Symplecticity-preserving continuous-stage Runge-Kutta-Nyström methods

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Abstract

We develop continuous-stage Runge-Kutta-Nyström (csRKN) methods for solving second order ordinary differential equations (ODEs) in this paper. The second order ODEs are commonly encountered in various fields and some of them can be reduced to the first order ODEs with the form of separable Hamiltonian systems. The symplecticity-preserving numerical algorithm is of interest for solving such special systems. We present a sufficient condition for a csRKN method to be symplecticity-preserving, and by using Legendre polynomial expansion we show a simple way to construct such symplectic RKN type method.

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

1. Introduction

It is well-known that Runge-Kutta (RK) methods, partitioned Runge-Kutta (PRK) methods and Runge-Kutta-Nyström (RKN) methods paly a central role in the context of numerical solution of ordinary differential equations (ODEs), and they were well-developed in the previous investigations [2, 6, 7].

More recently, numerical methods with infinitely many stages including continuous-stage Runge-Kutta (csRK) method, continuous-stage partitioned Runge-Kutta (csPRK) method have been investigated and discussed in [9, 15, 18, 17, 10, 16, 3]. It is found that based on such methods we can obtain many classical RK methods and PRK methods of arbitrarily high order by using quadrature formulae but without resort to solving the tedious nonlinear algebraic equations that stem from the order conditions with many unknown coefficients. The construction of continuous-stage numerical methods seems

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more easier than that of those classical methods, since the associated Butcher tableau coefficients belong to the space of continuous functions and they can be treated in use of orthogonal polynomial expansions [17, 16]. Moreover, as shown in [17, 16], numerical methods serving some special purpose including symplecticity-preserving methods for Hamiltonian systems, symmetric methods for reversible systems, energy-preserving methods for Hamiltonian systems, numerical methods with conjugate symplecticity (up to a finite order) for Hamiltonian systems can also be constructed and investigated based on such new framework.

It is worth mentioning that some methods with special purpose couldn't possibly exist in the classical context of numerical methods but it does within the new framework. For instance, [4] has proved that there is no energy-preserving RK methods for general Hamiltonian system excluding those polynomial system, but energy-preserving methods based on csRK obviously exist [9, 12, 1, 15, 18, 17, 10, 3]. It is also found that some Galerkin variational methods can be related to continuous-stage (P)RK methods, which can not be completely explained in the classical (P)RK framework [18, 19, 20]. As a consequence, the continuous-stage methods provide a new broader scope for numerical solution of ODEs and they are worth further investigating.

As is well known, the second order ODEs are commonly encountered in various fields including celestial mechanics, molecular dynamics, biological chemistry and so on [6, 13, 8]. In this paper, we are going to develop continuous-stage RKN (csRKN) methods for solving second order ODEs. In particular, there is a number of second order ODEs that can be reduced to the first order ODEs with the form of separable Hamiltonian systems, and the symplecticity-preserving discretization for such systems is of considerable interest [5, 13, 8]. For this sake, we will present a sufficient condition for a csRKN method to be symplecticity-preserving, and then show the construction of symplectic RKN type methods by using the Legendre polynomial expansion technique.

The outline of this paper is as follows. In the next section, we introduce the so-called csRKN methods for solving second order ODEs. After that we present the corresponding symplectic conditions and the order conditions, then we use the orthogonal polynomial expansion technique to construct symplecticity-preserving csRKN methods, which will be given in section 3-4. Section 5 is devoted to discuss the construction of diagonally implicit symplectic methods. At last, the concluding remarks will be given.

2. Continuous-stage RKN method

In the field of engineering and physics there are a large class of problems which can be expressed by a system of second order differential equations

$$\ddot{q} = f(t, q), \ q \in \mathbb{R}^d, \tag{2.1}$$ {eq:second}

where the double dots on q represent the second-order derivative with respect to t and $f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ is a sufficiently smooth vector function.

For system (2.1), the often used treatment is to write it as a first order differential system by introducing $p = \dot{q}$, namely

$$\begin{cases} \dot{q} = p, \\ \dot{p} = f(t, q). \end{cases} \tag{2.2}$$ {eq:first}

As presented in [16], by using a continuous-stage partitioned Runge-Kutta (csPRK) method to (2.2), it gives

$$Q_\tau = q_n + h \int_0^1 A_{\tau,\sigma} P_\sigma d\sigma, \quad \tau \in [0, 1], \tag{2.3a}$$ {eq:cs1}

$$P_\tau = p_n + h \int_0^1 \hat{A}_{\tau,\sigma} f(t_n + C_\sigma h, Q_\sigma) d\sigma, \quad \tau \in [0, 1], \tag{2.3b}$$ {eq:cs2}

$$q_{n+1} = q_n + h \int_0^1 B_\tau P_\tau d\tau, \quad n \in \mathbb{N}, \tag{2.3c}$$ {eq:cs3}

$$p_{n+1} = p_n + h \int_0^1 \hat{B}_\tau f(t_n + C_\tau h, Q_\tau) d\tau, \quad n \in \mathbb{N}, \tag{2.3d}$$ {eq:cs4}

where $A_{\tau,\sigma}$, $\hat{A}_{\tau,\sigma}$ are functions of two variables $\tau, \sigma \in [0, 1]$ and B_τ, $\hat{B}_\tau$, C_τ are functions of $\tau \in [0, 1]$. We call Q_τ and P_τ the internal continuous stages. In addition, here we assume that $\int_0^1 A_{\tau,\sigma} d\sigma = \int_0^1 \hat{A}_{\tau,\sigma} d\sigma = C_\tau$, and $\int_0^1 B_\tau d\tau = \int_0^1 \hat{B}_\tau d\tau = 1$.

By inserting (2.3b) into (2.3a), we derive

$$Q_\tau = q_n + h \int_0^1 A_{\tau,\sigma} \big(p_n + h \int_0^1 \hat{A}_{\sigma,\rho} f(t_n + C_\rho h, Q_\rho) d\rho\big) d\sigma \tag{2.4}$$

$$= q_n + hC_\tau p_n + h^2 \int_0^1 \bar{A}_{\tau,\rho} f(t_n + C_\rho h, Q_\rho) d\rho, \tag{2.5}$$

where we define $\bar{A}_{\tau,\rho} = \int_0^1 A_{\tau,\sigma} \hat{A}_{\sigma,\rho} d\sigma$ and here by hypothesis $C_\tau = \int_0^1 A_{\tau,\sigma} d\sigma$. Similarly, by inserting (2.3b) into (2.3c), we have

$$q_{n+1} = q_n + h \int_0^1 B_\tau \big(p_n + h \int_0^1 \hat{A}_{\tau,\sigma} f(t_n + C_\sigma h, Q_\sigma) d\sigma\big) d\tau \tag{2.6}$$

$$= q_n + hp_n + h^2 \int_0^1 \bar{B}_\sigma f(t_n + C_\sigma h, Q_\sigma) d\sigma \tag{2.7}$$

where we denote $\bar{B}_\sigma = \int_0^1 B_\tau \hat{A}_{\tau,\sigma} d\tau$, and note that $\int_0^1 B_\tau d\tau = 1$.

In summary, by using a csPRK method to (2.2) and eliminating the internal stage variable P_τ, we can obtain the method which is referred to as a continuous-stage Runge-Kutta-Nyström method in this paper.

Definition 2.1 (Continuous-stage Runge-Kutta-Nyström method)**.** *Let $\bar{A}_{\tau,\sigma}$ be a function of variables $\tau, \sigma \in [0, 1]$ and $\bar{B}_\tau$, $\hat{B}_\tau$, C_τ be functions of $\tau \in [0, 1]$.*

A continuous-stage Runge-Kutta-Nyström (csRKN) method for the solution of (2.1) *is given by*

$$Q_\tau = q_n + hC_\tau p_n + h^2 \int_0^1 \bar{A}_{\tau,\sigma} f(t_n + C_\sigma h, Q_\sigma) d\sigma, \quad \tau \in [0,1], \tag{2.8a}$$ {eq:csrkn1}

$$q_{n+1} = q_n + hp_n + h^2 \int_0^1 \bar{B}_\tau f(t_n + C_\tau h, Q_\tau) d\tau, \quad n \in \mathbb{N}, \tag{2.8b}$$ {eq:csrkn2}

$$p_{n+1} = p_n + h \int_0^1 \hat{B}_\tau f(t_n + C_\tau h, Q_\tau) d\tau, \quad n \in \mathbb{N}, \tag{2.8c}$$ {eq:csrkn3}

which can be characterized by the following Butcher tableau

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

3. Symplectic conditions for csRKN method

When the system (2.1) is autonomous (i.e., time-independent for the right-hand-side vector field) and f is the gradient of a scalar function, e.g.,

$$f(q) = -\nabla_q V(q),$$

then it becomes a separable Hamiltonian system in the form

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

with the Hamiltonian $\mathbf{H}(z) = \frac{1}{2} p^T p + V(q)$ and $J = \begin{pmatrix} 0 & I_{d\times d} \\ -I_{d\times d} & 0 \end{pmatrix}$, and such system possesses an intrinsic geometric structure called symplecticity. This states that the flow φ_t of the system is a symplectic transformation [8], i.e., $(\varphi_t')^T J \varphi_t' = J$, where φ_t' denotes the derivative of φ_t with respect to the initial values. For Hamiltonian system, symplectic numerical method is of considerable interest [5, 8], as it always exhibits bounded small energy errors for the exponentially long time, and can correctly mimic the qualitative behavior of the original system (e.g., preserving the quasi-periodic orbits (namely KAM tori) and chaotic regions of phase space [14]). A one-step method $\Phi_h : (p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$, when applied to a Hamiltonian system, is called symplectic if and only if $(\Phi_h')^T J \Phi_h' = J$, or equivalently $dp_{n+1} \wedge dq_{n+1} = dp_n \wedge dq_n$ (Here $\wedge$ denotes the standard wedge product in differential geometry).

3.1. The sufficient condition for symplecticity

{conditions: sym}

Theorem 3.1. *If a csRKN method denoted by* $(\bar{A}_{\tau,\sigma}, \bar{B}_\tau, \hat{B}_\tau, C_\tau)$ *satisfies*

$$\hat{B}_\tau (1 - C_\tau) = \bar{B}_\tau, \ \tau \in [0,1], \tag{3.1a}$$ {sym_cond_orig01}

$$\hat{B}_\tau (\bar{B}_\sigma - \bar{A}_{\tau,\sigma}) = \hat{B}_\sigma (\bar{B}_\tau - \bar{A}_{\sigma,\tau}), \ \tau, \sigma \in [0,1], \tag{3.1b}$$ {sym_cond_orig02}

then the method is symplectic for solving the autonomous second order differential equations (2.1) *with* $f(q) = -\nabla_q V(q)$ *(which can be rewritten as a Hamiltonian system).*

Proof. By the csRKN method (2.8a-2.8c), we have

$$\begin{aligned}
&dp_{n+1} \wedge dq_{n+1} \\
&= d(p_n + h\int_0^1 \hat{B}_\tau f(Q_\tau)d\tau) \wedge d(q_n + hp_n + h^2\int_0^1 \bar{B}_\tau f(Q_\tau)d\tau) \\
&= dp_n \wedge dq_n + h\int_0^1 (\hat{B}_\tau df(Q_\tau) \wedge dq_n)d\tau + hdp_n \wedge dp_n \\
&\quad + h^2\int_0^1 (\hat{B}_\tau df(Q_\tau) \wedge dp_n)d\tau + h^2\int_0^1 (\bar{B}_\tau dp_n \wedge df(Q_\tau))d\tau \\
&\quad + h^3\int_0^1\int_0^1 \hat{B}_\tau \bar{B}_\sigma df(Q_\tau) \wedge df(Q_\sigma)d\sigma d\tau
\end{aligned} \tag{3.2}$$ {eq:proofsym1}

Because of the skew symmetry of wedge product, the third term vanishes. By virtue of (2.8a), the second term can be recast as

$$\begin{aligned}
&h\int_0^1 (\hat{B}_\tau df(Q_\tau) \wedge dq_n)d\tau \\
&= h\int_0^1 \big(\hat{B}_\tau df(Q_\tau) \wedge d(Q_\tau - hC_\tau p_n - h^2\int_0^1 \bar{A}_{\tau,\sigma} f(Q_\sigma)d\sigma)\big)d\tau \\
&= h\int_0^1 (\hat{B}_\tau df(Q_\tau) \wedge dQ_\tau)d\tau - h^2\int_0^1 (\hat{B}_\tau C_\tau df(Q_\tau) \wedge dp_n)d\tau \\
&\quad - h^3\int_0^1 (\int_0^1 \hat{B}_\tau \bar{A}_{\tau,\sigma} df(Q_\tau) \wedge df(Q_\sigma)d\sigma)d\tau
\end{aligned} \tag{3.3}$$ {eq:sovqn}

Note that $f(q) = -\nabla_q V(q)$ and its Jacobian matrix is symmetric, the first term in the above equality vanishes. Then by substituting (3.3) into (3.2), it yields

$$\begin{aligned}
&dp_{n+1} \wedge dq_{n+1} \\
&= dp_n \wedge dq_n - h^2\int_0^1 (\hat{B}_\tau C_\tau df(Q_\tau) \wedge dp_n)d\tau \\
&\quad - h^3\int_0^1\int_0^1 (\hat{B}_\tau \bar{A}_{\tau,\sigma} df(Q_\tau) \wedge df(Q_\sigma))d\sigma d\tau + h^2\int_0^1 (\hat{B}_\tau df(Q_\tau) \wedge dp_n)d\tau \\
&\quad - h^2\int_0^1 (\bar{B}_\tau df(Q_\tau) \wedge dp_n)d\tau \ + h^3\int_0^1\int_0^1 \hat{B}_\tau \bar{B}_\sigma df(Q_\tau) \wedge df(Q_\sigma)d\sigma d\tau \\
&= dp_n \wedge dq_n + h^2\int_0^1 (-\hat{B}_\tau C_\tau + \hat{B}_\tau - \bar{B}_\tau)df(Q_\tau) \wedge dp_n d\tau \\
&\quad + h^3\int_0^1\int_0^1 (\hat{B}_\tau \bar{B}_\sigma - \hat{B}_\tau \bar{A}_{\tau,\sigma})df(Q_\tau) \wedge df(Q_\sigma)d\sigma d\tau
\end{aligned} \tag{3.4}$$ {eq:proofsym2}

The last term of the formula above can be reshaped as follows

$$
\begin{aligned}
& h^3 \int_0^1 \int_0^1 (\hat{B}_\tau \bar{B}_\sigma - \hat{B}_\tau \bar{A}_{\tau,\sigma}) df(Q_\tau) \wedge df(Q_\sigma) d\sigma d\tau \\
= & -\frac{h^3}{2} \int_0^1 \int_0^1 \big(\hat{B}_\tau \bar{A}_{\tau,\sigma} df(Q_\tau) \wedge df(Q_\sigma) + \hat{B}_\sigma \bar{A}_{\sigma,\tau} df(Q_\sigma) \wedge df(Q_\tau)\big) d\sigma d\tau \\
& + \frac{h^3}{2} \int_0^1 \int_0^1 \big(\hat{B}_\tau \bar{B}_\sigma df(Q_\tau) \wedge df(Q_\sigma) + \hat{B}_\sigma \bar{B}_\tau df(Q_\sigma) \wedge df(Q_\tau)\big) d\sigma d\tau \\
= & -\frac{h^3}{2} \int_0^1 \int_0^1 \big(\hat{B}_\tau \bar{A}_{\tau,\sigma} df(Q_\tau) \wedge df(Q_\sigma) - \hat{B}_\sigma \bar{A}_{\sigma,\tau} df(Q_\tau) \wedge df(Q_\sigma)\big) d\sigma d\tau \\
& + \frac{h^3}{2} \int_0^1 \int_0^1 \big(\hat{B}_\tau \bar{B}_\sigma df(Q_\tau) \wedge df(Q_\sigma) - \hat{B}_\sigma \bar{B}_\tau df(Q_\tau) \wedge df(Q_\sigma)\big) d\sigma d\tau \\
= & \frac{h^3}{2} \int_0^1 \int_0^1 (\hat{B}_\tau \bar{B}_\sigma - \hat{B}_\sigma \bar{B}_\tau - \hat{B}_\tau \bar{A}_{\tau,\sigma} + \hat{B}_\sigma \bar{A}_{\sigma,\tau}) df(Q_\tau) \wedge df(Q_\sigma) d\sigma d\tau
\end{aligned}
\tag{3.5}
$$

Therefore, if we require the condition given by (3.1a-3.1b), then the last two terms in (3.4) vanish, and it yields

$$dp_{n+1} \wedge dq_{n+1} = dp_n \wedge dq_n,$$

which implies the symplecticity. $\square$

A very special class of separable Hamiltonian systems commonly considered in practice is the system with Hamiltonian

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

where M (mass matrix) is a constant, symmetric and invertible matrix, and the corresponding Hamiltonian system becomes

$$\begin{cases} \dot{q} = M^{-1} p, \\ \dot{p} = -\nabla_q V(q). \end{cases}$$

If we let $\widetilde{p} = M^{-1} p$, then we get

$$\begin{cases} \dot{q} = \widetilde{p}, \\ \dot{\widetilde{p}} = -M^{-1} \nabla_q V(q), \end{cases}$$

which is in the form (2.2). By eliminating $\widetilde{p}$, it reads

$$\ddot{q} = -M^{-1} \nabla_q V(q). \tag{3.6}$$ {eq:Hs}

For such a second order system, the csRKN method is

$$
\begin{aligned}
&Q_\tau = q_n + hC_\tau \widetilde{p}_n + h^2 \int_0^1 \bar{A}_{\tau,\sigma} f(Q_\sigma) d\sigma, \quad \tau \in [0,1],\\
&q_1 = q_n + h\widetilde{p}_n + h^2 \int_0^1 \bar{B}_\tau f(Q_\tau) d\tau, \qquad\qquad (3.7) \quad \{\texttt{scheme1}\}\\
&\widetilde{p}_{n+1} = \widetilde{p}_n + h \int_0^1 \hat{B}_\tau f(Q_\tau) d\tau,
\end{aligned}
$$

where $f(q) = -M^{-1}\nabla_q V(q)$ and $\widetilde{p}_n = M^{-1}p_n$.

By Theorem 3.1, if we require (3.1a-3.1b), then the one-step method (3.7) mapping $(\widetilde{p}_n, q_n)$ to $(\widetilde{p}_{n+1}, q_{n+1})$ is symplectic, i.e.,

$$
d\widetilde{p}_{n+1} \wedge dq_{n+1} = d\widetilde{p}_n \wedge dq_n.
$$

However, we are interested in the method in terms of the variables p and q, rather than in terms of $\widetilde{p} = \dot{q}$ and q. To address this issue, we observe that (3.7) can be recast as

$$
\begin{aligned}
&Q_\tau = q_n + hC_\tau M^{-1} p_n + h^2 \int_0^1 \bar{A}_{\tau,\sigma} f(Q_\sigma) d\sigma, \quad \tau \in [0,1],\\
&q_1 = q_n + hM^{-1}p_n + h^2 \int_0^1 \bar{B}_\tau f(Q_\tau) d\tau, \qquad\qquad (3.8) \quad \{\texttt{scheme2}\}\\
&p_{n+1} = p_n + hM \int_0^1 \hat{B}_\tau f(Q_\tau) d\tau,
\end{aligned}
$$

where the last formula is derived by multiplying M from the left-hand side of (3.7). By the similar arguments as the proof of Theorem 3.1, we can prove that it still yields[1]

$$
dp_{n+1} \wedge dq_{n+1} = dp_n \wedge dq_n.
$$

Therefore, the csRKN method (3.8) remains symplectic under the conditions (3.1a-3.1b).

3.2. Further characterizations for symplecticity

In what follows, we will show another useful result which shows the characterizations for a csRKN method to be symplectic.

Now we introduce the ι-degree normalized shifted Legendre polynomial $P_\iota(x)$ by using the Rodrigues formula

$$
P_0(x) = 1,\; P_\iota(x) = \frac{\sqrt{2\iota+1}}{\iota!} \frac{\mathrm{d}^\iota}{\mathrm{d}x^\iota}\Big(x^\iota (x-1)^\iota\Big), \quad \iota = 1,2,3,\cdots.
$$

[1]A detailed proof will be found in our another coming paper.

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

$$\int_0^1 P_\iota(t)P_\kappa(t)\,\mathrm{d}t = \delta_{\iota\kappa}, \quad \iota,\, \kappa = 0, 1, 2, \cdots,$$

and they as well satisfy the following integration formulae

$$\begin{aligned}
&\int_0^x P_0(t)\,\mathrm{d}t = \xi_1 P_1(x) + \frac{1}{2}P_0(x),\\
&\int_0^x P_\iota(t)\,\mathrm{d}t = \xi_{\iota+1}P_{\iota+1}(x) - \xi_\iota P_{\iota-1}(x), \quad \iota = 1, 2, 3, \cdots,\\
&\int_x^1 P_\iota(t)\,\mathrm{d}t = \delta_{\iota 0} - \int_0^x P_\iota(t)\,\mathrm{d}t, \quad \iota = 0, 1, 2, \cdots,
\end{aligned} \tag{3.9}$$ {property}

where $\xi_\iota = \frac{1}{2\sqrt{4\iota^2-1}}$ and δ_{ij} is the Kronecker symbol.

Similarly as the continuous-stage (P)RK methods discussed in [16], we will use the simplifying hypothesis $\hat{B}_\tau = 1, C_\tau = \tau$ throughout this paper. By exploiting the orthogonal polynomial expansions we get the following result.

{construct_scsRKN}

Theorem 3.2. *The csRKN method denoted by* $(\bar{A}_{\tau,\sigma}, \bar{B}_\tau, \hat{B}_\tau, C_\tau)$ *with* $\hat{B}_\tau = 1, C_\tau = \tau$ *is symplectic for solving system* (2.1) *(as a separable Hamiltonian system), if* $\bar{A}_{\tau,\sigma}$ *and* $\bar{B}_\tau$ *take the following forms in terms of Legendre polynomials*

$$\begin{aligned}
\bar{B}_\tau &= 1 - \tau = \frac{1}{2}P_0(\tau) - \xi_1 P_1(\tau), \quad \tau \in [0, 1],\\
\bar{A}_{\tau,\sigma} &= \alpha_{(0,0)} + \alpha_{(0,1)}P_1(\sigma) + \alpha_{(1,0)}P_1(\tau) + \sum_{i+j>1} \alpha_{(i,j)}P_i(\tau)P_j(\sigma), \;\; \tau, \sigma \in [0, 1],
\end{aligned} \tag{3.10}$$ {sym_cond}

where the expansion coefficients $\alpha_{(i,j)}$ *as real parameters satisfy*

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

Proof. By the assumption $\hat{B}_\tau = 1, C_\tau = \tau$ and using (3.1a) we get

$$\bar{B}_\tau = 1 - \tau = \frac{1}{2}P_0(\tau) - \xi_1 P_1(\tau),$$

inserting it into (3.1b), then it ends up with

$$\bar{A}_{\tau,\,\sigma} - \bar{A}_{\sigma,\,\tau} = \tau - \sigma = \xi_1(P_1(\tau) - P_1(\sigma)) = \frac{\sqrt{3}}{6}(P_1(\tau) - P_1(\sigma)), \tag{3.11}$$ {eq:AB}

in which we have used the known 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

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

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

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

Substituting the above two expressions into (3.11) and collecting the like basis, it gives

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

which completes the proof. $\square$

4. Symplectic RKN methods based on csRKN

In this section, we discuss the construction of symplectic RKN methods based on csRKN.

It is almost mandatory that the practical implementation of the csRKN method (2.8a)-(2.8c) needs the use of numerical quadrature formula. By applying the quadrature formula $(b_i, c_i)_{i=1}^r$ of order p to (2.8a)-(2.8c), with abuse of notations $Q_i = Q_{c_i}$, we derive an r-stage classical RKN method

$$Q_i = q_n + hC_i p_n + h^2 \sum_{j=1}^{r} b_j \bar{A}_{ij} f(Q_j), \quad i = 1, \cdots, r, \tag{4.1a}$$ {eq:rkn1}

$$q_{n+1} = q_n + hp_n + h^2 \sum_{i=1}^{r} b_i \bar{B}_i f(Q_i), \quad n \in \mathbb{N}, \tag{4.1b}$$ {eq:rkn2}

$$p_{n+1} = p_n + h \sum_{i=1}^{r} b_i \hat{B}_i f(Q_i), \quad n \in \mathbb{N}, \tag{4.1c}$$ {eq:rkn3}

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

$$\begin{array}{c|ccc} C_1 & b_1\bar{A}_{11} & \cdots & b_r\bar{A}_{1r} \\ \vdots & \vdots & & \vdots \\ C_r & b_1\bar{A}_{r1} & \cdots & b_r\bar{A}_{rr} \\ \hline & b_1\bar{B}_1 & \cdots & b_r\bar{B}_r \\ \hline & b_1\hat{B}_1 & \cdots & b_r\hat{B}_r \end{array} \tag{4.2}$$ {tab:rknbutcher}

In particular, if we use the hypothesis $\bar{B}_\tau = \hat{B}_\tau(1 - C_\tau)$, $\hat{B}_\tau = 1$, $C_\tau = \tau$ for

$\tau \in [0,1]$, we then get an r-stage RKN method with tableau

$$\begin{array}{c|ccc} c_1 & b_1\bar{A}_{11} & \cdots & b_r\bar{A}_{1r} \\ \vdots & \vdots & & \vdots \\ c_r & b_1\bar{A}_{r1} & \cdots & b_r\bar{A}_{rr} \\ \hline & \bar{b}_1 & \cdots & \bar{b}_r \\ \hline & b_1 & \cdots & b_r \end{array} \tag{4.3}$$ {RKN:qua}

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

The following result implies that we can construct symplectic RKN method via symplectic csRKN method with the help of a quadrature formula.

Theorem 4.1. *If the csRKN method denoted by $(\bar{A}_{\tau,\sigma}, \bar{B}_\tau, \hat{B}_\tau, C_\tau)$ satisfies the symplectic condition (3.1a-3.1b), then the associated RKN method* (4.2) *derived by using a quadrature formula $(b_i, c_i)_{i=1}^r$ is still symplectic.*

Proof. Recall that the sufficient condition for a classical RKN method denoted by $(\bar{a}_{ij}, \bar{b}_i, b_i, c_i)$ to be symplectic is [13]

$$\begin{aligned} &\bar{b}_i = b_i(1-c_i), \quad i = 1, \cdots, r, \\ &b_i(\bar{b}_j - \bar{a}_{ij}) = b_j(\bar{b}_i - \bar{a}_{ji}), \quad i, j = 1, \cdots, r. \end{aligned}$$

By (3.1a-3.1b), we have the following equalities

$$\begin{aligned} &\bar{B}_i = \hat{B}_i(1-C_i), \quad i = 1, \cdots, r, \\ &\hat{B}_i(\bar{B}_j - \bar{A}_{ij}) = \hat{B}_j(\bar{B}_i - \bar{A}_{ji}), \quad i, j = 1, \cdots, r. \end{aligned}$$

Therefore, the coefficients $(b_j\bar{A}_{i,j},\ b_i\bar{B}_i,\ b_i\hat{B}_i,\ C_i)$ of the associated RKN method satisfy

$$\begin{aligned} &b_i\bar{B}_i = b_i\hat{B}_i(1-C_i), \quad i = 1, \cdots, r, \\ &b_i\hat{B}_i(b_j\bar{B}_j - b_j\bar{A}_{ij}) = b_j\hat{B}_j(b_i\bar{B}_i - b_i\bar{A}_{ji}), \quad i, j = 1, \cdots, r, \end{aligned}$$

which completes the proof by using the classical result. □

4.1. Order conditions for RKN type methods

To construct symplectic RKN method with a preassigned order, let us introduce the order conditions for RKN type methods.

It is known that the classical RKN method for solving (2.1) can be formulated as

$$Q_i = q_n + hc_ip_n + h^2\sum_{j=1}^r \bar{a}_{ij} f(t_n + c_jh, Q_j), \quad i = 1, \cdots, r, \tag{4.4a}$$ {eq:grkn1}

$$q_{n+1} = q_n + hp_n + h^2\sum_{i=1}^r \bar{b}_i f(t_n + c_ih, Q_i), \quad n \in \mathbb{N}, \tag{4.4b}$$ {eq:grkn2}

$$p_{n+1} = p_n + h\sum_{i=1}^r b_i f(t_n + c_ih, Q_i), \quad n \in \mathbb{N}, \tag{4.4c}$$ {eq:grkn3}

and as shown in [6], under the assumption

$$\bar{b}_i = b_i(1 - c_i), \quad i = 1, \ldots, r, \tag{4.5}$$

the number of order conditions are drastically reduced and there are rather fewer order conditions need to be further considered, as listed below [6]

$$\left|\begin{array}{l|l}
1)\ \sum\limits_{i=1}^{r} b_i = 1; & 2)\ \sum\limits_{i=1}^{r} b_i c_i = \frac{1}{2}; \\
3)\ \sum\limits_{i=1}^{r} b_i c_i^2 = \frac{1}{3}; & 4)\ \sum\limits_{i=1}^{r}\sum\limits_{j=1}^{r} b_i \bar{a}_{ij} = \frac{1}{6}; \\
5)\ \sum\limits_{i=1}^{r} b_i c_i^3 = \frac{1}{4}; & 6)\ \sum\limits_{i=1}^{r}\sum\limits_{j=1}^{r} b_i c_i \bar{a}_{ij} = \frac{1}{8}; \\
7)\ \sum\limits_{i=1}^{r}\sum\limits_{j=1}^{r} b_i \bar{a}_{ij} c_j = \frac{1}{24}; & 8)\ \sum\limits_{i=1}^{r} b_i c_i^4 = \frac{1}{5}; \\
9)\ \sum\limits_{i=1}^{r}\sum\limits_{j=1}^{r} b_i c_i^2 \bar{a}_{ij} = \frac{1}{10}; & 10)\ \sum\limits_{i=1}^{r}\sum\limits_{j=1}^{r}\sum\limits_{k=1}^{r} b_i \bar{a}_{ij} \bar{a}_{ik} = \frac{1}{20}; \\
11)\ \sum\limits_{i=1}^{r}\sum\limits_{j=1}^{r} b_i c_i \bar{a}_{ij} c_j = \frac{1}{30}; & 12)\ \sum\limits_{i=1}^{r}\sum\limits_{j=1}^{r} b_i \bar{a}_{ij} c_j^2 = \frac{1}{60}; \\
13)\ \sum\limits_{i=1}^{r}\sum\limits_{j=1}^{r}\sum\limits_{k=1}^{r} b_i \bar{a}_{ij} \bar{a}_{jk} = \frac{1}{120}; & 14)\ \cdots
\end{array}\right|$$

If the condition 1) holds, then the RKN method is of order 1; if conditions 1)-2) hold, then the RKN method is of order 2; if conditions 1)-4) hold, then the RKN method is of order 3; if conditions 1)-7) hold, then the RKN method is of order 4; if conditions 1)-13) hold, then the RKN method is of order 5.

Similarly as the classical case, under the assumption $\bar{B}_\tau = \hat{B}_\tau(1 - C_\tau)$, we have the following order conditions for csRKN method

$$\left|\begin{array}{l|l}
1)\ \int_0^1 \hat{B}_\tau d\tau = 1; & 2)\ \int_0^1 \hat{B}_\tau C_\tau d\tau = \frac{1}{2}; \\
3)\ \int_0^1 \hat{B}_\tau C_\tau^2 d\tau = \frac{1}{3}; & 4)\ \int_0^1\int_0^1 \hat{B}_\tau \bar{A}_{\tau,\sigma} d\sigma d\tau = \frac{1}{6}; \\
5)\ \int_0^1 \hat{B}_\tau C_\tau^3 d\tau = \frac{1}{4}; & 6)\ \int_0^1\int_0^1 \hat{B}_\tau C_\tau \bar{A}_{\tau,\sigma} d\sigma d\tau = \frac{1}{8}; \\
7)\ \int_0^1\int_0^1 \hat{B}_\tau \bar{A}_{\tau,\sigma} C_\sigma d\sigma d\tau = \frac{1}{24}; & 8)\ \int_0^1 \hat{B}_\tau C_\tau^4 d\tau = \frac{1}{5}; \\
9)\ \int_0^1\int_0^1 \hat{B}_\tau C_\tau^2 \bar{A}_{\tau,\sigma} d\sigma d\tau = \frac{1}{10}; & 10)\ \int_0^1\int_0^1\int_0^1 \hat{B}_\tau \bar{A}_{\tau,\sigma} \bar{A}_{\tau,\rho} d\rho d\sigma d\tau = \frac{1}{20}; \\
11)\ \int_0^1\int_0^1 \hat{B}_\tau C_\tau \bar{A}_{\tau,\sigma} C_\sigma d\sigma d\tau = \frac{1}{30}; & 12)\ \int_0^1\int_0^1 \hat{B}_\tau \bar{A}_{\tau,\sigma} C_\sigma^2 d\sigma d\tau = \frac{1}{60}; \\
13)\ \int_0^1\int_0^1\int_0^1 \hat{B}_\tau \bar{A}_{\tau,\sigma} \bar{A}_{\sigma,\rho} d\rho d\sigma d\tau = \frac{1}{120}; & 14)\ \cdots
\end{array}\right|$$

Note that $\bar{B}_\tau = \hat{B}_\tau(1 - C_\tau)$ is naturally satisfied by the hypothesis $\hat{B}_\tau = 1,\ C_\tau = \tau$. Moreover, if the condition 1) holds, then the csRKN method is of order 1; if conditions 1)-2) hold, then the csRKN method is of order 2; if conditions 1)-4) hold, then the csRKN method is of order 3; if conditions 1)-7) hold, then the csRKN method is of order 4; if conditions 1)-13) hold, then the csRKN method is of order 5.

It is obvious that the conditions 1)-2) always hold, so the csRKN methods presented in this paper are of order 2 at least. Moreover, it is found that conditions 2), 3), 5), 8) are also naturally satisfied, so other conditions will be further investigated when we try to construct higher order csRKN methods.

4.2. Construction of symplectic RKN methods

Though it is possible to construct RKN type methods with arbitrarily high order for some special purposes, here we will restrict ourselves on the construction of symplectic integrators. By using expansion of Legendre orthogonal polynomials, we have the following identities

$$\begin{aligned}
&1 = P_0(\tau),\\
&\tau = \frac{1}{2}P_0(\tau) + \frac{\sqrt{3}}{6}P_1(\tau),\\
&\tau^2 = \frac{1}{3}P_0(\tau) + \frac{\sqrt{3}}{6}P_1(\tau) + \frac{\sqrt{5}}{30}P_2(\tau),\\
&\tau^3 = \frac{1}{4}P_0(\tau) + \frac{3\sqrt{3}}{20}P_1(\tau) + \frac{\sqrt{5}}{20}P_2(\tau) + \frac{\sqrt{7}}{140}P_3(\tau),\\
&\cdots
\end{aligned} \tag{4.6}$$

which turn out to be very helpful for the investigation of the order conditions. For convenience, here we provide the former several Legendre polynomials

$$\begin{aligned}
&P_0(\tau) = 1,\\
&P_1(\tau) = \sqrt{3}(2\tau - 1),\\
&P_2(\tau) = \sqrt{5}(6\tau^2 - 6\tau + 1),\\
&P_3(\tau) = \sqrt{7}(20\tau^3 - 30\tau^2 + 12\tau - 1),\\
&\cdots
\end{aligned} \tag{4.7}$$

In what follows, we present the construction of symplectic integrators up to order 5 and some examples will be given.

4.2.1. 2-order symplectic integrators

Although the csRKN methods presented in this paper are always of order 2 at least, but for a symplectic csRKN method, the coefficient $\bar{A}_{\tau,\sigma}$ should be designed by Theorem 3.2, an example is given in what follows.

Example 4.1. *If we take the coefficients* $(\bar{A}_{\tau,\sigma}, \bar{B}_\tau, \hat{B}_\tau, C_\tau)$ *as*

$$\begin{aligned}
&\bar{A}_{\tau,\sigma} = \alpha + (\beta - \frac{\sqrt{3}}{6})P_1(\sigma) + \beta P_1(\tau),\\
&\bar{B}_\tau = 1 - \tau,\ \hat{B}_\tau = 1,\ C_\tau = \tau,
\end{aligned} \tag{4.8}$$ {eq:2coeff}

where α *and* β *are two real parameters, then we get a two-parameter family of* 2*-order symplectic csRKN methods.*

By using any numerical quadrature formula with order $p \geq 2$ *we can get the classical symplectic RKN methods of order*[2] 2*, e.g., Gaussian quadrature with*

[2]This can be easily checked by the classical order conditions that listed in subsection 4.1.

$$\begin{array}{c|c} \frac{1}{2} & \alpha \\ \hline & \frac{1}{2} \\ \hline & 1 \end{array} \qquad \begin{array}{c|cc} 0 & \frac{1}{4}\alpha - \frac{\sqrt{3}}{2}\beta + \frac{1}{8} & \frac{3}{4}\alpha - \frac{\sqrt{3}}{2}\beta - \frac{1}{8} \\ \frac{2}{3} & \frac{1}{4}\alpha - \frac{\sqrt{3}}{6}\beta + \frac{1}{8} & \frac{3}{4}\alpha + \frac{\sqrt{3}}{2}\beta - \frac{1}{8} \\ \hline & \frac{1}{4} & \frac{1}{4} \\ \hline & \frac{1}{4} & \frac{3}{4} \end{array}$$

$$\begin{array}{c|cc} \frac{1}{3} & \frac{3}{4}\alpha - \frac{\sqrt{3}}{2}\beta + \frac{1}{8} & \frac{1}{4}\alpha + \frac{\sqrt{3}}{6}\beta - \frac{1}{8} \\ 1 & \frac{3}{4}\alpha + \frac{\sqrt{3}}{2}\beta + \frac{1}{8} & \frac{1}{4}\alpha + \frac{\sqrt{3}}{2}\beta - \frac{1}{8} \\ \hline & \frac{1}{2} & 0 \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array} \qquad \begin{array}{c|cc} 0 & \frac{1}{2}\alpha - \sqrt{3}\beta + \frac{1}{4} & \frac{1}{2}\alpha - \frac{1}{4} \\ 1 & \frac{1}{2}\alpha + \frac{1}{4} & \frac{1}{2}\alpha + \sqrt{3}\beta - \frac{1}{4} \\ \hline & \frac{1}{2} & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Table 1: Symplectic RKN methods of order 2 by using different quadrature formulae. Top Left: by Gaussian quadrature, Top Right: by Radau-left quadrature, Bottom Left: by Radau-right quadrature, Bottom Right: by Lobatto quadrature. {exa:SRKN2}

1 node, Radau-left or Radau-right quadrature with 2 nodes, Lobatto quadrature with 2 nodes. The corresponding symplectic RKN methods obtained by using different quadrature formulae are shown in Table 1.

4.2.2. 3-order symplectic integrators

By inserting (3.10) into the fourth order condition and using the orthogonality of the Legendre polynomials, it gives

$$\int_0^1 \int_0^1 \hat{B}_\tau \bar{A}_{\tau,\sigma} d\sigma d\tau = \int_0^1 (\alpha_{(0,0)} + \alpha_{(1,0)} P_1(\tau) + \sum_{i>1} \alpha_{(i,0)} P_i(\tau)) d\tau = \alpha_{(0,0)} = \frac{1}{6}, \tag{4.9}$$

therefore, if we require $\alpha_{(0,0)} = \frac{1}{6}$, then we can get a class of 3-order symplectic csRKN methods.

Example 4.2. *If we take the coefficients $(\bar{A}_{\tau,\sigma}, \bar{B}_\tau, \hat{B}_\tau, C_\tau)$ as*

$$\begin{aligned} &\bar{A}_{\tau,\sigma} = \frac{1}{6} + (\alpha - \frac{\sqrt{3}}{6}) P_1(\sigma) + \alpha P_1(\tau) + \beta P_1(\tau) P_1(\sigma), \\ &\bar{B}_\tau = 1 - \tau,\ \hat{B}_\tau = 1,\ C_\tau = \tau, \end{aligned} \tag{4.10}$$ {eq:3coeff}

then we get a two-parameter family of 3-order symplectic csRKN methods.

By using any numerical quadrature formula with order $p \geq 3$ we can get the classical symplectic RKN methods of order 3, e.g., Gaussian quadrature with 2 nodes, Radau-left or Radau-right quadrature with 2 nodes, Lobatto quadrature with 3 nodes. The corresponding symplectic RKN methods obtained by using different quadrature formulae are shown in Table 2.

$$
\begin{array}{c|cc}
\frac{3-\sqrt{3}}{6} & \frac{1+\sqrt{3}}{12}-\alpha+\frac{1}{2}\beta & \frac{1-\sqrt{3}}{12}-\frac{1}{2}\beta \\
\frac{3+\sqrt{3}}{6} & \frac{1+\sqrt{3}}{12}-\frac{1}{2}\beta & \frac{1-\sqrt{3}}{12}+\alpha+\frac{1}{2}\beta \\
\hline
 & \frac{1}{4}+\frac{\sqrt{3}}{12} & \frac{1}{4}-\frac{\sqrt{3}}{12} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
\qquad
\begin{array}{c|cc}
0 & \frac{2-6\sqrt{3}\alpha+9\beta}{12} & -\frac{\sqrt{3}}{2}\alpha-\frac{3}{4}\beta \\
\frac{2}{3} & \frac{2-2\sqrt{3}\alpha-3\beta}{12} & \frac{\sqrt{3}}{2}\alpha+\frac{1}{4}\beta \\
\hline
 & \frac{1}{4} & \frac{1}{4} \\
\hline
 & \frac{1}{4} & \frac{3}{4}
\end{array}
$$

$$
\begin{array}{c|cc}
\frac{1}{3} & \frac{1-2\sqrt{3}\alpha+\beta}{4} & \frac{-1+2\sqrt{3}\alpha-3\beta}{12} \\
1 & \frac{1+2\sqrt{3}\alpha-3\beta}{4} & \frac{-1+6\sqrt{3}\alpha+9\beta}{12} \\
\hline
 & \frac{1}{2} & 0 \\
\hline
 & \frac{3}{4} & \frac{1}{4}
\end{array}
\qquad
\begin{array}{c|ccc}
0 & \frac{6-18\sqrt{3}\alpha+27\beta}{54} & \frac{1-6\sqrt{3}\alpha}{9} & -\frac{1}{18}-\frac{1}{2}\beta \\
\frac{1}{2} & \frac{1}{9}-\frac{\sqrt{3}}{6}\alpha & \frac{1}{9} & -\frac{1}{18}+\frac{\sqrt{3}}{6}\alpha \\
1 & \frac{1}{9}-\frac{1}{2}\beta & \frac{1+6\sqrt{3}\alpha}{9} & \frac{-1+6\sqrt{3}\alpha+9\beta}{18} \\
\hline
 & \frac{1}{6} & \frac{1}{3} & 0 \\
\hline
 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{array}
$$

Table 2: Symplectic RKN methods of order 3 by using different quadrature formulae. Top Left: by Gaussian quadrature, Top Right: by Radau-left quadrature, Bottom Left: by Radau-right quadrature, Bottom Right: by Lobatto quadrature. {exa:SRKN3}

4.2.3. 4-order symplectic integrators

By inserting (3.10) with $\alpha_{(0,0)} = \frac{1}{6}$ into the sixth order condition and using the orthogonality of the Legendre polynomials, it gives

$$
\begin{aligned}
&\int_0^1 \int_0^1 \hat{B}_\tau C_\tau \bar{A}_{\tau,\sigma} d\sigma d\tau \\
&= \int_0^1 \int_0^1 \tau \bar{A}_{\tau,\sigma} d\sigma d\tau \\
&= \int_0^1 (\frac{1}{2}P_0(\tau) + \frac{\sqrt{3}}{6}P_1(\tau))(\int_0^1 \bar{A}_{\tau,\sigma} d\sigma) d\tau \\
&= \int_0^1 (\frac{1}{2}P_0(\tau) + \frac{\sqrt{3}}{6}P_1(\tau))(\frac{1}{6} + \alpha_{(1,0)}P_1(\tau) + \sum_{i>1} \alpha_{(i,0)}P_i(\tau)) d\tau \\
&= \alpha_{(1,0)}\frac{\sqrt{3}}{6} + \frac{1}{12} = \frac{1}{8},
\end{aligned}
\tag{4.11}
$$

which provides $\alpha_{(1,0)} = \frac{\sqrt{3}}{12}$.

Similarly, by exploiting the seventh order condition we obtain $\alpha_{(0,1)} = -\frac{\sqrt{3}}{12}$, which coincides with the symplectic condition $\alpha_{(0,1)} - \alpha_{(1,0)} = -\frac{\sqrt{3}}{6}$ that given in Theorem 3.2. Therefore, if we require

$$
\alpha_{(0,0)} = \frac{1}{6},\ \alpha_{(1,0)} = \frac{\sqrt{3}}{12},\ \alpha_{(0,1)} = -\frac{\sqrt{3}}{12},
$$

then we can get a class of 4-order symplectic csRKN methods.

$$
\begin{array}{c|cc}
\frac{3-\sqrt{3}}{6} & \frac{1}{12}+\frac{1}{2}\alpha & \frac{1-\sqrt{3}}{12}-\frac{1}{2}\alpha \\
\frac{3+\sqrt{3}}{6} & \frac{1+\sqrt{3}}{12}-\frac{1}{2}\alpha & \frac{1}{12}+\frac{1}{2}\alpha \\
\hline
 & \frac{1}{4}+\frac{\sqrt{3}}{12} & \frac{1}{4}-\frac{\sqrt{3}}{12} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
$$

$$
\begin{array}{c|ccc}
0 & \frac{1+18\alpha}{54} & \frac{-11+4\sqrt{6}+(-36+54\sqrt{6})\alpha}{216} & \frac{-11-4\sqrt{6}+(-36-54\sqrt{6})\alpha}{216} \\
\frac{6-\sqrt{6}}{10} & \frac{28-3\sqrt{6}}{540}+\frac{(-15+15\sqrt{6})\alpha}{225} & \frac{16+\sqrt{6}}{216}+\frac{(12-3\sqrt{6})\alpha}{36} & \frac{98-53\sqrt{6}}{1080}+\frac{(-240+15\sqrt{6})\alpha}{900} \\
\frac{6+\sqrt{6}}{10} & \frac{28+3\sqrt{6}}{540}+\frac{(-15-15\sqrt{6})\alpha}{225} & \frac{98+53\sqrt{6}}{1080}-\frac{(240+15\sqrt{6})\alpha}{900} & \frac{16-\sqrt{6}}{216}+\frac{(12+3\sqrt{6})\alpha}{36} \\
\hline
 & \frac{1}{9} & \frac{7+2\sqrt{6}}{36} & \frac{7-2\sqrt{6}}{36} \\
\hline
 & \frac{1}{9} & \frac{16+\sqrt{6}}{36} & \frac{16-\sqrt{6}}{36}
\end{array}
$$

$$
\begin{array}{c|ccc}
\frac{4-\sqrt{6}}{10} & \frac{16-\sqrt{6}}{216}+\frac{(12+3\sqrt{6})\alpha}{36} & \frac{62-43\sqrt{6}}{1080}-\frac{(240+15\sqrt{6})\alpha}{900} & -\frac{8+3\sqrt{6}}{540}+\frac{-(15+15\sqrt{6})\alpha}{225} \\
\frac{4+\sqrt{6}}{10} & \frac{62+43\sqrt{6}}{1080}-\frac{(240-15\sqrt{6})\alpha}{900} & \frac{16+\sqrt{6}}{216}+\frac{(12-3\sqrt{6})\alpha}{36} & -\frac{8-3\sqrt{6}}{540}+\frac{-(15-15\sqrt{6})\alpha}{225} \\
1 & \frac{43+2\sqrt{6}}{216}+\frac{-(6+9\sqrt{6})\alpha}{36} & \frac{43-2\sqrt{6}}{216}+\frac{-(6-9\sqrt{6})\alpha}{36} & \frac{1+18\alpha}{54} \\
\hline
 & \frac{9+\sqrt{6}}{36} & \frac{9-\sqrt{6}}{36} & 0 \\
\hline
 & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9}
\end{array}
$$

$$
\begin{array}{c|ccc}
0 & \frac{1+18\alpha+12\sqrt{5}\beta}{36} & \frac{-1+6\sqrt{5}\beta}{18} & \frac{-2-18\alpha+12\sqrt{5}\beta}{36} \\
\frac{1}{2} & \frac{5+6\sqrt{5}\beta}{72} & \frac{1-6\sqrt{5}\beta}{9} & \frac{-1+6\sqrt{5}\beta}{72} \\
1 & \frac{2-9\alpha+6\sqrt{5}\beta}{18} & \frac{5+6\sqrt{5}\beta}{18} & \frac{1+18\alpha+12\sqrt{5}\beta}{36} \\
\hline
 & \frac{1}{6} & \frac{1}{3} & 0 \\
\hline
 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{array}
$$

Table 3: Symplectic RKN methods of order 4 by using different quadrature formulae. First: by Gaussian quadrature, Second: by Radau-left quadrature ($\beta = 0$), Third: by Radau-right quadrature ($\beta = 0$), Fourth: by Lobatto quadrature. {exa:SRKN4}

Example 4.3. *If we take the coefficients $(\bar{A}_{\tau,\sigma},\, \bar{B}_\tau,\, \hat{B}_\tau,\, C_\tau)$ as*

$$\begin{aligned} &\bar{A}_{\tau,\sigma} = \frac{1}{6} + \frac{\tau-\sigma}{2} + \alpha P_1(\tau)P_1(\sigma) + \beta(P_2(\tau)+P_2(\sigma)), \\ &\bar{B}_\tau = 1-\tau,\ \hat{B}_\tau = 1,\ C_\tau = \tau, \end{aligned} \tag{4.12}$$ {eq:4coeff}

then we get a two-parameter family of 4*-order symplectic csRKN methods.*

By using any numerical quadrature formula with order $p \geq 4$ we can get the classical symplectic RKN methods of order 4*, e.g., Gaussian quadrature with* 2 *nodes, Radau-left or Radau-right quadrature with* 3 *nodes, Lobatto quadrature with* 3 *nodes. The corresponding symplectic RKN methods obtained by using different quadrature formulae are shown in Table 3. Note that, actually, more free parameters can be taken into account.*

4.2.4. 5*-order symplectic integrators*

By the previous discussions we have obtained that $\alpha_{(0,0)} = \frac{1}{6}$, $\alpha_{(1,0)} = \frac{\sqrt{3}}{12}$, $\alpha_{(0,1)} = -\frac{\sqrt{3}}{12}$, now we shall insert (3.10) into the remaining order conditions.

For condition 9): We compute

$$\begin{aligned} &\int_0^1\int_0^1 \hat{B}_\tau C_\tau^2 \bar{A}_{\tau,\sigma} d\sigma d\tau \\ &= \int_0^1\int_0^1 \tau^2 \bar{A}_{\tau,\sigma} d\sigma d\tau \\ &= \int_0^1 (\frac{1}{3}P_0(\tau) + \frac{\sqrt{3}}{6}P_1(\tau) + \frac{\sqrt{5}}{30}P_2(\tau))(\int_0^1 \bar{A}_{\tau,\sigma} d\sigma) d\tau \\ &= \int_0^1 (\frac{1}{3}P_0(\tau) + \frac{\sqrt{3}}{6}P_1(\tau) + \frac{\sqrt{5}}{30}P_2(\tau))(\alpha_{(0,0)} + \alpha_{(1,0)}P_1(\tau) + \sum_{i>1}\alpha_{(i,0)}P_i(\tau)) d\tau \\ &= \frac{1}{3}\alpha_{(0,0)} + \frac{\sqrt{3}}{6}\alpha_{(1,0)} + \frac{\sqrt{5}}{30}\alpha_{(2,0)} = \frac{1}{10}, \end{aligned}$$

which then gives $\alpha_{(2,0)} = \frac{\sqrt{5}}{60}$.

For condition 10): Since

$$\begin{aligned} &\int_0^1\int_0^1\int_0^1 \hat{B}_\tau \bar{A}_{\tau,\sigma}\bar{A}_{\tau,\rho} d\rho d\sigma d\tau \\ &= \int_0^1 (\int_0^1 \bar{A}_{\tau,\sigma} d\sigma)(\int_0^1 \bar{A}_{\tau,\rho} d\rho) d\tau \\ &= \int_0^1 (\alpha_{(0,0)} + \alpha_{(1,0)}P_1(\tau) + \sum_{i>1}\alpha_{(i,0)}P_i(\tau))^2 d\tau \\ &= \alpha_{(0,0)}^2 + \alpha_{(1,0)}^2 + \sum_{i>1}\alpha_{(i,0)}^2 = \frac{1}{20}, \end{aligned}$$

substituting the values of $\alpha_{(0,0)}$, $\alpha_{(1,0)}$, $\alpha_{(2,0)}$ into it, then we get $\sum\limits_{i>2} \alpha^2_{(i,0)} = 0$ which means $\alpha_{(i,0)} = 0$ for all $i > 2$.

For condition 11): Since

$$\begin{aligned}
&\int_0^1 \int_0^1 \hat{B}_\tau C_\tau \bar{A}_{\tau,\sigma} C_\sigma d\sigma d\tau \\
&= \int_0^1 \tau\big(\int_0^1 \bar{A}_{\tau,\sigma}\sigma d\sigma\big) d\tau \\
&= \int_0^1 (\frac{1}{2}P_0(\tau) + \frac{\sqrt{3}}{6}P_1(\tau))\big[\int_0^1 \Big(\alpha_{(0,0)} + \alpha_{(0,1)}P_1(\sigma) + \alpha_{(1,0)}P_1(\tau) \\
&\quad + \sum_{i+j>1} \alpha_{(i,j)}P_i(\tau)P_j(\sigma)\Big)\big(\frac{1}{2}P_0(\sigma) + \frac{\sqrt{3}}{6}P_1(\sigma)\big)d\sigma\big] d\tau \\
&= \int_0^1 (\frac{1}{2}P_0(\tau) + \frac{\sqrt{3}}{6}P_1(\tau))\big(\frac{1}{2}\alpha_{(0,0)} + \frac{1}{2}\alpha_{(1,0)}P_1(\tau) + \frac{1}{2}\sum_{i>1}\alpha_{(i,0)}P_i(\tau) \\
&\quad + \frac{\sqrt{3}}{6}\alpha_{(0,1)} + \frac{\sqrt{3}}{6}\sum_{i>0}\alpha_{(i,1)}P_i(\tau)\big)d\tau \\
&= \frac{1}{4}\alpha_{(0,0)} + \frac{\sqrt{3}}{12}\alpha_{(0,1)} + \frac{\sqrt{3}}{12}\alpha_{(1,0)} + \frac{1}{12}\alpha_{(1,1)} = \frac{1}{30},
\end{aligned}$$

this gives $\alpha_{(1,1)} = -\frac{1}{10}$.

For condition 12): By the very similar deduction as that for (9) we get

$$\frac{1}{3}\alpha_{(0,0)} + \frac{\sqrt{3}}{6}\alpha_{(0,1)} + \frac{\sqrt{5}}{30}\alpha_{(0,2)} = \frac{1}{60}, \tag{4.13}$$

which provides $\alpha_{(0,2)} = \frac{\sqrt{5}}{60}$.

For condition 13): We have

$$\begin{aligned}
&\int_0^1 \int_0^1 \int_0^1 \hat{B}_\tau \bar{A}_{\tau,\sigma} \bar{A}_{\sigma,\rho} d\rho d\sigma d\tau \\
&= \int_0^1 (\int_0^1 \bar{A}_{\tau,\sigma} d\tau)(\int_0^1 \bar{A}_{\sigma,\rho} d\rho) d\sigma \\
&= \int_0^1 \Big(\alpha_{(0,0)} + \alpha_{(0,1)}P_1(\sigma) + \sum_{j>1}\alpha_{(0,j)}P_j(\sigma)\Big)\Big(\alpha_{(0,0)} + \alpha_{(1,0)}P_1(\sigma) \\
&\quad + \sum_{i>1}\alpha_{(i,0)}P_i(\sigma)\Big) d\sigma \\
&= \alpha^2_{(0,0)} + \alpha_{(0,1)}\alpha_{(1,0)} + \sum_{j>1}\alpha_{(0,j)}\alpha_{(j,0)} = \frac{1}{120},
\end{aligned}$$

After substituting the values of $\alpha_{(0,0)}$, $\alpha_{(0,1)}$, $\alpha_{(1,0)}$, $\alpha_{(2,0)}$ into it, it brings out that $\sum\limits_{j>2} \alpha_{(0,j)}\alpha_{(j,0)} = 0$. In addition, by Theorem 3.2 we have $\alpha_{(0,j)} = \alpha_{(j,0)}$ for

$\frac{5-\sqrt{15}}{10}$	$\frac{2-90\alpha+60\beta}{135}$	$\frac{19-6\sqrt{15}+180\alpha-120\beta}{270}$	$\frac{62-15\sqrt{15}+120\beta}{540}$
$\frac{1}{2}$	$\frac{19+6\sqrt{15}+180\alpha-120\beta}{432}$	$\frac{1+15\beta}{27}$	$\frac{19-6\sqrt{15}-180\alpha-120\beta}{432}$
$\frac{5+\sqrt{15}}{10}$	$\frac{62+15\sqrt{15}+120\beta}{540}$	$\frac{19+6\sqrt{15}-180\alpha-120\beta}{270}$	$\frac{2+90\alpha+60\beta}{135}$
	$\frac{5+\sqrt{15}}{36}$	$\frac{2}{9}$	$\frac{5-\sqrt{15}}{36}$
	$\frac{5}{18}$	$\frac{4}{9}$	$\frac{5}{18}$

0	$\frac{1-60\sqrt{15}\alpha}{270}$	$\frac{-4-19\sqrt{6}+(240\sqrt{15}-180\sqrt{10})\alpha}{2160}$	$\frac{-4+19\sqrt{6}+(240\sqrt{15}+180\sqrt{10})\alpha}{2160}$
$\frac{6-\sqrt{6}}{10}$	$\frac{181-36\sqrt{6}+(84\sqrt{15}-72\sqrt{10})\alpha}{2700}$	$\frac{17+2\sqrt{6}+60\sqrt{15}\alpha}{540}$	$\frac{301-136\sqrt{6}-(384\sqrt{15}-72\sqrt{10})\alpha}{2700}$
$\frac{6+\sqrt{6}}{10}$	$\frac{181+36\sqrt{6}+(84\sqrt{15}+72\sqrt{10})\alpha}{2700}$	$\frac{301+136\sqrt{6}-(384\sqrt{15}+72\sqrt{10})\alpha}{2700}$	$\frac{17-2\sqrt{6}+60\sqrt{15}\alpha}{540}$
	$\frac{1}{9}$	$\frac{7+2\sqrt{6}}{36}$	$\frac{7-2\sqrt{6}}{36}$
	$\frac{1}{9}$	$\frac{16+\sqrt{6}}{36}$	$\frac{16-\sqrt{6}}{36}$

$\frac{4-\sqrt{6}}{10}$	$\frac{17-2\sqrt{6}-60\sqrt{15}\alpha}{540}$	$\frac{211-104\sqrt{6}+(384\sqrt{15}+72\sqrt{10})\alpha}{2700}$	$\frac{1+6\sqrt{6}-(84\sqrt{15}+72\sqrt{10})\alpha}{2700}$
$\frac{4+\sqrt{6}}{10}$	$\frac{211+104\sqrt{6}+(384\sqrt{15}-72\sqrt{10})\alpha}{2700}$	$\frac{17+2\sqrt{6}-60\sqrt{15}\alpha}{540}$	$\frac{1-6\sqrt{6}-(84\sqrt{15}-72\sqrt{10})\alpha}{2700}$
1	$\frac{536+79\sqrt{6}-(240\sqrt{15}+180\sqrt{10})\alpha}{2160}$	$\frac{536-79\sqrt{6}-(240\sqrt{15}-180\sqrt{10})\alpha}{2160}$	$\frac{1+60\sqrt{15}\alpha}{270}$
	$\frac{9+\sqrt{6}}{36}$	$\frac{9-\sqrt{6}}{36}$	0
	$\frac{16-\sqrt{6}}{36}$	$\frac{16+\sqrt{6}}{36}$	$\frac{1}{9}$

Table 4: Symplectic RKN methods of order 5 by using different quadrature formulae. First: by Gaussian quadrature, Second: by Radau-left quadrature ($\beta = 0$), Third: by Radau-right quadrature ($\beta = 0$). {exa:SRKN5}

$j > 2$, then it follows that

$$\alpha_{(0,j)} = \alpha_{(j,0)} = 0, \quad j > 2.$$

In summary, for obtaining a symplectic csRKN method of order 5, we should require that

$$\begin{aligned} &\alpha_{(0,0)} = \frac{1}{6},\, \alpha_{(1,0)} = \frac{\sqrt{3}}{12},\, \alpha_{(0,1)} = -\frac{\sqrt{3}}{12}, \\ &\alpha_{(1,1)} = -\frac{1}{10},\, \alpha_{(2,0)} = \alpha_{(0,2)} = \frac{\sqrt{5}}{60}, \\ &\alpha_{(0,j)} = \alpha_{(j,0)} = 0, \quad j > 2, \end{aligned} \tag{4.14}$$ {coef: fifth}

and other parameters $\alpha_{(i,j)}$ can be freely assigned.

Example 4.4. *If we take the coefficients* $(\bar{A}_{\tau,\sigma},\, \bar{B}_\tau,\, \hat{B}_\tau,\, C_\tau)$ *as*

$$\begin{aligned} \bar{A}_{\tau,\sigma} = \sum_{i+j\leq 2} \alpha_{(i,j)} P_i(\tau)P_j(\sigma) + \alpha\Big(P_1(\tau)P_2(\sigma) + P_2(\tau)P_1(\sigma)\Big) + \beta P_2(\tau)P_2(\sigma), \\ \bar{B}_\tau = 1-\tau,\ \hat{B}_\tau = 1,\ C_\tau = \tau, \end{aligned} \tag{4.15}$$ {eq:5coeff}

where $\alpha_{(i,j)}$, $i+j \leq 2$ satisfy (4.14) and α, β are real parameters, then we get a two-parameter family of 5-order symplectic csRKN methods.

By using any numerical quadrature formula with order $p \geq 5$ we can get the classical symplectic RKN methods of order 5, e.g., Gaussian quadrature with 3 nodes, Radau-left or Radau-right quadrature with 3 nodes, Lobatto quadrature with 4 nodes. The corresponding symplectic RKN methods obtained by using different quadrature formulae are shown in Table 4.

Notice that based on 4-nodes Lobatto qudrature, the 4-stage 5-order symplectic RKN method with coefficients denoted by $(\bar{A}, \bar{b}, b, c)$ is too lengthy to be shown in a Butcher tableau, we present it as follows in use of Matlab notations

$$
\begin{aligned}
\bar{A} =& [\frac{1-60\sqrt{15}\alpha+150\beta}{360}, \frac{-5-3\sqrt{5}-(300\sqrt{3}-60\sqrt{15})\alpha-300\beta}{720},\\
& \frac{-5+3\sqrt{5}+(300\sqrt{3}+60\sqrt{15})\alpha-300\beta}{720}, \frac{2+75\beta}{180};\\
& \frac{29}{720}-\frac{11\sqrt{5}+(100\sqrt{3}-20\sqrt{15})\alpha+100\beta}{1200}, \frac{11+60\sqrt{3}\alpha+30\beta}{360},\\
& \frac{29-15\sqrt{5}+30\beta}{360}, -\frac{1}{720}+\frac{\sqrt{5}-(20\sqrt{15}+100\sqrt{3})\alpha-100\beta}{1200};\\
& \frac{29}{720}+\frac{11\sqrt{5}+(100\sqrt{3}+20\sqrt{15})\alpha-100\beta}{1200}, \frac{29+15\sqrt{5}+30\beta}{360},\\
& \frac{11-60\sqrt{3}\alpha+30\beta}{360}, -\frac{1}{720}-\frac{\sqrt{5}+(20\sqrt{15}-100\sqrt{3})\alpha+100\beta}{1200};\\
& \frac{17+75\beta}{180}, \frac{145+33\sqrt{5}-(60\sqrt{15}+300\sqrt{3})\alpha-300\beta}{720},\\
& \frac{145-33\sqrt{5}-(60\sqrt{15}-300\sqrt{3})\alpha-300\beta}{720}, \frac{1+60\sqrt{15}\alpha+150\beta}{360}],\\
\bar{b} =& [\frac{1}{12}, \frac{5+\sqrt{5}}{24}, \frac{5-\sqrt{5}}{24}, 0],\ b=[\frac{1}{12}, \frac{5}{12}, \frac{5}{12}, \frac{1}{12}],\ c=[0, \frac{5-\sqrt{5}}{10}, \frac{5+\sqrt{5}}{10}, 1].
\end{aligned}
$$

5. Diagonally implicit symplectic RKN methods

It is known that diagonally implicit methods are more attractive than fully implicit methods for the sake of time cost savings and high efficiency in the numerical computations. A diagonally implicit RKN method is a method (4.4a-4.4c) with coefficient $(\bar{a}_{ij}, \bar{b}_i, b_i, c_i)$ satisfying

$$\bar{a}_{ij} = 0,\ j > i. \tag{5.1}$$ {diag imp:condi}

By setting more parameters and solving a linear algebraic system, it is possible to get diagonally implicit symplectic integrators.

For example, let us take

$$
\begin{aligned}
&\bar{A}_{\tau,\sigma} = \alpha + (\beta - \frac{\sqrt{3}}{6})P_1(\sigma) + \beta P_1(\tau) + \gamma P_1(\tau)P_1(\sigma),\\
&\bar{B}_\tau = 1-\tau,\ \hat{B}_\tau = 1,\ C_\tau = \tau,
\end{aligned}
\tag{5.2}
$$ {diag imp:2coeff}

where three real parameters α, β, γ are included. In such a case, by using Radau-left, Radau-right and Lobatto quadrature with 2 nodes, respectively, it gives

$$\begin{array}{c|cc} 0 & \frac{1}{8}+\frac{1}{4}\alpha-\frac{\sqrt{3}}{2}\beta+\frac{3}{4}\gamma & -\frac{1}{8}+\frac{3}{4}\alpha-\frac{\sqrt{3}}{2}\beta-\frac{3}{4}\gamma \\ \frac{2}{3} & \frac{1}{8}+\frac{1}{4}\alpha-\frac{\sqrt{3}}{6}\beta-\frac{1}{4}\gamma & -\frac{1}{8}+\frac{3}{4}\alpha+\frac{\sqrt{3}}{2}\beta+\frac{1}{4}\gamma \\ \hline & \frac{1}{4} & \frac{1}{4} \\ \hline & \frac{1}{4} & \frac{3}{4} \end{array} \tag{5.3}$$ {fully:RL}

$$\begin{array}{c|cc} \frac{1}{3} & \frac{1}{8}+\frac{3}{4}\alpha-\frac{\sqrt{3}}{2}\beta+\frac{1}{4}\gamma & -\frac{1}{8}+\frac{1}{4}\alpha+\frac{\sqrt{3}}{6}\beta-\frac{1}{4}\gamma \\ 1 & \frac{1}{8}+\frac{3}{4}\alpha+\frac{\sqrt{3}}{2}\beta-\frac{3}{4}\gamma & -\frac{1}{8}+\frac{1}{4}\alpha+\frac{\sqrt{3}}{2}\beta+\frac{3}{4}\gamma \\ \hline & \frac{1}{2} & 0 \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array} \tag{5.4}$$ {fully:RR}

$$\begin{array}{c|cc} 0 & \frac{1}{4}+\frac{\alpha}{2}-\sqrt{3}\beta+\frac{3\gamma}{2} & -\frac{1}{4}+\frac{\alpha}{2}-\frac{3\gamma}{2} \\ 1 & \frac{1}{4}+\frac{\alpha}{2}-\frac{3\gamma}{2} & -\frac{1}{4}+\frac{\alpha}{2}+\sqrt{3}\beta+\frac{3\gamma}{2} \\ \hline & \frac{1}{2} & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \tag{5.5}$$ {fully:LO}

and all of which are of order 2. If we impose the diagonally implicit requirements (5.1), then by eliminating γ we then get the following two-parameter families of diagonally implicit symplectic integrators

$$\begin{array}{c|cc} 0 & \alpha-\sqrt{3}\beta & 0 \\ \frac{2}{3} & \frac{1}{6} & -\frac{1}{6}+\alpha+\frac{\sqrt{3}}{3}\beta \\ \hline & \frac{1}{4} & \frac{1}{4} \\ \hline & \frac{1}{4} & \frac{3}{4} \end{array} \tag{5.6}$$ {diag:RL}

$$\begin{array}{c|cc} \frac{1}{3} & \alpha-\frac{\sqrt{3}}{3}\beta & 0 \\ 1 & \frac{1}{2} & -\frac{1}{2}+\alpha+\sqrt{3}\beta \\ \hline & \frac{1}{2} & 0 \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array} \tag{5.7}$$ {diag:RR}

$$\begin{array}{c|cc} 0 & \alpha-\sqrt{3}\beta & 0 \\ 1 & \frac{1}{2} & -\frac{1}{2}+\alpha+\sqrt{3}\beta \\ \hline & \frac{1}{2} & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \tag{5.8}$$ {diag:LO}

We point out that, if we further require the following conditions for explicit RKN schemes (as a very special type of diagonally implicit schemes)

$$\bar{a}_{ij} = 0,\ j \geq i, \tag{5.9}$$ {expl:condi}

then we derive a linear algebraic system in terms of α, β, γ for each case, which can be easily solved and their solutions are

(a) $\alpha = \frac{1}{8}$, $\beta = \frac{\sqrt{3}}{24}$, $\gamma = -\frac{1}{8}$ for (5.3);

(b) $\alpha = \frac{1}{8}$, $\beta = \frac{\sqrt{3}}{8}$, $\gamma = -\frac{1}{8}$ for (5.4);

(c) $\alpha = \frac{1}{4}$, $\beta = \frac{\sqrt{3}}{12}$, $\gamma = -\frac{1}{12}$ for (5.5).

Consequently, by substituting them into (5.3), (5.4) and (5.5), it yields the following three explicit symplectic integrators

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{2}{3} & \frac{1}{6} & 0 \\ \hline & \frac{1}{4} & \frac{1}{4} \\ \hline & \frac{1}{4} & \frac{3}{4} \end{array} \qquad \begin{array}{c|cc} \frac{1}{3} & 0 & 0 \\ 1 & \frac{1}{2} & 0 \\ \hline & \frac{1}{2} & 0 \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array} \qquad \begin{array}{c|cc} 0 & 0 & 0 \\ 1 & \frac{1}{2} & 0 \\ \hline & \frac{1}{2} & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

It is worth mentioning that the right-hand tableau provides the well-known Störmer-Verlet scheme, which has been the most widely used scheme by far in many fields such as astronomy, molecular dynamics and so on [8].

More higher order diagonally implicit symplectic integrators with more stages can be constructed by the same techniques. For instance, a 3-stage 4-order integrator can be obtained by imposing the diagonally implicit conditions to the last table shown in Table 3, which means we should take $\alpha = 0$, $\beta = \frac{\sqrt{5}}{30}$. However, it is difficult to construct higher order explicit symplectic integrators along the same line, as an explicit symplectic integrators generally can be completely determined by the nodes c_i of a quadrature formula [11], which means we can not get explicit symplectic integrators by using a given quadrature formula (e.g. the commonly used Gaussian, Radau and Lobatto type quadrature). However, it is possible that an explicit symplectic integrator stems from a csRKN method by using the associated quadrature formula.

6. Concluding remarks

We propose the continuous-stage Runge-Kutta-Nyström (csRKN) methods for solving second order ordinary differential equations in this paper, and the construction of symplecticity-preserving integrators for separable Hamiltonian systems is investigated. It is shown that the construction of csRKN methods heavily relies on the Legendre polynomial expansion technique coupling with the symplectic conditions and order conditions. Based on symplectic csRKN methods, several new classes of symplectic RKN methods are obtained in use of the quadrature formulae, and some free parameters are included in the Butcher tableaux. It is interesting to see that we can use different quadrature formulae to get different RKN schemes even for the same csRKN coefficients. In addition, we can set many free parameters to get more methods, though we only provides the methods with two free parameters. We have only considered the methods up to order 5 in this paper, but it is possible to construct more higher order methods with the same technique. It is stressed that our approach seems more easier to construct RKN type methods than the traditional approaches which in general have to solve the tedious nonlinear algebraic equations that stem from the order conditions with many unknown coefficients.

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