau}) - B_{1-\sigma} + \tilde{A}_{1-\tau,1-\sigma},
\]
\[
\tilde{B}_\tau = B_{1-\tau} - \tilde{B}_{1-\tau},
\]
\[
B_\tau = B_{1-\tau},
\]
for \( \forall \tau, \sigma \in I \).
By using (4.10) and (4.25), it yields

Analogously to the proof of Theorem 4.4, let us consider the expansion of \( \bar{A}_{\tau,\sigma} \) in terms of the orthogonal polynomials \( P_n(x) \) in \( L_w^2(I) \)

\[
\bar{A}_{\tau,\sigma} = B_{\sigma} \left( \alpha_{(0,0)} + \alpha_{(0,1)} P_1(\sigma) + \alpha_{(1,0)} P_1(\tau) + \sum_{i+j \text{ is even} \quad 1<i+j<\infty} \alpha_{(i,j)} P_i(\tau) P_j(\sigma) \right), \quad \alpha_{(i,j)} \in \mathbb{R}, \quad (4.24)
\]

with \( B_{\sigma} \equiv B_{1-\sigma} \), where \( \alpha_{(0,1)} = -\alpha_{(1,0)} = -\frac{1}{2} \langle x, P_1(x) \rangle_w \), provided that the orthogonal polynomials \( P_n(x) \) satisfy

\[
P_n(1-x) = (-1)^n P_n(x), \quad n \in \mathbb{Z}. \quad (4.25)
\]

Proof. We only give the proof for the necessity, seeing that the sufficiency part is rather trivial. Since under the assumption \( w(x) \equiv w(1-x) \), we get (4.23). Hence, by using \( C_{\tau} = \tau, B_{\tau} = B_{\tau}(1-C_{\tau}) \) and \( B_{\sigma} \equiv B_{1-\sigma} \), the second formula of (4.23) becomes

\[
\bar{A}_{\tau,\sigma} = \bar{B}_{1-\tau,1-\sigma} = B_\sigma(\tau - \sigma),
\]

which leads to

\[
\frac{\bar{A}_{\tau,\sigma}}{B_\sigma} - \frac{\bar{A}_{1-\tau,1-\sigma}}{B_{1-\sigma}} = \tau - \sigma. \quad (4.26)
\]

Analogously to the proof of Theorem 4.4, let us consider the expansion of \( \bar{A}_{\tau,\sigma}/B_\sigma \) given by (4.10). By using (4.10) and (4.25), it yields

\[
\bar{A}_{1-\tau,1-\sigma}/B_{1-\sigma} = \alpha_{(0,0)} - \alpha_{(0,1)} P_1(\sigma) - \alpha_{(1,0)} P_1(\tau) + \sum_{i+j>1} (-1)^{i+j} \alpha_{(i,j)} P_i(\tau) P_j(\sigma).
\]

By substituting (4.10) and the above formula into (4.26) and comparing the like basis, it gives (4.24). \( \square \)

For the sake of employing Theorem 4.13, we also need some useful results which are quoted from [47].

Theorem 4.14. If \( w(x) \) is an even function, i.e., satisfying \( w(-x) \equiv w(x) \), then the shifted function defined by \( \bar{w}(x) = w(2\theta x - \theta) \) satisfies the symmetry relation: \( \bar{w}(x) \equiv \bar{w}(1-x) \). Here \( \theta \) is a non-zero constant.
Theorem 4.15. [47] If a sequence of polynomials \( \{P_n(x)\}_{n=0}^{\infty} \) satisfy the symmetry relation
\[
P_n(-x) = (-1)^nP_n(x), \quad n \in \mathbb{Z},
\]
then the shifted polynomials defined by \( \tilde{P}_n(x) = P_n(2\theta x - \theta) \) are bound to satisfy the property (4.25). Here \( \theta \) is a non-zero constant.

Theorem 4.16. [47] If a sequence of polynomials \( \{P_n(x)\}_{n=0}^{\infty} \) satisfy (4.25), then we have
\[
\int_0^1 P_j(x) \, dx = 0, \text{ for } j \text{ is odd},
\]
and the following function
\[
B_\sigma = \sum_{j=0}^{\xi-1} \int_0^1 P_j(x) \, dx P_j(\sigma) + \sum_{\text{even } j \geq \xi} \lambda_j P_j(\sigma), \quad \xi \geq 1,
\]
always satisfies \( B_\sigma \equiv B_{1-\sigma} \).

As pointed out in [47], many classical (standard) orthogonal polynomials including Hermite polynomials, Legendre polynomials, Chebyshev polynomials of the first and second kind, and any other general Gegenbauer polynomials etc., do not satisfy (4.25), but they possess the symmetry property (4.27). Nevertheless, by using Theorem 4.15 we can always shift them to a suitable interval such that the condition (4.25) is fulfilled. With these discussions, we can also propose an operational procedure for constructing symmetric integrators in a similar way as that given in the preceding subsection.

4.3. Some examples

In the following, we provide some examples for illustrating the application of our theoretical results. On account of (4.11), we only present the values of \( \alpha_{(i,j)} \) with \( i \leq j \) in our examples. Besides, the Gaussian-Christoffel’s quadrature rules (please see (3.8)) will be used, which means the quadrature nodes \( c_1, c_2, \ldots, c_s \) are exactly the zeros of the normalized orthogonal polynomial \( P_s(x) \) in \( L^2_w(I) \). For the sake of deriving symmetric methods we mainly consider the weighted orthogonal polynomials shifted into a suitable interval.

Example 4.1. Consider using the shifted normalized Legendre polynomials which are orthogonal with respect to the weight function \( w(x) = 1 \) on \([0,1] \). These Legendre polynomials \( L_n(x) \) can be defined by Rodrigues’ formula [13]
\[
L_0(x) = 1, \quad L_n(x) = \frac{\sqrt{2n+1}}{n!} \frac{d^n}{dx^n} \left( t^n(t-1)^n \right), \quad x \in [0,1], \quad n = 1, 2, \ldots.
\]

Let \( \xi = 3, \eta = 2, \rho = 2 \) in (4.14), \( r = 2 \) and thus the number of degrees of freedom is \((r+1)(r+2)/2 = 6\). For simplicity, we set \( \alpha_{(i,j)} = 0 \) for \( 0 \leq i, j \leq 2, i + j > 2 \). After some elementary calculations, it gives
\[
\alpha_{(0,0)} = \frac{1}{6}, \quad \alpha_{(0,1)} = -\frac{\sqrt{3}}{12}, \quad \alpha_{(1,1)} = \mu, \quad \alpha_{(0,2)} = \frac{\sqrt{5}}{60},
\]
Table 4.1: A family of 2-stage 4-order symmetric and symplectic RKN methods, based on the shifted Legendre polynomials $L_n(x)$.

|    | $\frac{3-\sqrt{3}}{6}$ | $1+\frac{\sqrt{3}}{12}$ | $\frac{1}{12} + \gamma$ | $\frac{1-\sqrt{3}}{12} - \gamma$ |
|----|------------------------|--------------------------|--------------------------|--------------------------|
| 2  | $\frac{3+\sqrt{3}}{6}$ | $1+\frac{\sqrt{3}}{12}$ | $\frac{1}{12} + \gamma$ | $\frac{1-\sqrt{3}}{12} - \gamma$ |
| 1  | $\frac{3+\sqrt{3}}{12}$ | $\frac{3-\sqrt{3}}{12}$ |

Table 4.2: A family of 3-stage 4-order symmetric and symplectic RKN methods, based on the shifted Chebyshev polynomials of the first kind $T_n(x)$.

|    | $\frac{2-\sqrt{3}}{4}$ | $\frac{13}{216} + \gamma$ | $\frac{85-60\sqrt{3}}{864}$ | $\frac{13-12\sqrt{3}}{216} - \gamma$ |
|----|------------------------|--------------------------|--------------------------|--------------------------|
| 1  | $\frac{3+\sqrt{3}}{4}$ | $\frac{17+12\sqrt{3}}{432}$ | $\frac{5}{108}$ | $\frac{17-12\sqrt{3}}{432}$ |
| 2  | $\frac{2+\sqrt{3}}{18}$ | $\frac{13+12\sqrt{3}}{216} - \gamma$ | $\frac{85-60\sqrt{3}}{864}$ | $\frac{13}{216} + \gamma$ |
| 0  | $\frac{2+\sqrt{3}}{18}$ | $\frac{5}{18}$ | $\frac{2-\sqrt{3}}{18}$ |

where $\alpha_{(1,1)} = \mu$ is a free parameter, then we get a $\mu$-parameter family of symmetric (by Theorem 4.13) and symplectic csRKN methods of order 4. By using Gauss-Christoffel’s quadrature rules with 2 nodes, we get a family of symmetric and symplectic RKN methods of order 4 which are shown in Tab. 4.1 with $\gamma = \frac{1}{2}\mu$. It is found that this family of methods coincides with the methods presented in [39].

**Example 4.2.** Consider using the shifted normalized Chebyshev polynomials of the first kind which are orthogonal with respect to the weight function $w(x) = \frac{1}{2\sqrt{x(1-x)}}$ on $[0,1]$. These Chebyshev polynomials $T_n(x)$ can be defined by [45]

$T_0(x) = \frac{\sqrt{2}}{\sqrt{\pi}}, \ T_n(x) = \frac{2 \cos \left(n \arccos(2x - 1)\right)}{\sqrt{\pi}}, \ x \in [0,1], \ n = 1, 2, \cdots$

Let $\xi = 3$, $\eta = 2$, $\rho = 2$ in (4.14) and set $\alpha_{(i,j)} = 0$ for $0 \leq i, j \leq 2, i + j > 2$. After some elementary calculations, it gives

$\alpha_{(0,0)} = \frac{5}{24}, \ \alpha_{(0,1)} = -\frac{\sqrt{\pi}}{8}, \ \alpha_{(1,1)} = \mu, \ \alpha_{(0,2)} = \frac{\sqrt{2}}{64}\pi,$

where $\alpha_{(1,1)} = \mu$ is a free parameter, then we get a $\mu$-parameter family of symplectic csRKN methods of order at least 3. However, since we have $\alpha_{(0,1)} = -\frac{1}{2} \langle x, T_1(x) \rangle_w = -\frac{\sqrt{\pi}}{8}$ and other conditions of Theorem 4.13 are fulfilled, the newly-derived methods are symmetric and of an even order 4. By using Gauss-Christoffel’s quadrature rules with 3 nodes, we get a family of symmetric and symplectic RKN methods of order 4 which are shown in Tab. 4.2 with $\gamma = \frac{2\mu}{3\pi}$.

**Example 4.3.** Consider using the shifted normalized Hermite polynomials which are orthogonal with respect to the weight function $\hat{w}(x) = e^{-(2x-1)^2}$ on $(-\infty, +\infty)$. These Hermite polynomials $\hat{H}_n(x)$ can be defined by [47]

$\hat{H}_n(x) = \sqrt{2}H_n(2x - 1), \ x \in (-\infty, +\infty), \ n = 0, 1, \cdots,$
where $H_n(x)$ is the standard normalized $n$-degree Hermite polynomial
\[
H_0(x) = \frac{1}{\pi^{\frac{1}{4}}}, \quad H_n(x) = \frac{(-1)^n e^{-x^2}}{\sqrt{2^n n! \pi^{\frac{n+1}{2}}}} \frac{d^n}{dx^n} (e^{-x^2}), \quad x \in (-\infty, +\infty), \quad n = 1, 2, \cdots, 
\]
with the weight function given by $w(x) = e^{-x^2}$.

Let $\xi = 3$, $\eta = 2$, $\rho = 2$ in (4.14) and set $\alpha(i,j) = 0$ for $0 \leq i, j \leq 2, i + j > 2$. After some elementary calculations, it gives
\[
\alpha(0,0) = \frac{5}{24}, \quad \alpha(0,1) = -\frac{\pi}{8}, \quad \alpha(1,1) = \mu, \quad \alpha(0,2) = \frac{\sqrt{2\pi}}{32},
\]
where $\alpha(1,1) = \mu$ is a free parameter, then we get a $\mu$-parameter family of symplectic csRKN methods of order at least 3. However, since we have $\alpha(0,1) = -\frac{\pi}{8}$ and other conditions of Theorem 4.13 are fulfilled, the newly-derived methods are symmetric and of an even order 4. By using Gauss-Christoffel’s quadrature rules with 3 nodes, we get a family of symmetric and symplectic RKN methods of order 4 which are shown in Tab. 4.3 with the weight function given by $w(x) = e^{-x^2}$.

We claim that if we do not use the shifted Hermite polynomials $H_n(x)$, then it may result in symplectic methods without the symmetric property. Let us consider using $H_n(x)$ to construct symplectic methods, take the same $\xi = 3$, $\eta = 2$, $\rho = 2$, and also set $\alpha(i,j) = 0$ for $0 \leq i, j \leq 2, i + j > 2$. Additionally, we impose $\alpha(0,1) = -\frac{1}{2} \langle x, \tilde{H}_1(x) \rangle \hat{w} = -\frac{\pi}{8}$, then we get
\[
\alpha(0,0) = \frac{7}{12}, \quad \alpha(0,1) = -\frac{\sqrt{2\pi} \frac{1}{4}}, \quad \alpha(1,1) = -\frac{\sqrt{2\pi}}{2}, \quad \alpha(0,2) = \frac{\sqrt{2\pi}}{4}.
\]
In such a case, we get a symplectic csRKN method with order 3. One can verify that such method does not satisfy all the bushy tree order condition for order 4 (see $B(\xi)$), e.g.,
\[
\int_{-\infty}^{+\infty} B_\tau \hat{w}(\tau) C_\tau^3 d\tau = \int_{-\infty}^{+\infty} \frac{7 + 6\tau - 2\tau^2}{6\sqrt{\pi}} e^{-\tau^2} \tau^3 d\tau = \frac{3}{4} \neq \frac{1}{4},
\]

Table 4.3: A family of 3-stage 4-order symmetric and symplectic RKN methods, based on the shifted Hermite polynomials $\tilde{H}_n(x)$.

| $\alpha$ | $\beta$ | $\gamma$ | $\delta$ |
|---------|---------|---------|---------|
| $\frac{2-\sqrt{6}}{4}$ | $\frac{11}{216} + \gamma$ | $\frac{91-42\sqrt{6}}{432}$ | $\frac{11-6\sqrt{6}}{216} - \gamma$ |
| $\frac{1}{2}$ | $\frac{13+6\sqrt{6}}{432}$ | $\frac{7}{108}$ | $\frac{13-6\sqrt{6}}{432}$ |
| $\frac{2+\sqrt{6}}{4}$ | $\frac{11+6\sqrt{6}}{216} - \gamma$ | $\frac{91+42\sqrt{6}}{432}$ | $\frac{11}{216} + \gamma$ |

Table 4.4: A 3-stage 3-order symplectic RKN method (non-symmetric), based on the Hermite polynomials $H_n(x)$.

| $\alpha$ | $\beta$ | $\gamma$ | $\delta$ |
|---------|---------|---------|---------|
| $\frac{\sqrt{6}}{2}$ | $\frac{4-3\sqrt{6}}{2} \cdot 70 \cdot 21 \sqrt{6}$ | $\frac{40+87\sqrt{6}}{432}$ | $\frac{70-21\sqrt{6}}{108} \cdot 432$ |
| $0$ | $\frac{216}{216}$ | $\frac{7}{108}$ | $\frac{7-6\sqrt{6}}{216}$ |
| $\frac{\sqrt{6}}{2}$ | $\frac{40-87\sqrt{6}}{432}$ | $\frac{70+21\sqrt{6}}{108} \cdot 432$ | $\frac{4+3\sqrt{6}}{108} \cdot 432$ |
| $\frac{2}{36}$ | $\frac{36}{36}$ | $\frac{9}{36}$ | $\frac{9}{36}$ |

\[
\int_{-\infty}^{+\infty} B_\tau \hat{w}(\tau) C_\tau^3 d\tau = \int_{-\infty}^{+\infty} \frac{7 + 6\tau - 2\tau^2}{6\sqrt{\pi}} e^{-\tau^2} \tau^3 d\tau = \frac{3}{4} \neq \frac{1}{4},
\]

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hence it is of an odd order and can not be a symmetric method. Besides, by using corresponding Gauss-Christoffel’s quadrature rules with 3 nodes, we get a 3-stage 3-order symplectic RKN method which is shown in Tab. 4.4. Although it looks like as if the quadrature weights and nodes possess a kind of “symmetry”, the method is essentially not symmetric according to the classical symmetric conditions for RKN methods [25].

5. Numerical tests

In this section, we perform some numerical tests to verify our theoretical results. For ease of description and comparison studies, we denote our methods shown in Tab. 4.1-4.4 (with $\gamma = 0$) by Legendre-4, Chebyshev-4, Hermite-4 and Hermite-3 in turn and all of them will be applied to two classical mechanical problems.

**Example 5.1.** Consider the numerical integration of the well-known Kepler’s problem [16]. The Kepler’s problem describes the motion of two bodies which attract each other under the universal gravity. The motion of two-bodies can be described by

$$q_1'' = -\frac{q_1}{(q_1^2 + q_2^2)^{\frac{3}{2}}}, \quad q_2'' = -\frac{q_2}{(q_1^2 + q_2^2)^{\frac{3}{2}}}.$$

(5.1)

By introducing the momenta $p_1 = q_1', p_2 = q_2'$, we can transform (5.1) into a nonlinear Hamiltonian system with Hamiltonian

$$H = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}}.$$

Beside the Hamiltonian, the system possesses other two invariants: the quadratic angular momentum

$$I = q_1 p_2 - q_2 p_1 = q^T \left( \begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array} \right) q, \quad q = \left( \begin{array}{c} q_1 \\ q_2 \end{array} \right),$$

and the Runge-Lenz-Pauli-vector (RLP) invariant

$$L = \left( \begin{array}{c} p_1 \\ p_2 \\ 0 \end{array} \right) \times \left( \begin{array}{c} 0 \\ 0 \\ q_1 p_2 - q_2 p_1 \end{array} \right) - \frac{1}{\sqrt{q_1^2 + q_2^2}} \left( \begin{array}{c} q_1 \\ q_2 \\ 0 \end{array} \right).$$

In our numerical tests, we take the initial values as

$$q_1(0) = 1, \quad q_2(0) = 0, \quad p_1(0) = 0, \quad p_2(0) = 1,$$

and the corresponding exact solution is

$$q_1(t) = \cos(t), \quad q_2(t) = \sin(t), \quad p_1(t) = -\sin(t), \quad p_2(t) = \cos(t).$$

Applying our symplectic integrators to (5.1), we compute the approximation errors of the numerical solution to the exact solution, as well as the errors in terms of the above three invariants. These errors are shown in Fig. 5.1-5.4, where the errors at each time step are carried out in the maximum norm $||x||_\infty = \max(|x_1|, \cdots, |x_n|)$ for $x = (x_1, \cdots, x_n) \in \mathbb{R}^n$. It indicates that all the
Figure 5.1: Energy (Hamiltonian) errors by four new symplectic RKN methods for Kepler’s problem, with step size $h = 0.1$.

Figure 5.2: Angular momentum errors by four new symplectic RKN methods for Kepler’s problem, with step size $h = 0.1$. 
Figure 5.3: RLP invariant errors by four new symplectic RKN methods for Kepler’s problem, with step size $h = 0.1$.

Figure 5.4: Solution errors by four new symplectic RKN methods for Kepler’s problem, with step size $h = 0.1$. 
symplectic integrators show a near-preservation of the Hamiltonian and RLP invariant, and a practical preservation (up to the machine precision) of the quadratic angular momentum — symplectic RKN methods can preserve all quadratic invariants of the form $q^T D q'$ with $D$ a skew-symmetric matrix (see [16], page 104). The solution errors of $p$-variable and $q$-variable measured in Euclidean norm are shown in Fig. 5.4 which implies a linear error growth. It is observed that amongst four methods the Hermite-4 method gives the best result, while the Hermite-3 method is inferior to other three methods due to its lower accuracy. Moreover, all the numerical orbits by four methods (see Fig. 5.5) are in the shape of an ellipse, closely approximating to the exact one (we do not show it here). These numerical observations have well conformed with the common features of symplectic integration.

Example 5.2. Consider the numerical integration of the well-known Hénon-Heiles model problem [16], which was created for describing stellar motion. The problem can be described by

$$
q_1'' = -q_1 - 2q_1q_2, \quad q_2'' = -q_2 - q_1^2 + q_2^2.
$$

It is clear to see that (5.2) can be reduced to a first-order Hamiltonian system determined by the Hamiltonian

$$
H = \frac{1}{2} (p_1^2 + p_2^2) + \frac{1}{2} (q_1^2 + q_2^2) + q_1^2 q_2 - \frac{1}{3} q_2^3.
$$

In our experiment, the initial values are taken as

$$
q_1(0) = 0.1, \quad q_2(0) = -0.5, \quad p_1(0) = 0, \quad p_2(0) = 0,
$$

which will result in a chaotic behavior and the chaotic orbits should stay in the interior zone of an equilateral triangle [16, 26]. We present our numerical results in Fig. 5.6 and 5.7. It is observed
Figure 5.6: Energy (Hamiltonian) errors by four new symplectic RKN methods for Hénon-Heiles model problem, with step size $h = 0.1$.

Figure 5.7: Chaotic orbits by four new symplectic RKN methods for Hénon-Heiles model problem, with step size $h = 0.1$. 
that all the symplectic methods have a well near-preservation of the energy (see Fig. 5.6) and they numerically reproduce the correct behavior of the original system without points escaping from the equilateral triangle (see Fig. 5.7).

6. Concluding remarks

The constructive theory of continuous-stage Runge-Kutta-Nyström methods is examined in this paper. We establish a new framework for such methods by leading weight function into the formalism and imposing the range of integration to be a general interval $I$ (finite or infinite). Particularly, we intensively discuss its applications in the geometric integration of second-order differential equations. A systematic way for deriving symplectic and symmetric integrators is presented. We stress that our crucial technique for deriving these geometric integrators is the orthogonal polynomial expansion and the simplifying assumptions for order conditions. It is hoped that in the forthcoming future other new applications of the presented theoretical results will be discovered.

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