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

Wensheng Tang\textsuperscript{a}, Yajuan Sun\textsuperscript{b,*}, Jingjing Zhang\textsuperscript{c},

\textsuperscript{a}College of Mathematics and Computational Science
Changsha University of Science and Technology
Changsha 410114, China
\textsuperscript{b}LSEC, Academy of Mathematics and Systems Science
Chinese Academy of Sciences, Beijing 100190, P. R. China
\textsuperscript{c}School of Mathematics and Information Science,
Henan Polytechnic University, Jiaozuo 454001, China

Abstract

In this article, we develop high order symplectic integrators based on the recently developed continuous-stage Runge-Kutta Nyström (csRKN) methods for solving second order ordinary differential equations (ODEs) when written as separable Hamiltonian systems. The construction of such methods heavily relies on the Legendre polynomial expansion technique coupling with the simplifying assumptions and symplectic conditions. As the detail illustrations, we present three new one-parameter families of symplectic RKN methods of orders 4, 6 and 8 based on Gaussian type quadrature.

Keywords: Hamiltonian systems; Symplecticity-preserving; Runge-Kutta Nyström methods; Legendre polynomial; Symplectic conditions.

1. Introduction

In the last few decades, geometric structure preserving algorithms (also called geometric numerical integration) for conservative differential equations have drawn increasing attention of mathematicians and scientists. The most significant advantage of employing such algorithms is that they usually provide a more accurate long-time integration than those traditional methods for general purpose use, and they can correctly capture the qualitative features of the exact flow of original systems. As is well known, classical numerical methods such as Runge-Kutta (RK) methods, partitioned Runge-Kutta (PRK) methods and Runge-Kutta Nyström (RKN) methods play an important role in the field of numerical solution of ordinary differential equations (ODEs) and they
have reached a certain maturity up to now \cite{3, 9, 10}. Moreover, as expected, it is shown that based on such three classes of numerical methods the structure-preserving integrators can be established, and these algorithms are very practical for use as well as rather popular owing to their simpleness and convenience for application \cite{11, 13, 7, 8}.

As an extension of numerical methods with finite stages (e.g., classical RK method), numerical methods with infinitely many stages including continuous-stage Runge-Kutta (csRK) method, continuous-stage partitioned Runge-Kutta (csPRK) method and continuous-stage Runge-Kutta Nyström (csRKN) method have been proposed and discussed in some recent literatures \cite{12, 18, 21, 20, 13, 14, 4, 24}. It turned out that based on the so-called continuous-stage methods we can construct many classical RK, PRK and RKN methods of arbitrary order by using quadrature formulae, without resort to solving the tedious nonlinear algebraic equations that stem from the order conditions with a huge number of unknown coefficients. The construction of continuous-stage numerical methods seems more easier than that of those traditional methods with finite stages, as the associated Butcher coefficients are viewed as continuous functions and they can be handled by orthogonal polynomial expansions coupling with some simplifying assumptions \cite{20, 19, 24}. As shown in \cite{20, 19, 24, 13, 4}, numerical methods serving some special purpose including symplecticity-preserving methods for Hamiltonian systems, symmetric methods for reversible systems, energy-preserving methods for conservative systems can also be established within this new framework that formed by numerical methods with continuous stage.

Besides, it is found that some methods for special purpose couldn’t possibly exist in the context of classical numerical methods but it does under the new insights given by the continuous-stage methods. A well-known example we have to mention here is that no RK methods is energy-preserving for general Hamiltonian system except for those polynomial system \cite{5}, but under the csRK framework this difficult can be easily get around \cite{12, 14, 21, 20, 13, 4}. In addition, as presented in \cite{21, 22, 23}, 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. Therefore, continuous-stage methods have created a larger realm for numerical solution of differential equations and they provide us a new insight in geometric integration.

Based on our previous work \cite{24}, we are going to develop high order symplectic integrators in virtue of csRKN methods for solving second order ordinary differential equations. The construction of such methods heavily relies on the Legendre polynomial expansion technique, the simplifying assumptions for order conditions and the sufficient conditions for symplecticity. We will show the close relationship between csRKN methods and RKN methods, and based on this, by using Gaussian quadrature formulae we present several new classes of symplecticity-preserving RKN schemes with high order for practical use.

The outline of this paper is as follows. In the next section, we introduce the so-called csRKN methods for solving second order ordinary differential equations. After that we establish the order theory for csRKN methods, which will be given in Section 3. In Section 4, by coupling the orthogonal polyno-
mial expansion technique with the symplectic conditions, we present the new characterizations for symplecticity and in the sequel section we construct high order symplecticity-preserving integrators based on this. At last, the concluding remarks will be given.

2. Continuous-stage RKN method

Consider an initial value problem given by the following second order differential equations

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

where the double dots on \( q \in \mathbb{R}^d \) represents the second-order derivative with respect to \( t \). A well-known numerical method for solving (2.1) is the so-called Runge-Kutta Nyström (RKN) method, which can be defined below.

**Definition 2.1** (RKN method [11]). For the special second order differential equations (2.1), the Runge-Kutta Nyström method as a one-step method mapping \((q_0, q'_0)\) to \((q_1, q'_1)\) is defined by

\[
Q_i = q_0 + h c_i q'_0 + h^2 \sum_{j=1}^{s} \bar{a}_{ij} f(t_0 + c_j h, Q_j), \quad i = 1, \ldots, s, \tag{2.2a}
\]

\[
q_1 = q_0 + h q'_0 + h^2 \sum_{i=1}^{s} \bar{b}_i f(t_0 + c_i h, Q_i), \tag{2.2b}
\]

\[
q'_1 = q'_0 + h \sum_{i=1}^{s} b_i f(t_0 + c_i h, Q_i), \tag{2.2c}
\]

which can be characterized by the following Butcher tableau

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

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

Similarly as the classical RKN method, the continuous-stage Runge-Kutta Nyström (csRKN) method can be formally defined, which has been introduced in [24].

**Definition 2.2** (csRKN method [24]). 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 \( \tau \in [0, 1] \). For the special second order differential equations (2.1), the continuous-stage Runge-Kutta Nyström method
as a one-step method mapping \((q_0, q'_0)\) to \((q_1, q'_1)\) is given by

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

(2.3a)

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

(2.3b)

\[
q'_1 = q'_0 + h \int_0^1 B_{\tau} f(t_0 + C_\tau h, Q_\tau) d\tau,
\]

(2.3c)

which can be characterized by the following Butcher tableau

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

3. Order theory for RKN type method

A RKN type method (including the classical and the continuous-stage case) is of order \(p\), if for sufficiently smooth problem (2.1) the following two formulae hold [9]

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

3.1. Order theory for RKN method

For constructing arbitrary order RKN methods, the following simplifying assumptions for order conditions were proposed [9, 11]

\[
B(\xi) : \sum_{i=1}^s b_i e_i^{\kappa-1} = \frac{1}{\kappa}, \quad 1 \leq \kappa \leq \xi,
\]

\[
CN(\eta) : \sum_{j=1}^s \bar{a}_{ij} e_j^{\kappa-1} = \frac{e_i^{\kappa+1}}{\kappa(\kappa + 1)}, \quad 1 \leq i \leq s, \quad 1 \leq \kappa \leq \eta - 1,
\]

\[
DN(\zeta) : \sum_{i=1}^s b_i e_i^{\kappa-1} a_{ij} = \frac{b_j e_j^{\kappa+1}}{\kappa(\kappa + 1)} - \frac{b_i e_i^{\kappa+1}}{\kappa + 1} + \frac{b_j}{\kappa + 1}, \quad 1 \leq j \leq s, \quad 1 \leq \kappa \leq \zeta - 1,
\]

(3.1)

and the following theorem is based on these simplifying assumptions.

**Theorem 3.1.** [4] If the RKN method (2.2a-2.2c) with its coefficients satisfying the simplifying assumptions \(B(p)\), \(CN(\eta)\), \(DN(\zeta)\), and if \(\bar{b}_i = b_i(1 - c_i)\) is satisfied for all \(i = 1, \ldots, s\), then the method is of order \(\min\{p, 2\eta + 2, \eta + \zeta\}\).
3.2. Order theory for csRKN method

Very similarly as the classical case, we propose the following simplifying assumptions for csRKN method

\[ B(\xi) : \int_0^1 B_\tau C_\tau^{\kappa-1} \, d\tau = \frac{1}{\kappa}, \quad 1 \leq \kappa \leq \xi, \]

\[ CN(\eta) : \int_0^1 \bar{A}_{\tau, \sigma} C_\sigma^{\kappa-1} \, d\sigma = \frac{C_\tau^{\kappa+1}}{\kappa(\kappa + 1)}, \quad 1 \leq \kappa \leq \eta - 1, \]

\[ DN(\zeta) : \int_0^1 B_\tau C_\tau^{\kappa-1} \bar{A}_{\tau, \sigma} \, d\tau = \frac{B_\sigma C_\sigma^{\kappa+1}}{\kappa(\kappa + 1)} - \frac{B_\sigma C_\sigma}{\kappa + 1}, \quad 1 \leq \kappa \leq \zeta - 1, \]

where \( \tau, \sigma \in [0, 1] \).

**Theorem 3.2.** If the csRKN method (2.3a-2.3c) with its coefficients satisfying the simplifying assumptions \( B(\xi), CN(\eta), DN(\zeta) \), and if \( \bar{B}_\tau = B_\tau(1 - C_\tau) \) is satisfied for \( \tau \in [0, 1] \), then the method is of order \( \min\{p, 2\eta + 2, \eta + \zeta\} \).

**Proof.** This result can be proved similarly as the classical result given by Theorem 3.1, in which the SN-trees have to be considered [9]. \( \square \)

To proceed our discussions, let us introduce the \( \iota \)-degree normalized shifted Legendre polynomial denoted by \( P_\iota(t) \), which can be explicitly computed by the Rodrigues formula

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

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

\[ \int_0^1 P_\iota(t)P_\kappa(t) \, dt = \delta_{\iota\kappa}, \quad \iota, \kappa = 0, 1, 2, \ldots, \]

and they as well satisfy the following integration formulae

\[ \int_0^x P_0(t) \, dt = \xi_1 P_1(x) + \frac{1}{2} P_0(x), \]

\[ \int_0^x P_\iota(t) \, dt = \xi_{\iota+1} P_{\iota+1}(x) - \xi_\iota P_{\iota-1}(x), \quad \iota = 1, 2, 3, \ldots, \]

\[ \int_x^1 P_\iota(t) \, dt = \delta_{\iota0} - \int_0^x P_\iota(t) \, dt, \quad \iota = 0, 1, 2, \ldots, \]  

where \( \xi_\iota = \frac{1}{2\sqrt{\iota(\iota + 1)}} \) and \( \delta_{\iota\kappa} \) is the Kronecker delta.

In what follows, as the case for csRK and csPRK method discussed in [20, 19], we will use the hypothesis \( \bar{B}_\tau = 1, C_\tau = \tau \) throughout this paper. In such a case, the first simplifying assumption \( B(\xi) \) can be reduced to

\[ \int_0^1 \tau^{\kappa-1} \, d\tau = \frac{1}{\kappa}, \quad \kappa = 1, \ldots, \xi, \]
which always holds for any positive integer $\xi$, for convenience we denote this fact by $B(\infty)$. In addition, by taking the derivative with respect to $\tau$ and $\sigma$ respectively, it follows from $CN(\eta), DN(\zeta)$ that

\[
CN'(\eta) : \int_0^1 \frac{d}{d\tau} \tilde{A}_{\tau, \sigma} \sigma^{\kappa-1} d\sigma = \frac{\tau^\kappa}{\kappa} = \int_0^\tau \sigma^{\kappa-1} d\sigma, \quad 1 \leq \kappa \leq \eta - 1,
\]
\[
DN'(\zeta) : \int_0^1 \sigma^{\kappa-1} \frac{d}{d\sigma} \tilde{A}_{\tau, \sigma} d\tau = \frac{\sigma^\kappa}{\kappa} - \frac{1}{\kappa} = -\int_\sigma^1 \tau^{\kappa-1} d\tau, \quad 1 \leq \kappa \leq \zeta - 1.
\]

(3.3)

Remark that $CN'(\eta)$ (resp. $DN'(\zeta)$) is only necessary for $CN(\eta)$ (resp. $DN(\zeta)$), hence we should additionally require that

\[
\int_0^1 \tilde{A}_{0, \sigma} \sigma^{\kappa-1} d\sigma = 0, \quad 1 \leq \kappa \leq \eta - 1,
\]
for $CN(\eta)$, and

\[
\int_0^1 \tau^{\kappa-1} \tilde{A}_{\tau, 0} d\tau = \frac{1}{\kappa + 1} = \int_0^1 \tau^\kappa d\tau, \quad 1 \leq \kappa \leq \zeta - 1,
\]
for $DN(\zeta)$. For convenience to use, we can rewrite the formula above as

\[
\int_0^1 \tau^{\kappa-1} (\tilde{A}_{\tau, 0} - \tau) d\tau = 0, \quad 1 \leq \kappa \leq \zeta - 1.
\]
(3.5)

As all the Legendre polynomials form a complete orthogonal set in the interval $[0, 1]$, we can expand $\frac{d}{d\tau} A_{\tau, \sigma}$ (with $\tau$ being fixed) and $\frac{d}{d\sigma} A_{\tau, \sigma}$ (with $\sigma$ being fixed) respectively as

\[
\frac{d}{d\tau} A_{\tau, \sigma} = \sum_{i=0}^\infty \gamma_i(\tau) P_i(\sigma),
\]
\[
\frac{d}{d\sigma} A_{\tau, \sigma} = \sum_{i=0}^\infty \lambda_i(\sigma) P_i(\tau),
\]
(3.6)

where $\gamma_i(\tau), \lambda_i(\sigma)$ are the unknown coefficient functions. Consider that (3.3) implies

\[
CN'(\eta) : \int_0^1 \frac{d}{d\tau} A_{\tau, \sigma} P_{\kappa-1}(\sigma) d\sigma = \int_0^\tau P_{\kappa-1}(\sigma) d\sigma, \quad 1 \leq \kappa \leq \eta - 1,
\]
\[
DN'(\zeta) : \int_0^1 P_{\kappa-1}(\tau) \frac{d}{d\sigma} A_{\tau, \sigma} d\tau = -\int_\sigma^1 P_{\kappa-1}(\tau) d\tau, \quad 1 \leq \kappa \leq \zeta - 1,
\]
which result in

\[
\gamma_i(\tau) = \int_0^\tau P_i(\sigma) d\sigma, \quad 0 \leq i \leq \eta - 2,
\]
\[
\lambda_i(\sigma) = -\int_\sigma^1 P_i(\tau) d\tau, \quad 0 \leq i \leq \zeta - 2.
\]
(3.8)
Substituting (3.8) into (3.6) and by virtue of (3.2) it gives
\[
\frac{d}{d\tau} \bar{A}_{\tau, \sigma} = \sum_{i=0}^{\eta-2} \int_{0}^{\tau} P_i(x) \, dx \, P_i(\sigma) + \sum_{i \geq \eta-1} \gamma_i(\tau) P_i(\sigma)
\]
\[
= \frac{1}{2} + \sum_{i=0}^{\eta-2} \xi_{i+1} P_{i+1}(\tau) P_i(\sigma) - \sum_{i=0}^{\eta-3} \xi_{i+1} P_{i+1}(\sigma) P_i(\tau) + \sum_{i \geq \eta-1} \gamma_i(\tau) P_i(\sigma),
\]
\[\text{(3.9)}\]
\[
\frac{d}{d\sigma} \bar{A}_{\tau, \sigma} = -\sum_{i=0}^{\zeta-2} \int_{\sigma}^{1} P_i(x) \, dx \, P_i(\tau) + \sum_{i \geq \zeta-1} \lambda_i(\sigma) P_i(\tau)
\]
\[
= -\frac{1}{2} - \sum_{i=0}^{\zeta-3} \xi_{i+1} P_{i+1}(\tau) P_i(\sigma) + \sum_{i=0}^{\zeta-2} \xi_{i+1} P_{i+1}(\sigma) P_i(\tau) + \sum_{i \geq \zeta-1} \lambda_i(\sigma) P_i(\tau).
\]
\[\text{(3.10)}\]

It is evident that (3.4) and (3.5) give rise to
\[
\int_{0}^{1} \bar{A}_{0, \sigma} P_{\kappa-1}(\sigma) \, d\sigma = 0, \quad 1 \leq \kappa \leq \eta - 1,
\]
\[
\int_{0}^{1} P_{\kappa-1}(\sigma)(\bar{A}_{\tau, 0} - \tau) \, d\tau = 0, \quad 1 \leq \kappa \leq \zeta - 1.
\]
\[\text{(3.11)}\]

Let us consider the following orthogonal polynomial expansions
\[
\bar{A}_{0, \sigma} = \sum_{i=0}^{\infty} \alpha_i P_i(\sigma),
\]
\[
\bar{A}_{\tau, 0} - \tau = \sum_{i=0}^{\infty} \beta_i P_i(\tau),
\]
\[\text{(3.12)}\]

where the unknown expansion coefficients \(\alpha_i, \beta_i\) are real numbers, then from (3.11) we get
\[
\alpha_i = 0, \quad 0 \leq \kappa \leq \eta - 2,
\]
\[
\beta_i = 0, \quad 0 \leq \kappa \leq \zeta - 2.
\]
\[\text{(3.13)}\]

Therefore, it follows from (3.12) that
\[
\bar{A}_{0, \sigma} = \sum_{i \geq \eta-1} \alpha_i P_i(\sigma),
\]
\[
\bar{A}_{\tau, 0} = \tau + \sum_{i \geq \zeta-1} \beta_i P_i(\tau).
\]
\[\text{(3.14)}\]
By integrating (3.9) with respect to $\tau$ and (3.10) with respect to $\sigma$, it yields

$$\bar{A}_{\tau, \sigma} - \bar{A}_{\tau, 0} = \frac{1}{2}\tau + \sum_{i=0}^{\eta-2} \xi_{i+1} \int_0^{\tau} P_{i+1}(x) \, dx \, P_i(\sigma)$$

$$- \sum_{i=0}^{\eta-3} \xi_{i+1} P_{i+1}(\sigma) \int_0^{\tau} P_i(x) \, dx + \sum_{i \geq \eta-1} \int_0^{\tau} \gamma_i(x) \, dx \, P_i(\sigma),$$

$$\bar{A}_{\tau, \sigma} - \bar{A}_{\tau, 0} = -\frac{1}{2}\sigma - \sum_{i=0}^{\zeta-3} \xi_{i+1} P_{i+1}(\tau) \int_0^{\sigma} P_i(x) \, dx$$

$$+ \sum_{i=0}^{\zeta-2} \xi_{i+1} \int_0^{\sigma} P_{i+1}(x) \, dx \, P_i(\tau) + \sum_{i \geq \zeta-1} \int_0^{\sigma} \lambda_i(x) \, dx \, P_i(\tau).$$

By using the known equality $\tau = \frac{1}{2} P_0(\tau) + \xi_1 P_1(\tau)$ and inserting (3.14) into the two formulae above, it then gives

$$\bar{A}_{\tau, \sigma} = \frac{1}{4} P_0(\tau) + \frac{1}{2} \xi_1 P_1(\tau) + \sum_{i=0}^{\eta-2} \xi_{i+1} \int_0^{\tau} P_{i+1}(x) \, dx \, P_i(\sigma)$$

$$- \sum_{i=0}^{\eta-3} \xi_{i+1} P_{i+1}(\sigma) \int_0^{\tau} P_i(x) \, dx + \sum_{i \geq \eta-1} (\alpha_i + \int_0^{\tau} \gamma_i(x) \, dx) \, P_i(\sigma),$$

$$\bar{A}_{\tau, \sigma} = \frac{1}{4} P_0(\tau) + \xi_1 P_1(\tau) - \frac{1}{2} \xi_1 P_1(\sigma) - \sum_{i=0}^{\zeta-3} \xi_{i+1} P_{i+1}(\tau) \int_0^{\sigma} P_i(x) \, dx$$

$$+ \sum_{i=0}^{\zeta-2} \xi_{i+1} \int_0^{\sigma} P_{i+1}(x) \, dx \, P_i(\tau) + \sum_{i \geq \zeta-1} (\beta_i + \int_0^{\sigma} \lambda_i(x) \, dx) \, P_i(\tau).$$

By exploiting (3.2) once again, it ends up with

$$\bar{A}_{\tau, \sigma} = \frac{1}{6} - \frac{1}{2} \xi_1 P_1(\sigma) + \frac{1}{2} \xi_1 P_1(\tau) + \sum_{i=0}^{\eta-3} \xi_i \xi_{i+1} P_{i+1}(\tau) P_{i+1}(\sigma)$$

$$- \sum_{i=1}^{\eta-1} (\xi_i^2 + \xi_{i+1}^2) P_i(\tau) P_i(\sigma) + \sum_{i=1}^{\eta-1} \xi_i \xi_{i+1} P_{i+1}(\tau) P_{i-1}(\sigma)$$

$$+ \sum_{i \geq \eta-1} (\alpha_i + \int_0^{\tau} \gamma_i(x) \, dx) \, P_i(\sigma),$$

8
For simplicity, we denote that

\[ \tilde{\lambda}_i(\tau) = \alpha_i + \int_0^\tau \xi_i(\tau) \, d\tau, \quad \tau \geq \eta - 1, \]

\[ \tilde{\alpha}_i(\sigma) = \beta_i + \int_0^\sigma \lambda_i(\sigma) \, d\sigma, \quad \sigma \geq \zeta - 1, \]

all of which are arbitrary functions, as here \( \alpha_i, \beta_i \) can be arbitrary real numbers and \( \gamma_i(x), \lambda_i(x) \) can be arbitrary functions.

We summarize the results above in the following lemma.

**Lemma 3.3.** For the csRKN method (2.3a–2.3c) denoted by \( (\tilde{A}_{r,\sigma}, \tilde{B}_r, B_r, C_r) \) with the assumption \( B_r = 1, C_r = \tau \), we have the following statements:

(I) The second simplifying assumption \( \mathcal{CN}(\eta) \) is equivalent to the fact that \( \tilde{A}_{r,\sigma} \) takes the form

\[
\tilde{A}_{r,\sigma} = \frac{1}{6} - \frac{1}{2} \xi_1 P_1(\sigma) + \frac{1}{2} \xi_1 P_1(\tau) + \sum_{i=1}^{\eta-3} \xi_i \xi_{i+1} P_{i-1}(\tau) P_{i+1}(\sigma) \\
- \sum_{i=1}^{\eta-2} (\xi_i^2 + \xi_{i+1}^2) P_i(\tau) P_i(\sigma) + \sum_{i=1}^{\eta-1} \xi_i \xi_{i+1} P_{i+1}(\tau) P_{i-1}(\sigma) \\
+ \sum_{i=\eta-1}^\eta \tilde{\tau}_i(\tau) P_i(\sigma),
\]

where \( \xi_i = \frac{1}{2\sqrt{4\tau^2 - 1}} (i \geq 1) \) and \( \tilde{\tau}_i(\tau) (i \geq \eta - 1) \) are arbitrary functions;

(II) The third simplifying assumption \( \mathcal{DN}(\zeta) \) is equivalent to the fact that \( \tilde{A}_{r,\sigma} \) takes the form

\[
\tilde{A}_{r,\sigma} = \frac{1}{6} - \frac{1}{2} \xi_1 P_1(\sigma) + \frac{1}{2} \xi_1 P_1(\tau) + \sum_{i=1}^{\zeta-1} \xi_i \xi_{i+1} P_{i-1}(\tau) P_{i+1}(\sigma) \\
- \sum_{i=1}^{\zeta-2} (\xi_i^2 + \xi_{i+1}^2) P_i(\tau) P_i(\sigma) + \sum_{i=1}^{\zeta-3} \xi_i \xi_{i+1} P_{i+1}(\tau) P_{i-1}(\sigma) \\
+ \sum_{i=\zeta-1}^\zeta \tilde{\alpha}_i(\sigma) P_i(\tau),
\]

where \( \xi_i = \frac{1}{2\sqrt{4\tau^2 - 1}} (i \geq 1) \) and \( \tilde{\alpha}_i(\sigma) (i \geq \zeta - 1) \) are arbitrary functions.
Theorem 3.4. For the csRKN method (2.3a-2.3c) 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:

(I) Both $\mathcal{C}N(\eta)$ and $\mathcal{D}N(\zeta)$ hold;

(II) The coefficient $\bar{A}_{\tau,\sigma}$ possesses the following form

$$
\bar{A}_{\tau,\sigma} = \frac{1}{6} - \frac{1}{2} \xi_1 P_1(\sigma) + \frac{1}{2} \xi_1 P_1(\tau) + \sum_{i=1}^{N_1} \xi_i \xi_{i+1} P_{\tau-1}(\tau) P_{\sigma+1}(\sigma) - \sum_{i=1}^{N_2} (\xi_i^2 + \xi_{i+1}^2) P_i(\tau) P_i(\sigma) + \sum_{i=1}^{N_3} \xi_i \xi_{i+1} P_{\tau+1}(\tau) P_{\tau-1}(\sigma)
$$

(3.17)

where $\xi_1 = \frac{1}{2\sqrt{2\eta^2 - 1}}$, $N_1 = \max\{\eta - 3, \zeta - 1\}$, $N_2 = \max\{\eta - 2, \zeta - 2\}$, $N_3 = \max\{\eta - 1, \zeta - 3\}$ and $\omega_{(i,j)}$ are arbitrary real numbers.

Proof. By Lemma 3.3 consider that we can further expand $\overline{\gamma}_i(\tau)$ and $\overline{\lambda}_i(\sigma)$ by using the Legendre polynomials as follows

$$
\overline{\gamma}_i(\tau) = \sum_{i=0}^{\infty} \mu_i^\tau P_i(\tau), \quad i \geq \eta - 1,
$$

$$
\overline{\lambda}_i(\sigma) = \sum_{j=0}^{\infty} \nu_j^\sigma P_j(\sigma), \quad i \geq \zeta - 1,
$$

where the expansion coefficients $\mu_i^\tau, \nu_j^\sigma$ are real numbers. Inserting them into (3.15) and (3.16) respectively, and by comparing the expansion coefficients associated with the orthogonal basis functions in $[0, 1] \times [0, 1]$ namely

$$
\{ P_i(\tau) P_j(\sigma), \ i, j = 0, 1, 2, \cdots \}
$$

we then get the final result. 

Recall that we already have $\mathcal{B}(\infty)$ by the hypothesis $B_\tau = 1, C_\tau = \tau$, thus the above theorem implies that we can construct a csRKN method with order $\min\{\infty, 2\eta + 2, \eta + \zeta\} = \min\{2\eta + 2, \eta + \zeta\}$, which is directly concluded by using Theorem 3.2.

Remark 3.5. For the sake of obtaining a practical csRKN method, we need to get a finite form for the coefficient $\bar{A}_{\tau,\sigma}$, hence it is necessary to truncate the series (3.17), or equivalently, impose infinitely many parameters $\omega_{(i,j)}$ to be zero after a certain term. In such a case, we get a coefficient $\bar{A}_{\tau,\sigma}$ which is a bivariate polynomial in variables $\tau$ and $\sigma$. 

10
3.3. RKN methods based on csRKN

It is known that the practical implementation of the csRKN method (2.3a)-(2.3c) needs the use of numerical quadrature formula. Therefore, we are interested in the relationship between csRKN and RKN methods, this will be illustrated hereafter.

By applying a quadrature formula denoted by \((b_i, c_i)_{i=1}^s\) to (2.3a)-(2.3c), with abuse of notations \(Q_i = Q_{c_i}\), we derive an \(s\)-stage RKN method below

\[
Q_i = q_0 + hC_i q_0' + h^2 \sum_{j=1}^s b_j \bar{A}_{ij} f(t_0 + C_j h, Q_j), \quad i = 1, \cdots, s, \tag{3.18a}
\]

\[
q_1 = q_0 + h q_0' + h^2 \sum_{i=1}^s b_i \tilde{B}_i f(t_0 + C_i h, Q_i), \tag{3.18b}
\]

\[
q_1' = q_0' + h \sum_{i=1}^s b_i B_i f(t_0 + C_i h, Q_i), \tag{3.18c}
\]

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

\[
\begin{array}{cccc}
C_1 & b_1 \bar{A}_{11} & \cdots & b_s \bar{A}_{1s} \\
\vdots & \vdots & & \vdots \\
C_s & b_1 \bar{A}_{s1} & \cdots & b_s \bar{A}_{ss} \\
\hline
& b_1 \tilde{B}_1 & \cdots & b_s \tilde{B}_s \\
& b_1 \bar{B}_1 & \cdots & b_s \bar{B}_s \\
\end{array} \tag{3.19}
\]

Particularly, by the hypothesis \(\bar{B}_\tau = B_\tau(1 - C_\tau), B_\tau = 1, C_\tau = \tau\) for \(\tau \in [0, 1]\), we actually get an \(s\)-stage RKN method with tableau

\[
\begin{array}{cccc}
c_1 & b_1 \bar{A}_{11} & \cdots & b_s \bar{A}_{1s} \\
\vdots & \vdots & & \vdots \\
c_s & b_1 \bar{A}_{s1} & \cdots & b_s \bar{A}_{ss} \\
\hline
& b_1 & \cdots & b_s \\
\end{array} \tag{3.20}
\]

where \(\bar{b}_i = b_i(1 - c_i), \ i = 1, \cdots, s\).

Linked with Remark 3.5, we have the following order result for the RKN method based on csRKN.

**Theorem 3.6.** Assume \(\bar{A}_{\tau,\sigma}\) is a bivariate polynomial of degree \(d^\tau\) in \(\tau\) and degree \(d^\sigma\) in \(\sigma\), and the quadrature formula \((b_i, c_i)_{i=1}^s\) is of order \(p\). If a csRKN method (2.23) denoted by \((\bar{A}_{\tau,\sigma}, \tilde{B}_\tau, B_\tau, C_\tau)\) with the assumptions \(\bar{B}_\tau = \ldots\)
$B_\tau(1 - C_\tau), B_\tau = 1, C_\tau = \tau, \tau \in [0, 1]$ (then $B(\infty)$ holds) and both $CN(\eta), DN(\zeta)$ hold, then the RKN method with tableau \(3.20\) is at least of order

$$\min(p, 2\alpha + 2, \alpha + \beta),$$

where $\alpha = \min(\eta, p - d^\tau + 1)$ and $\beta = \min(\zeta, p - d^\tau + 1)$.

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

$$\sum_{i=1}^s b_i \nu_i^{\kappa - 1} = \frac{1}{\kappa}, \kappa = 1, \ldots, p,$$

$$\sum_{j=1}^s (b_j \bar{A}_{ij}) \nu_j^{\kappa - 1} = \frac{c_i^{\kappa + 1}}{\kappa(\kappa + 1)}, i = 1, \ldots, s, \kappa = 1, \ldots, \alpha - 1,$$

$$\sum_{i=1}^s b_i \nu_i^{\kappa - 1} (b_j \bar{A}_{ij}) = \frac{b_j \nu_j^{\kappa + 1}}{\kappa(\kappa + 1)} - \frac{b_j c_j}{\kappa} + \frac{b_j}{\kappa + 1}, j = 1, \ldots, s, \kappa = 1, \ldots, \beta - 1,$$

where $\alpha = \min(\eta, p - d^\tau + 1)$ and $\beta = \min(\zeta, p - d^\tau + 1)$. Note that in the last formula, we have multiplied a factor $b_j$ afterwards from both sides of the original identity. These formulae imply that the RKN method \((3.20)\) satisfies $B(p), CN(\alpha)$ and $DN(\beta)$, and it is observed that $b_i = b_i(1 - c_i)$ is naturally satisfied for each $i = 1, \ldots, s$, all of these conditions give rise to the order of the method by the classical result (see Theorem 3.1).

**Remark 3.7.** If the second order equation \((2.1)\) is a polynomial system namely $f$ is a polynomial (vector) function of $t$ and $q$, then $Q_\tau$ in Definition \(2.2\) is also a polynomial with the same degree of $\bar{A}_{\tau, \sigma}$ in $\tau$, this implies that we can always accurately compute the integrals of the csRKN scheme by using a quadrature formula with high enough order. In such a case, the associated RKN method obtained by exploiting a high-order quadrature formula can be viewed as a perfectly implementation of the original csRKN method.

### 4. Characterizations for symplecticity of csRKN method

Hamiltonian system has attracted a wide range of scientists in various fields \[1\], and it forms one of the most important class of dynamical systems in the context of geometric integration \[6, 11, 15, 7, 8\]. Such a system can be written in the form

$$\dot{z} = J^{-1} \nabla_z H(z), \ z \in \mathbb{R}^{2d},$$

where $J \in \mathbb{R}^{2d \times 2d}$ is a skew-symmetric canonical structure matrix, and it is equipped with an intrinsic geometric structure called symplecticity which states that the flow $\varphi_t$ of the system is a symplectic transformation \[1\], i.e.,

$$d\varphi_t(z_0) \land Jd\varphi_t(z_0) = dz_0 \land Jdz_0, \ z_0 \in D,$$
where $\wedge$ represents the standard wedge product, and $D$ is an open subset in the phase space $\mathbb{R}^{2d}$. For Hamiltonian system, symplecticity-preserving numerical method is of considerable interest [6, 15, 11], as such algorithm always exhibits bounded small energy errors for the exponentially long time [11], and it can correctly reproduce some qualitative behaviors of the original system such as preserving the quasi-periodic orbits (namely KAM tori) and chaotic regions of phase space by numerical KAM theorem [16]. A one-step method $\Phi_h : z_0 = (p_0, q_0) \mapsto (p_1, q_1) = z_1$, when applied to a Hamiltonian system, is called symplectic if and only if [6, 15, 11]

$$d\Phi_h(z_0) \wedge Jd\Phi_h(z_0) = dz_0 \wedge Jdz_0, \quad z_0 \in D,$$

or equivalently,

$$dp_1 \wedge dq_1 = dp_0 \wedge dq_0, \quad (p_0, q_0) \in D.$$

A very special class of Hamiltonian systems frequently encountered in practice is the so-called separable Hamiltonian system. The well-known separable Hamiltonian system is the system with the Hamiltonian (namely the total energy) in the form

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

where $M$ is a constant symmetric matrix. In such a case, the corresponding Hamiltonian system becomes

$$\begin{align*}
\dot{p} &= -\nabla_q V(q), \\
\dot{q} &= Mp,
\end{align*}$$

which is equivalent to the following second order system

$$\ddot{q} = -M\nabla_q V(q).$$

In the sequel we denote $f(q) = -M\nabla_q V(q)$ and $g(q) = -\nabla_q V(q)$, then for solving this special autonomous second order equation (4.2), we propose the following csRKN method

$$\begin{align*}
Q_\tau &= q_0 + hC\tau M p_0 + h^2 \int_0^1 \bar{A}_{\tau, \sigma} f(Q_\sigma) d\sigma, \quad \tau \in [0, 1], \\
q_1 &= q_0 + hMp_0 + h^2 \int_0^1 \bar{B}_{\tau} f(Q_{\tau}) d\tau, \\
p_1 &= p_0 + h \int_0^1 B_{\tau} g(Q_{\tau}) d\tau,
\end{align*}$$

which is derived by replacing the variable $q'$ with $Mp$ in the Definition [2.2] but with $M$ dropped in the last formula. It is evident that this small modification for the last formula does not influence (at least not decrease) the order of the method since $M$ is a constant matrix.

Next, we present the conditions under which the csRKN method above is symplectic and after that a useful result for constructing symplectic csRKN methods will be given.
Theorem 4.1. If a csRKN method denoted by \((\bar{A}_{\tau,\sigma}, \bar{B}_{\tau}, B_{\tau}, C_{\tau})\) satisfies
\[
\bar{B}_{\tau} = B_{\tau}(1 - C_{\tau}), \quad \tau \in [0, 1], \quad (4.4a)
\]
\[
B_{\tau}(\bar{B}_{\sigma} - \bar{A}_{\tau,\sigma}) = B_{\sigma}(\bar{B}_{\tau} - \bar{A}_{\sigma,\tau}), \quad \tau, \sigma \in [0, 1], \quad (4.4b)
\]
then the method is symplectic for solving the autonomous second order differential equations \((4.2)\).

Proof. By the csRKN scheme \((4.3a-4.3c)\), we have
\[
dp_1 \wedge dq_1 = d(p_0 + h \int_0^1 B_{\tau}g(Q_{\tau})d\tau) \wedge dq_0 + h M p_0 + h^2 \int_0^1 \bar{B}_{\tau} f(Q_{\tau})d\tau
\]
\[
= dp_0 \wedge dq_0 + h \int_0^1 (B_{\tau} dg(Q_{\tau}) \wedge dq_0) d\tau + h dp_0 \wedge M dp_0 + h^2 \int_0^1 (\bar{B}_{\tau} dp_0 \wedge df(Q_{\tau})) d\tau
\]
\[
+ h^3 \int_0^1 \int_0^1 B_{\tau} \bar{A}_{\tau,\sigma} dg(Q_{\tau}) \wedge df(Q_{\sigma}) d\sigma d\tau.
\]

As a result of the symmetry of \(M\) and the skew symmetry of wedge product, the third term vanishes. By virtue of \((4.3a)\), the second term can be recast as
\[
h \int_0^1 (B_{\tau} dg(Q_{\tau}) \wedge dq_0) d\tau
\]
\[
= h \int_0^1 (B_{\tau} dg(Q_{\tau}) \wedge d(Q_{\tau} - h C_{\tau} M p_0 - h^2 \int_0^1 \bar{A}_{\tau,\sigma} f(Q_{\sigma})d\sigma)) d\tau
\]
\[
= h \int_0^1 (B_{\tau} dg(Q_{\tau}) \wedge dQ_{\tau}) d\tau - h^2 \int_0^1 (B_{\tau} C_{\tau} dg(Q_{\tau}) \wedge M dp_0) d\tau
\]
\[
- h^3 \int_0^1 \int_0^1 B_{\tau} \bar{A}_{\tau,\sigma} dg(Q_{\tau}) \wedge df(Q_{\sigma}) d\sigma d\tau.
\]

Note that the Jacobian matrix of \(g(q) = -\nabla_q V(q)\) is symmetric and the wedge product is skew-symmetric, the first term of the above formula vanishes. By substituting \((4.6)\) into \((4.5)\), and note that
\[
df(Q_{\tau}) \wedge dp_0 = M dg(Q_{\tau}) \wedge dp_0 = dg(Q_{\tau}) \wedge M^T dp_0 = dg(Q_{\tau}) \wedge M dp_0,
\]
then it yields
\[
dp_1 \wedge dq_1
\]
\[
= dp_0 \wedge dq_0 - h^2 \int_0^1 (B_\tau C_\tau dg(Q_\tau) \wedge M dp_0) d\tau
\]
\[
- h^3 \int_0^1 \int_0^1 (B_\tau \bar{A}_{\tau,\sigma} dg(Q_\tau) \wedge df(Q_\sigma)) d\sigma d\tau + h^2 \int_0^1 (B_\tau dg(Q_\tau) \wedge M dp_0) d\tau
\]
\[
- h^2 \int_0^1 (\bar{B}_\tau df(Q_\tau) \wedge dp_0) d\tau + h^3 \int_0^1 \int_0^1 B_\tau B_\sigma dg(Q_\tau) \wedge df(Q_\sigma) d\sigma d\tau
\]
\[
= dp_0 \wedge dq_0 + h^2 \int_0^1 (-B_\tau C_\tau + B_\tau - \bar{B}_\tau) dg(Q_\tau) \wedge M dp_0 d\tau
\]
\[
+ h^3 \int_0^1 \int_0^1 (B_\tau \bar{B}_\sigma - B_\tau \bar{A}_{\tau,\sigma}) dg(Q_\tau) \wedge df(Q_\sigma) d\sigma d\tau.
\]
\[(4.7)\]

For the last term of the formula above, we deal with the integrand separately in what follows. First, we compute
\[
\int_0^1 \int_0^1 B_\tau \bar{B}_\sigma dg(Q_\tau) \wedge df(Q_\sigma) d\sigma d\tau
\]
\[
= \frac{1}{2} \int_0^1 \int_0^1 (B_\tau \bar{B}_\sigma dg(Q_\tau) \wedge df(Q_\sigma) + B_\sigma \bar{B}_\tau dg(Q_\sigma) \wedge df(Q_\tau)) d\sigma d\tau
\]
\[(4.8)\]
\[
= \frac{1}{2} \int_0^1 \int_0^1 (B_\tau \bar{B}_\sigma dg(Q_\tau) \wedge df(Q_\sigma) - B_\sigma \bar{B}_\tau df(Q_\tau) \wedge dg(Q_\sigma)) d\sigma d\tau
\]
\[
= \frac{1}{2} \int_0^1 \int_0^1 (B_\tau \bar{B}_\sigma - B_\sigma \bar{B}_\tau) dg(Q_\tau) \wedge df(Q_\sigma) d\sigma d\tau,
\]
where we have used a simple fact
\[
df(Q_\tau) \wedge dg(Q_\sigma) = M dg(Q_\tau) \wedge dq_\sigma = dq_\tau \wedge M^T dg(Q_\sigma) = dq_\tau \wedge df(Q_\sigma),
\]
which is owing to the symmetry of the matrix $M$. Similarly,
\[
\int_0^1 \int_0^1 -B_\tau \bar{A}_{\tau,\sigma} dg(Q_\tau) \wedge df(Q_\sigma) d\sigma d\tau
\]
\[
= \frac{1}{2} \int_0^1 \int_0^1 (-B_\tau \bar{A}_{\tau,\sigma} dg(Q_\tau) \wedge df(Q_\sigma) - B_\sigma \bar{A}_{\tau,\sigma} dg(Q_\sigma) \wedge df(Q_\tau)) d\sigma d\tau
\]
\[
= \frac{1}{2} \int_0^1 \int_0^1 (-B_\tau \bar{A}_{\tau,\sigma} dg(Q_\tau) \wedge df(Q_\sigma) + B_\sigma \bar{A}_{\tau,\sigma} df(Q_\tau) \wedge dg(Q_\sigma)) d\sigma d\tau
\]
\[
= \frac{1}{2} \int_0^1 \int_0^1 (-B_\tau \bar{A}_{\tau,\sigma} + B_\sigma \bar{A}_{\tau,\sigma}) dg(Q_\tau) \wedge df(Q_\sigma) d\sigma d\tau.
\]
\[(4.9)\]
By using (4.8) and (4.9), the last term of (4.7) becomes
\[
\begin{aligned}
&\int_0^1 \int_0^1 (B_\tau \tilde{B}_\sigma - B_\sigma \tilde{A}_{\tau,\sigma}) dg(\tau,Q_\tau) \wedge df(Q_\sigma) d\sigma d\tau \\
&= \frac{h^3}{2} \int_0^1 \int_0^1 (B_\tau \tilde{B}_\sigma - B_\sigma \tilde{B}_\tau - B_\tau \tilde{A}_{\tau,\sigma} + B_\sigma \tilde{A}_{\sigma,\tau}) dg(\tau,Q_\tau) \wedge df(Q_\sigma) d\sigma d\tau.
\end{aligned}
\]

Therefore, if we require the conditions given by (4.4a-4.4b), then the last two terms in (4.7) vanish, and it gives rise to
\[
d p_1 \wedge dq_1 = d p_0 \wedge dq_0,
\]
which implies the symplecticity.

Remark 4.2. From the process of the proof we can see that if we directly require
\[
\tilde{B}_\tau = B_\tau (1 - C_\tau), \quad \tau \in [0,1],
\]
\[
B_\tau (\tilde{B}_\sigma - \tilde{A}_{\tau,\sigma}) = 0, \quad \tau, \sigma \in [0,1],
\]
in (4.7), then it also results in the symplecticity. However, the conditions given in (4.11) are contained in the conditions that given in the theorem.

Remark 4.3. It is stressed that Theorem 4.1 has generalized the corresponding result presented in [24], in which the system (4.2) with \( M \) a invertible matrix is considered, whereas in this paper we get rid off the invertibility of \( M \).

Theorem 4.4. The csRKN method denoted by \((\tilde{A}_{\tau,\sigma}, \tilde{B}_\tau, B_\tau, C_\tau)\) with \( B_\tau = 1, C_\tau = \tau \) is symplectic for solving the second order system (4.2), if \( \tilde{A}_{\tau,\sigma} \) and \( \tilde{B}_\tau \) possess the following forms in terms of Legendre polynomials
\[
\tilde{B}_\tau = 1 - \tau = \frac{1}{2} P_0(\tau) - \xi_1 P_1(\tau), \quad \tau \in [0,1],
\]
\[
\tilde{A}_{\tau,\sigma} = \alpha_{(0,0)} + \alpha_{(0,1)} P_1(\sigma) + \alpha_{(1,0)} P_1(\tau) + \sum_{i+j>1} \alpha_{(i,j)} P_i(\tau) P_j(\sigma), \quad \tau, \sigma \in [0,1],
\]
(4.12)
where \( \alpha_{(0,0)} \) is an arbitrary real number, \( \alpha_{(0,1)} - \alpha_{(1,0)} = -\xi_1 = -\frac{\sqrt{3}}{6} \), and the parameters \( \alpha_{(i,j)} \) are symmetric, i.e., \( \alpha_{(i,j)} = \alpha_{(j,i)} \) for \( i + j > 1 \).

Proof. By the assumption \( B_\tau = 1, C_\tau = \tau \) and using (4.4b), we get
\[
\tilde{B}_\tau = 1 - \tau = \frac{1}{2} P_0(\tau) - \xi_1 P_1(\tau),
\]
inserting it into (4.4b), then it ends up with
\[
\tilde{A}_{\tau,\sigma} - \tilde{A}_{\sigma,\tau} = \tau - \sigma = \xi_1 (P_1(\tau) - P_1(\sigma)) = \frac{\sqrt{3}}{6} (P_1(\tau) - P_1(\sigma)),
\]
(4.13)
in which we have used the equality $\tau = \frac{1}{2} P_0(\tau) + \xi_1 P_1(\tau)$.

Next, assume $\bar{A}_{\tau, \sigma}$ can be expanded as a series in terms of the orthogonal basis $\{ P_i(\tau) P_j(\sigma) \}_{i,j=0}^{\infty}$ in $[0,1] \times [0,1]$, written in the form

$$\bar{A}_{\tau, \sigma} = \sum_{0 \leq i,j \in \mathbb{Z}} \alpha_{(i,j)} P_i(\tau) P_j(\sigma), \quad \alpha_{ij} \in \mathbb{R},$$

then by exchanging $\tau$ and $\sigma$ we have

$$\bar{A}_{\sigma, \tau} = \sum_{0 \leq i,j \in \mathbb{Z}} \alpha_{(i,j)} P_i(\sigma) P_j(\tau) = \sum_{0 \leq i,j \in \mathbb{Z}} \alpha_{(j,i)} P_j(\sigma) P_i(\tau),$$

where we have interchanged the indexes $i$ and $j$. Substituting the above two expressions into (4.13) and collecting the like basis, it gives

$$\alpha_{(0,0)} \in \mathbb{R}, \quad \alpha_{(0,1)} - \alpha_{(1,0)} = -\xi_1 = -\frac{\sqrt{3}}{6}, \quad \alpha_{(i,j)} = \alpha_{(j,i)}, \quad i+j > 1,$$

which completes the proof. \qed

As a consequence, by combining Theorem 3.4 and Theorem 4.4 with suitable truncation of the series, we can construct symplectic csRKN methods of arbitrarily high order.

5. High order symplectic RKN method

According to the discussions in subsection 3.3, we can also consider the construction of symplectic RKN method by using quadrature formulae based on csRKN. Firstly, we provide the following theorem which tells us that we can naturally get symplectic RKN methods via symplectic csRKN methods.

**Theorem 5.1.** [24] If the csRKN method denoted by $(\bar{A}_{\tau, \sigma}, \bar{B}_{\tau}, B_{\tau}, C_{\tau})$ satisfies the symplectic conditions (4.4a-4.4b), then the associated RKN method (3.19) derived by using a quadrature formula $(b_i, c_i)_{i=1}^{s}$ is still symplectic.

**Proof.** The conditions for a classical RKN method denoted by $(\bar{a}_{ij}, \bar{b}_i, b_i, c_i)$ to be symplectic are [17, 15, 11]

$$\bar{b}_i = b_i(1-c_i), \quad i = 1, \ldots, s,$$

$$b_i(\bar{b}_j - \bar{a}_{ij}) = b_j(\bar{b}_i - a_{ji}), \quad i, j = 1, \ldots, s.$$

By (4.4a-4.4b), we have the following equalities

$$\bar{B}_i = B_i(1-C_i), \quad i = 1, \ldots, s,$$

$$B_i(\bar{B}_j - \bar{A}_{ij}) = B_j(B_i - A_{ji}), \quad i, j = 1, \ldots, s.$$

Therefore, the coefficients $(b_j, \bar{A}_{ij}, \bar{b}_i, b_i, B_i, C_i)$ of the associated RKN method satisfy

$$b_i \bar{B}_i = b_i B_i(1-C_i), \quad i = 1, \ldots, s,$$

$$b_i B_i(b_j \bar{B}_j - b_j \bar{A}_{ij}) = b_j B_j(b_i \bar{B}_i - b_i \bar{A}_{ji}), \quad i, j = 1, \ldots, s,$$

which completes the proof. \qed
In [24], the authors have constructed several classes of symplectic RKN type methods of order up to 5, and their similar techniques can be exploited for obtaining higher order methods. However, it seems somewhat not very simple and convenient for constructing methods with arbitrarily higher order, as the techniques should be performed step by step with each step increasing only one order. In contrast, if we combine Theorem 4.4 and Theorem 3.3 then we can directly obtain classes of symplectic RKN type methods with any order.

In what follows, to exemplify the application of Theorem 3.4, Theorem 3.6, Theorem 4.4 and Theorem 5.1, we will show the construction of symplectic RKN methods by using Gaussian quadrature formulae, and several classes of symplectic integrators with order 4, 6 and 8 respectively will be given. It is stressed that other quadrature formulae such as Radau or Lobatto type quadrature can be similarly considered for constructing many other symplectic integrators.

For convenience, here we provide the former several Legendre polynomials as listed below

\[
\begin{align*}
P_0(t) &= 1, \\
P_1(t) &= \sqrt{3}(2t - 1), \\
P_2(t) &= \sqrt{5}(6t^2 - 6t + 1), \\
P_3(t) &= \sqrt{7}(20t^3 - 30t^2 + 12t - 1), \\
P_4(t) &= \sqrt{9}(70t^4 - 140t^3 + 90t^2 - 20t + 1), \\
&\cdots
\end{align*}
\] (5.1)

5.1. 4-order symplectic integrators

By Theorem 3.4 if we take \( \eta, \zeta \) as one of the following cases: (a) \( \eta = 1, \zeta = 3; \) (b) \( \eta = 2, \zeta = 2; \) (c) \( \eta = 3, \zeta = 1, \) then the resulting csRKN method is of order \( \min\{2\eta + 2, \eta + \zeta\} = 4. \)

As an illustration, we only consider the case with \( \eta = \zeta = 2, \) in which it gives rise to \( N_1 = 1, N_2 = 0, N_3 = 1, \) and then (3.17) becomes

\[
\bar{A}_{\tau, \sigma} = \frac{1}{6} - \frac{1}{2} \xi_1 P_1(\tau) + \frac{1}{2} \xi_1 \xi_2 P_0(\tau) P_2(\sigma) \\
+ \xi_1 \xi_2 P_2(\tau) P_0(\sigma) + \sum_{i \geq 1, j \geq 1} \omega_{i,j} P_i(\tau) P_j(\sigma),
\] (5.2)

where \( \xi_i = \frac{1}{2\sqrt{4i-1}} \) and \( \omega_{i,j} \) are arbitrary real numbers. We still take \( B_\tau = 1 - \tau, \ B_\tau = 1, \ C_\tau = \tau. \) Coupling with Theorem 4.4 to simplify, we assume that

\[
\omega_{i,j} = \begin{cases} 
\theta, & i=1, j=1; \\
0, & \text{other wise.}
\end{cases}
\]

where we set only one real parameter \( \theta, \) one should take notice that more parameters can be introduced.
As a consequence, by using Gaussian quadrature a one-parameter family of 2-stage 4-order symplectic RKN methods denoted by \((\bar{A}, \bar{b}, b, c)\) can be described as follows

\[
\bar{A} = \begin{bmatrix}
\frac{1 + 6\theta}{12}, & \frac{1 - \sqrt{3} - 6\theta}{12}, & \frac{1 + \sqrt{3} - 6\theta}{12}, & \frac{1 + 6\theta}{12}
\end{bmatrix},
\]

\[
\bar{b} = \begin{bmatrix}
\frac{3 + \sqrt{3}}{12}, & \frac{3 - \sqrt{3}}{12}, & \frac{1}{2}, & \frac{1}{2}
\end{bmatrix},
\]

\[
b = \begin{bmatrix}
\frac{3}{6}, & \frac{3}{6}, & \frac{3}{6}, & \frac{3}{6}
\end{bmatrix},
\]

\[
c = \begin{bmatrix}
\frac{3 - \sqrt{3}}{6}, & \frac{3 + \sqrt{3}}{6}
\end{bmatrix},
\]

(5.3)

where we have used the usual Matlab notations.

5.2. 6-order symplectic integrators

If we take \(\eta, \zeta\) as one of the following cases: (a) \(\eta = 2, \zeta = 4\); (b) \(\eta = 3, \zeta = 3\); (c) \(\eta = 4, \zeta = 2\); (c) \(\eta = 5, \zeta = 1\), then the resulting csRKN method is of order \(\min\{2\eta + 2, \eta + \zeta\}\) = 6.

Now we consider the case with \(\eta = \zeta = 3\), which implies that \(N_1 = 2, N_2 = 1, N_3 = 2\), and thus (3.17) becomes

\[
\bar{A}_{\tau, \sigma} = \frac{1}{6} - \frac{1}{2} \xi_1 P_1(\sigma) + \frac{1}{2} \xi_1 P_1(\tau) + \sum_{i=1}^{2} \xi_i \xi_{i+1} P_{i-1}(\tau) P_{i+1}(\sigma)
\]

\[- (\xi_1^2 + \xi_2^2) P_1(\tau) P_1(\sigma) + \sum_{i=1}^{2} \xi_i \xi_{i+1} P_{i-1}(\tau) P_{i+1}(\sigma)
\]

\[+ \sum_{i=2}^{\infty} \sum_{j=2}^{\infty} \omega(i, j) P_i(\tau) P_j(\sigma),\]

(5.4)

where \(\xi_i = \frac{1}{2\sqrt{i-1}}\) and \(\omega(i, j)\) are arbitrary real numbers. In addition, we set

\[
\omega(i, j) = \begin{cases} 
\theta, & i=2, j=2; \\
0, & \text{otherwise.}
\end{cases}
\]

where only one real parameter namely \(\theta\) is introduced.

As a consequence, by using Gaussian quadrature a one-parameter family of 3-stage 6-order symplectic RKN methods denoted by \((\bar{A}, \bar{b}, b, c)\) can be described as follows

\[
\bar{A} = \begin{bmatrix}
\frac{2 + 30\theta}{135}, & \frac{19 - 6\sqrt{15} - 120\theta}{270}, & \frac{62 - 15\sqrt{15} + 120\theta}{540}, & \frac{19 + 6\sqrt{15} - 120\theta}{432}, & \frac{1 + 15\theta}{27}, & \frac{19 + 6\sqrt{15} - 120\theta}{432}, & \frac{62 + 15\sqrt{15} + 120\theta}{540}, & \frac{2 + 30\theta}{135}
\end{bmatrix};
\]

\[
\bar{b} = \begin{bmatrix}
\frac{5 + \sqrt{15}}{36}, & \frac{2}{9}, & \frac{5 - \sqrt{15}}{36}
\end{bmatrix},
\]

\[
b = \begin{bmatrix}
\frac{5}{18}, & \frac{4}{9}, & \frac{5}{18}
\end{bmatrix},
\]

\[
c = \begin{bmatrix}
\frac{5 - \sqrt{15}}{10}, & \frac{1}{2}, & \frac{5 + \sqrt{15}}{10}
\end{bmatrix},
\]

(5.5)

where we have used the usual Matlab notations.
5.3. 8-order symplectic integrators

Similarly, if we take \( \eta, \zeta \) as one of the following cases: (a) \( \eta = 3, \zeta = 5 \); (b) \( \eta = 4, \zeta = 4 \); (c) \( \eta = 5, \zeta = 3 \); (d) \( \eta = 6, \zeta = 2 \); (d) \( \eta = 7, \zeta = 1 \), then the resulting csRKN method is of order min\( \{2\eta + 2, \eta + \zeta\} = 8 \).

Now we consider the case with \( \eta = \zeta = 4 \), which implies that \( N_1 = 3, N_2 = 2, N_3 = 3 \), hence (3.17) becomes

\[
\bar{A}_{r, \sigma} = \frac{1}{6} \xi_1 P_1(\sigma) + \frac{1}{2} \xi_1 P_1(\tau) + \sum_{i=1}^{3} \xi_i \xi_{i+1} P_{i-1}(\tau) P_{i+1}(\sigma)
\]

\[
- \sum_{i=1}^{2} (\xi_i^2 + \xi_{i+1}^2) P_i(\tau) P_i(\sigma) + \sum_{i=1}^{3} \xi_i \xi_{i+1} P_{i+1}(\tau) P_{i-1}(\sigma)
\]

\[
+ \sum_{i \geq 3} \omega(i, j) P_i(\tau) P_j(\sigma),
\]

where \( \xi_i = \frac{1}{2\sqrt{4i^2 - 1}} \) and \( \omega(i, j) \) are arbitrary real numbers. In addition, we set

\[
\omega(i, j) = \begin{cases} 
\theta, & i=3, j=3; \\
0, & \text{otherwise.}
\end{cases}
\]

where still only one real parameter \( \theta \) is settled down.

As a consequence, by using Gaussian quadrature a one-parameter family of 4-stage 8-order symplectic RKN methods denoted by \( (\bar{A}, \bar{b}, b, c) \) can be described as follows

\[
\bar{A} = \begin{pmatrix}
\frac{3\sqrt{30}}{280} & + & \frac{3\sqrt{30}}{280} & + & \frac{\sqrt{30}\theta}{40} & + & \frac{\sqrt{30}}{4136} & - & \frac{\sqrt{630 + 84\sqrt{30}}}{560} \\
\frac{\sqrt{30\theta}}{40} & + & \frac{\sqrt{30\theta}}{4136} & - & \frac{\sqrt{30\theta}}{560} & + & \frac{\sqrt{30\theta}}{4136} & - & \frac{\sqrt{30\theta}}{4136} \\
\frac{\sqrt{30\theta}}{40} & + & \frac{\sqrt{30\theta}}{4136} & - & \frac{\sqrt{30\theta}}{560} & + & \frac{\sqrt{30\theta}}{4136} & - & \frac{\sqrt{30\theta}}{4136} \\
\frac{\sqrt{30\theta}}{40} & + & \frac{\sqrt{30\theta}}{4136} & - & \frac{\sqrt{30\theta}}{560} & + & \frac{\sqrt{30\theta}}{4136} & - & \frac{\sqrt{30\theta}}{4136} \\
\frac{\sqrt{30\theta}}{40} & + & \frac{\sqrt{30\theta}}{4136} & - & \frac{\sqrt{30\theta}}{560} & + & \frac{\sqrt{30\theta}}{4136} & - & \frac{\sqrt{30\theta}}{4136} \\
\frac{\sqrt{30\theta}}{40} & + & \frac{\sqrt{30\theta}}{4136} & - & \frac{\sqrt{30\theta}}{560} & + & \frac{\sqrt{30\theta}}{4136} & - & \frac{\sqrt{30\theta}}{4136} \\
\frac{\sqrt{30\theta}}{40} & + & \frac{\sqrt{30\theta}}{4136} & - & \frac{\sqrt{30\theta}}{560} & + & \frac{\sqrt{30\theta}}{4136} & - & \frac{\sqrt{30\theta}}{4136} \\
\frac{\sqrt{30\theta}}{40} & + & \frac{\sqrt{30\theta}}{4136} & - & \frac{\sqrt{30\theta}}{560} & + & \frac{\sqrt{30\theta}}{4136} & - & \frac{\sqrt{30\theta}}{4136}
\end{pmatrix}
\]
\[
\begin{align*}
&= \sqrt{30} \, \frac{\sqrt{630 + 84\sqrt{30}} + \sqrt{630 - 84\sqrt{30}}}{336} + \sqrt{525 + 70\sqrt{30}} \, \frac{\sqrt{14}}{2016} + \sqrt{630 - 84\sqrt{30}} \, \frac{\sqrt{14} + \sqrt{140} + 3}{56 + 56} + \sqrt{630 - 84\sqrt{30}} \, \frac{-\sqrt{30}}{2016}, \\
&= \sqrt{630 - 84\sqrt{30}} \, \frac{3\sqrt{105} + 3\sqrt{105\theta}}{560} - \sqrt{30} \, \frac{\sqrt{630 + 70\sqrt{30}}}{140} - \sqrt{30} \, \frac{\sqrt{630 - 70\sqrt{30}}}{140}, \\
&= \sqrt{630 - 84\sqrt{30}} \, \frac{\sqrt{560}}{1008} + \sqrt{30} \, \frac{\sqrt{30} + 10\theta}{40}, \\
&= \sqrt{30} \, \frac{\sqrt{630 + 84\sqrt{30}} - \sqrt{630 - 84\sqrt{30}}}{336} + \sqrt{525 - 70\sqrt{30}} \, \frac{\sqrt{14}}{490} - \sqrt{630 - 84\sqrt{30}} \, \frac{3\sqrt{105} + 3\sqrt{105\theta}}{1225} - \sqrt{630 - 84\sqrt{30}} \, \frac{\sqrt{140} + \sqrt{140\theta}}{1008}, \\
&= \sqrt{630 - 84\sqrt{30}} \, \frac{\sqrt{560}}{280} + \sqrt{30} \, \frac{-\sqrt{30} - 10}{40} \theta + \sqrt{30} - 6\sqrt{14} \theta \, \frac{\sqrt{30} + 18}{280} + \sqrt{630 + 84\sqrt{30}} \, \frac{\sqrt{140} + \sqrt{140\theta}}{560}, \\
&= \sqrt{30} \, \frac{\sqrt{560}}{560} + \sqrt{30} \, \frac{\sqrt{30} - 10}{40} \theta + \sqrt{30} + 6\sqrt{14} \theta \, \frac{\sqrt{30} + 18}{280}, \\
&= \sqrt{30} \, \frac{\sqrt{630 + 84\sqrt{30}} + \sqrt{630 - 84\sqrt{30}}}{336} + \sqrt{525 + 70\sqrt{30}} \, \frac{\sqrt{14}}{2016} + \sqrt{630 - 84\sqrt{30}} \, \frac{3\sqrt{105} + 3\sqrt{105\theta}}{1225} - \sqrt{630 - 84\sqrt{30}} \, \frac{\sqrt{140} + \sqrt{140\theta}}{1008}, \\
&= \sqrt{630 - 84\sqrt{30}} \, \frac{\sqrt{560}}{1008} + \sqrt{30} \, \frac{-\sqrt{30} - 10}{40} \theta + \sqrt{30} - 6\sqrt{14} \theta \, \frac{\sqrt{30} + 18}{280}, \\
&= \sqrt{30} \, \frac{\sqrt{630 + 84\sqrt{30}} + \sqrt{630 - 84\sqrt{30}}}{336} + \sqrt{525 + 70\sqrt{30}} \, \frac{\sqrt{14}}{2016} + \sqrt{630 - 84\sqrt{30}} \, \frac{3\sqrt{105} + 3\sqrt{105\theta}}{1225} - \sqrt{630 - 84\sqrt{30}} \, \frac{\sqrt{140} + \sqrt{140\theta}}{1008}, \\
&= \sqrt{630 - 84\sqrt{30}} \, \frac{\sqrt{560}}{1008} + \sqrt{30} \, \frac{-\sqrt{30} - 10}{40} \theta + \sqrt{30} - 6\sqrt{14} \theta \, \frac{\sqrt{30} + 18}{280}, \\
&= \sqrt{30} \, \frac{\sqrt{630 + 84\sqrt{30}} + \sqrt{630 - 84\sqrt{30}}}{336} + \sqrt{525 + 70\sqrt{30}} \, \frac{\sqrt{14}}{2016} + \sqrt{630 - 84\sqrt{30}} \, \frac{3\sqrt{105} + 3\sqrt{105\theta}}{1225} - \sqrt{630 - 84\sqrt{30}} \, \frac{\sqrt{140} + \sqrt{140\theta}}{1008},
\end{align*}
\]

where we have used the usual Matlab notations.
6. Concluding remarks

In this article, we consider high order symplectic integrators within the newly developed framework of continuous-stage Runge-Kutta Nyström (csRKN) methods. It states that the construction of such integrators heavily relies on the Legendre polynomial expansion technique associated with the simplifying assumptions for order conditions and the symplectic conditions for RKN type methods. Several new one-parameter families of symplectic RKN methods of orders 4, 6 and 8 are obtained in use of Gaussian quadrature formulae. It is stressed that we can use any other quadrature formulae to get other symplectic RKN integrators and more than one free parameters can be embedded in the formulae. It is possible to construct more higher order methods with the same technique. As a consequence, it turned out that our approach seems more easier to construct RKN type methods of arbitrarily high order than the conventional approaches which generally resort to solving the tedious nonlinear algebraic equations that stem from the order conditions with a huge number of unknown coefficients.

Acknowledgements

The first author was supported by the Foundation of NNSFC (11401055) and the Foundation of Education Department of Hunan Province (15C0028). The second author was supported by the Foundation of NNSFC (No.11271357), the Foundation for Innovative Research Groups of the NNSFC (No.11321061) and ITER-China Program (No.2014GB124005). The third author was supported by...

References

[1] V.I. Arnold, Mathematical methods of classical mechanics, Vol. 60, Springer, 1989.

[2] L. Brugnano, F. Iavernaro, D. Trigiante, Hamiltonian boundary value methods: energy preserving discrete line integral methods, J. Numer. Anal., Indust. Appl. Math., 5 (1–2) (2010), 17–37.

[3] J. C. Butcher, The Numerical Analysis of Ordinary Differential Equations: Runge-Kutta and General Linear Methods, John Wiley & Sons, 1987.

[4] J. C. Butcher, Y. Miyatake, A characterization of energy-preserving methods and the construction of parallel integrators for Hamiltonian systems, arXiv preprint arXiv:1505.02537, 2015.

[5] E. Celledoni, R. I. McLachlan, D. McLaren, B. Owren, G. R. W. Quispel, W. M. Wright., Energy preserving Runge-Kutta methods, M2AN 43 (2009), 645–649.
[6] K. Feng, *On difference schemes and symplectic geometry*, Proceedings of the 5-th Inter., Symposium of Differential Geometry and Differential Equations, Beijing, 1984, 42-58.

[7] K. Feng, *K. Feng’s Collection of Works*, Vol. 2, Beijing: National Defence Industry Press, 1995.

[8] K. Feng, M. Qin, *Symplectic Geometric Algorithms for Hamiltonian Systems*, Springer and Zhejiang Science and Technology Publishing House, Heidelberg, Hangzhou, First edition, 2010.

[9] E. Hairer, S. P. Nørsett, G. Wanner, *Solving Ordinary Differential Equations I: Nonstiff Problems*, Springer Series in Computational Mathematics, 8, Springer-Verlag, Berlin, 1993.

[10] E. Hairer, G. Wanner, *Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems*, Second Edition, Springer Series in Computational Mathematics, 14, Springer-Verlag, Berlin, 1996.

[11] E. Hairer, C. Lubich, G. Wanner, *Geometric Numerical Integration: Structure-Preserving Algorithms For Ordinary Differential Equations*, Second edition. Springer Series in Computational Mathematics, 31, Springer-Verlag, Berlin, 2006.

[12] E. Hairer, *Energy-preserving variant of collocation methods*, JNAIAM J. Numer. Anal. Indust. Appl. Math., 5 (2010), 73–84.

[13] Y. Miyatake, *An energy-preserving exponentially-fitted continuous stage Runge-Kutta methods for Hamiltonian systems*, BIT Numer. Math., DOI 10.1007/s10543-014-0474-4, 2014.

[14] G. R. W. Quispel, D. I. McLaren, *A new class of energy-preserving numerical integration methods*, J. Phys. A: Math. Theor., 41 (2008) 045206.

[15] J. M. Sanz-Serna, M. P. Calvo, *Numerical Hamiltonian problems*, Chapman & Hall, 1994.

[16] Z. Shang, *K.A.M theorem of symplectic algorithms for Hamiltonian systems*, Numerische Mathematik, 83 (1999), 477–496.

[17] Y. B. Suris, *Canonical transformations generated by methods of Runge-Kutta type for the numerical integration of the system x'' = −∂U/∂x*, Zh. Vychisl. Mat. i Mat. Fiz., 29 (1989), 202–211.

[18] W. Tang, Y. Sun, *A new approach to construct Runge-Kutta type methods and geometric numerical integrators*, AIP. Conf. Proc., 1479 (2012), 1291-1294.

[19] W. Tang, G. Lang, X. Luo, *Construction of symplectic (partitioned) Runge-Kutta methods with continuous stage*, submitted, 2015.
[20] W. Tang, Y. Sun, *Construction of Runge-Kutta type methods for solving ordinary differential equations*, Appl. Math. Comput., 234 (2014), 179–191.

[21] W. Tang, Y. Sun, *Time finite element methods: A unified framework for numerical discretizations of ODEs*, Appl. Math. Comput. 219 (2012), 2158–2179.

[22] W. Tang, Y. Sun, *Symplecticity-preserving discontinuous Galerkin methods for Hamiltonian systems*, preprint, 2015.

[23] W. Tang, Y. Sun, W. Cai, *Discontinuous Galerkin methods for Hamiltonian ODEs and PDEs*, preprint, 2015.

[24] W. Tang, J. Zhang, *Symplecticity-preserving continuous-stage Runge-Kutta Nyström methods*, preprint, 2015.