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ENERGY AND QUADRATIC INVARIANTS PRESERVING METHODS FOR HAMILTONIAN SYSTEMS WITH HOLONOMIC CONSTRAINTS*

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Abstract

We introduce a new class of parametrized structure–preserving partitioned Runge-Kutta (α-PRK) methods for Hamiltonian systems with holonomic constraints. The methods are symplectic for any fixed scalar parameter α, and are reduced to the usual symplectic PRK methods like Shake-Rattle method or PRK schemes based on Lobatto IIIA-IIIB pairs when $\alpha = 0$. We provide a new variational formulation for symplectic PRK schemes and use it to prove that the α-PRK methods can preserve the quadratic invariants for Hamiltonian systems subject to holonomic constraints. Meanwhile, for any given consistent initial values (p_0, q_0) and small step size $h > 0$, it is proved that there exists $\alpha^* = \alpha(h, p_0, q_0)$ such that the Hamiltonian energy can also be exactly preserved at each step. Based on this, we propose some energy and quadratic invariants preserving α-PRK methods. These α-PRK methods are shown to have the same convergence rate as the usual PRK methods and perform very well in various numerical experiments.

Mathematics subject classification: 65P10, 65L05.
Key words: Hamiltonian systems, Holonomic constraints, symplecticity, Quadratic invariants, Partitioned Runge-Kutt methods.

1. Introduction

For a given differential equation, a numerical method is called a geometric numerical integrator if it can accurately preserve some of the geometric characteristics of the solution to the original equation [16]. The structure–preserving algorithms of differential equations have been enlarged by a lot of important developments. The idea of maintaining important structures of the original differential equation in numerical methods is widely accepted. For the Hamiltonian systems, the symplectic integrators preserving the symplectic geometry property of the solutions have been proved to own various excellent properties such as very good orbital tracking ability [12, 13, 16, 20]. Many effective methods for constructing symplectic integrators, such as the methods based on variational integrators [20], generating functions [13], Rung-Kutta (RK) methods [26,27] and composition method [32] have been developed and investigated. The

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theory of symplectic integrators for Hamiltonian systems has become more complete with the establishment of backward error analysis [4, 28] and discrete KAM theory [25]. Recently, some related numerical methods such as multi-symplectic methods for Hamiltonian partial differential equations [23] and stochastic symplectic methods for stochastic Hamiltonian systems [10] have been well developed. In addition to the symplectic property, another extremely important feature of the Hamiltonian system is the conservation of energy. Some important energy preserving methods include discrete gradient method [15, 21], average vector field method [24], HBVMs [7] and spectral methods [1].

When multiple important structures or physical quantities exist for a system, such as the symplectic structure and the energy for Hamiltonian system, a natural question arises: is it possible to construct a numerical method that preserves several of them? Regarding the symplectic structure and the energy for Hamiltonian system, one has unfortunately a negative answer in general with a constant step size. In fact, it is proved [14] that for non-integrable systems if a numerical method is symplectic and can conserve the Hamiltonian energy exactly, then it is the time advance map for the exact Hamiltonian systems up to a reparametrization of time. A similar negative result is proved in [9] for general Hamiltonian system by B-series method. However, the above negative results do not prevent people from constructing numerical methods to maintain both the energy and symplectic structure of the Hamilton system in some weaker sense.

A breakthrough work in this regard is the parameterized Gauss collocation method firstly developed by Brugnano et.al. [8]. Consider the canonical Hamiltonian systems in the form

$$\begin{cases} \dot{y} = J\nabla H(y), \\ y(t_0) = y_0 \in \mathbb{R}^{2d}, \end{cases} \qquad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \in \mathbb{R}^{2d\times 2d}, \tag{1.1}$$

where $y = (p^T, q^T)^T$ and I is the identity matrix and H is the Hamiltonian energy. Brugnano et.al. introduced a nice idea to develop a new family of Gauss type methods which share both the symplecticity-like and energy conservation features under suitable conditions. More precisely, they define a family of RK methods $y_1(\alpha) = \Phi_h(y_0, \alpha)$, where h is the step size of integration, α is a real parameter. This method satisfies the following three conditions simultaneously: (i) for $\alpha = 0$ one gets the Gauss collocation method of order $2s$, s is the number of stages of the RK method; (ii) for any fixed choice of $\alpha \neq 0$, the corresponding method is of order $2s-2$ and satisfies the conditions $b_i a_{i,j} + b_j a_{j,i} = b_i b_j$, thus being a quadratic invariant-preserving symplectic RK method; (iii) for any choice of y_0 and in a neighborhood of h, there exists a value of parameter $\alpha^* = \alpha^*(y_0, h)$ such that $H(y_1) = H(y_0)$(energy conservation). The resulting method $y_1 = \Phi_h(y_0, \alpha^*)$ has order $2s$, preserving the energy and quadratic invariants [1)] .

This method [8] has been rewritten in the framework of discrete linear integral methods [5], which leads to a more refined theoretical analysis and a nice practical implementation strategy for seeking the parameter α^*. Another extension from α-RK to α-PRK to make use of the additive structure of Hamiltonian system is given in [29]. This method is also used to construct

[1)] For standard RK method (c, A, b) with constant step size $h > 0$, the sufficient condition of symplecticity is given by $b_i a_{i,j} + b_j a_{j,i} = b_i b_j$ for all $i, j = 1, 2, ..., s$. For irreducible RK method, which can be intuitively understood to mean that this RK method is not equivalent to a RK method with a lower series, see more details in [17, pp.187], this condition is also necessary, and also sufficient and necessary for quadratic invariants-preserving. However, for the parametric α-RK methods $y_1(\alpha) = \Phi_h(y_0, \alpha^*)$ that preserve the energy, the parameter depends on the initial values, i.e., $\alpha^* = \alpha^*(y_0, h)$. Then, α-RK methods with condition $b_i a_{i,j} + b_j a_{j,i} = b_i b_j$ are in general not symplectic from the definition, but can preserve all the quadratic invariants.

energy conservation multi-symplectic schemes for Hamiltonian wave equations [11]. The key of constructing parametric RK or PRK methods in [8, 29] lies in the so-called W-transform technique. However, this technique is in general not suitable for constrained Hamiltonian systems since it will break the manifold constraint. See more details in Section 4.

In this paper, we focus on the geometric integrators for Hamiltonian systems subject to holonomic constraints. Consider the Hamiltonian with holonomic constraints (constraints that depend on q only) [16, Chap. VII] $\widetilde{H}(p,q,\lambda) = H(p,q) + g(q)^T\lambda$, where $H : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is the Hamiltonian function without constraint and $g(\cdot) : \mathbb{R}^d \to \mathbb{R}^m$ is the constraint function. Here, $\lambda \in \mathbb{R}^m$ is the Lagrangian multiplier. The corresponding ODE is given by (see [16, VII.1.2])

$$\begin{aligned} \dot{q} &= \nabla_p H(p,q) =: H_p(p,q), \\ \dot{p} &= -\nabla_q H(p,q) - G^T(q)\lambda =: -H_q(p,q) - G^T(q)\lambda, \\ 0 &= g(q), \end{aligned} \tag{1.2}$$

where we introduced $G(q) = \left(\frac{\partial g_i}{\partial q_j}\right)_{m\times d}$ to be the Jacobian matrix of $g(q)$ so that $G^T(q) = \nabla_q g \in \mathbb{R}^{d\times m}$. Note that we use the convention $(\nabla_q g)_{ij} = \frac{\partial g_j}{\partial q_i}$ which is commonly used in the community of fluid mechanics. Throughout this paper, we assume that the matrix $G(q)$ has full rank and $G(q)H_{pp}(p,q)G(q)^T$ is invertible, which will allow us to express λ in terms of (p,q). The dynamics given by (1.2) is on the manifold

$$\mathcal{M} = \{(p,q); \quad g(q) = 0,\ G(q)H_p(p,q) = 0\}, \tag{1.3}$$

which is the cotangent bundle of the manifold given by $\mathcal{Q} := \{q : g(q) = 0\}$. See [16, VII.1.2] for more details. The constraint $G(q)H_p(p,q) = 0$ is also called the hidden constraint.

It is easy to verify that the ODE (1.2) has many geometric structures. First of all, the Hamiltonian (or energy) H is preserved:

$$\frac{d}{dt}H(p(t),q(t)) = 0. \tag{1.4}$$

Secondly, the symplecticity is also preserved. Consider a map $\varphi : \mathcal{M} \to \mathcal{M}$ and its tangent map $\varphi' : T_x\mathcal{M} \to T_{\varphi(x)}\mathcal{M}$. One says the map φ is symplectic if

$$(\varphi'(x)\xi_1)^T J(\varphi'(x)\xi_2) = \xi_1^T J\xi_2, \quad \forall \xi_1, \xi_2 \in T_x\mathcal{M}. \tag{1.5}$$

For $\mathcal{M}$ being a submanifold of $\mathbb{R}^{2d}$, $\varphi' = (\nabla_x\varphi)^T$ so that $\varphi'\xi = \xi \cdot \nabla_x\varphi = \frac{d}{d\tau}\big|_{\tau=0}\varphi(\gamma(\tau))$ for any smooth curve γ in $\mathcal{M}$ satisfying $\gamma(0) = x, \gamma'(0) = \xi$. It can be shown that the flow map of (1.2) is symplectic. Plainly speaking, the symplecticity means that the flow preserves the quadratic forms, which further implies that the volume form is conserved (see the introduction of [18]).

From the point view of structure-preserving methods, if one solves the Hamiltonian system (1.2) numerically, besides the basic requirement that the solution falls onto the manifold $\mathcal{M}$, one also tends to ask that the energy preservation or the symplecticity to be satisfied. This additional requirement for staying on manifold $\mathcal{M}$ for constrained Hamiltonian systems brings new difficulties in the construction of structure–preserving numerical schemes.

There are several symplectic methods for the holonomic constrained Hamiltonian systems. One typical class is the PRK methods as detailed in [18–20]. The first order method in [16, sec VII.1.3] and the Shake-Rattle method in [2, 16] are special cases of the PRK methods.

Symplectic variational integrators for constrained Hamiltonian systems are developed in [20, 31]. Those methods are symplectic and preserve the manifolds $\mathcal{M}$ exactly, but they are not energy–conserving. The second order energy–conserving method in the line integral framework developed in [6] is not symplectic in general and can not conserve the the hidden constraint $G(q)H_p(p,q)=0$. The projected RK methods are proposed in [30], but it is not symplectic.

The goal of this work is to introduce a parameter in the PRK methods so that both the energy and the quadratic invariants can be preserved for the constrained Hamiltonian system following the spirit of [8,29]. Note that if we do this method for every trajectory, then the energy can be preserved for all trajectories but the method is in general not symplectic. However, if we fix down the parameters, the method is symplectic and can be preserve energy for one trajectory.

The rest of the paper is arranged as follows. In section 2, we recall some of the basic concepts and properties of symplectic PRK methods for constrained Hamiltonian systems. In order to show that the symplectic PRK methods preserve the quadratic invariants for Hamiltonian systems subject to holonomic constraints, we provide a new variational formulation for symplectic PRK methods in section 3. In section 4, we construct energy and quadratic invariants preserving parametric α-PRK methods based on Shake-Rattle method and Lobatto IIIA-IIIB pairs, and check various properties of the new methods. Numerical examples are included in section 5 to illustrate the energy and quadratic invariants conservations for the α-PRK methods.

2. Symplectic Partitioned Runge-Kutta Methods

In this subsection, we give a brief review of the symplectic PRK methods. See [16, 18] for more details. The s-stage PRK method denoted by $\left(c, A, b; \widehat{A}, \widehat{b}\right)$ for the Hamiltonian ODE (1.2) is given by the following

$$\begin{aligned}
&p_1 = p_0 + h\sum_{i=1}^{s}\hat{b}_i\ell_i, \quad q_1 = q_0 + h\sum_{i=1}^{s} b_i k_i.\\
&\ell_i = -H_q(P_i,Q_i) - G^T(Q_i)\Lambda_i,\ k_i = H_p(P_i,Q_i),\ g(Q_i)=0,\\
&P_i = p_0 + h\sum_{j=1}^{s}\hat{a}_{ij}\ell_j, \quad Q_i = q_0 + h\sum_{j=1}^{s} a_{ij}k_j.
\end{aligned} \tag{2.1}$$

The equations considered here are autonomous, so the parameters $c=(c_1,\ldots,c_s)$ for the Runge-Kutta methods are absent in (2.1). See section 4.1.2 for more details.

Lemma 2.1 ([18]). *For a given PRK method, if the conditions*

$$b_i = \hat{b}_i, \quad b_i\hat{a}_{ij} + \hat{b}_j a_{ji} = b_i\hat{b}_j, \tag{2.2}$$

are satisfied, then the method for Hamiltonian systems with holonomic constraints is symplectic.

For s-stage PRK methods, if $a_{ij}, \hat{a}_{ij}, b_i, \hat{b}_i$ are given, then there are $3s$ equations for the $3s$ unknowns (P_i, Q_i, Λ_i). However, for general symplectic PRK methods, (p_1, q_1) may not fall onto $\mathcal{M}$. To ensure that q_1 satisfies the constraint, it is suggested in [18] to impose the conditions

$$a_{1j} = 0, a_{sj} = b_j,\ 1 \le j \le s, \tag{2.3}$$

so that

$$Q_1 \equiv q_0, \quad Q_s \equiv q_1. \tag{2.4}$$

With this, one has correspondingly

$$\hat{a}_{js} = 0, \quad \hat{a}_{j1} = b_1, \qquad j = 1, ..., s, \tag{2.5}$$

from the symplectic condition given in Lemma 2.1. This requirement removes the unknowns Q_1, Λ_s and the equations $g(Q_1) = 0$, $Q_1 = q_0 + h\sum_{j=1}^{s} a_{ij}k_j$. Hence, the number of equations is now equal to the number of unknowns $(Q_2, \ldots, Q_s, P_1, \ldots, P_s, \Lambda_1, \ldots, \Lambda_{s-1})$. In fact, it is shown in [18] that these variables can be uniquely solved when h is small enough under some reasonable assumptions on H and $\left(c, A, b; \widehat{A}, \widehat{b}\right)$. We remark that even though one imposes $Q_1 = q_0$, the Lagrange multiplier Λ_1 is still in the system of equations. Lastly, p_1 and Λ_s can be determined by the hidden constraint condition $0 = G(q_1) \cdot H_p(p_1, q_1)$.

For the PRK methods suggested in [18], we thus solve the next two nonlinear systems in turn at each step. The first one

$$\begin{cases} Q_i = q_0 + h\sum\limits_{j=1}^{s} a_{ij} H_p(P_j, Q_j), \\ P_i = p_0 - h\sum\limits_{j=1}^{s-1} \hat{a}_{ij}\left(H_q(P_j, Q_j) - G^T(Q_j)\Lambda_j\right), \\ 0 = g(Q_i). \end{cases} \tag{2.6}$$

with $Q_1 \equiv q_0, Q_s \equiv q_1$. Then, we can solve (p_1, Λ_s) by

$$\begin{cases} p_1 = p_0 - h\sum\limits_{i=1}^{s-1} \hat{b}_i\left(H_q(P_i, Q_i) - G^T(Q_i)\Lambda_i\right) - h\hat{b}_s\left(H_q(P_s, Q_s) - G^T(Q_s)\Lambda_s\right), \\ 0 = G(q_1)H_p(p_1, q_1). \end{cases} \tag{2.7}$$

As commented in [16, sec VI.6.2], the symplectic schemes can be written as certain variational integrators. In [16, sec VI.6.3], it was explained in detail how a PRK scheme for unconstrained problems can be formulated into a variational integrator. The same is true for Hamiltonian systems with holonomic constraints. In fact, Marsden and West addressed this issue in [20, section 3.5.6]. In particular, given $(q_0, q_1) \in \mathbb{R}^d \times \mathbb{R}^d$, one can implicitly define quantities $\left(\bar{p}_0, \bar{p}_1, \bar{Q}_i, \bar{P}_i, \dot{\bar{P}}_i, \dot{\bar{Q}}_i\right)$ for $i = 1, \ldots, s$ and $\bar{\Lambda}_i$ for $i = 2, \ldots, s-1$ through the following system of equations

$$\begin{aligned} & q_1 = q_0 + h\sum_{j=1}^{s} b_j \dot{\bar{Q}}_j, \qquad \bar{p}_1 = \bar{p}_0 + h\sum_{j=1}^{s} \hat{b}_j \dot{\bar{P}}_j, \\ & \bar{Q}_i = q_0 + h\sum_{j=1}^{s} a_{ij} \dot{\bar{Q}}_j, \qquad \bar{P}_i = \bar{p}_0 + h\sum_{j=1}^{s} \hat{a}_{ij} \dot{\bar{P}}_j, \qquad i = 1, \ldots, s, \\ & \dot{\bar{Q}}_i = H_p(\bar{Q}_i, \quad \bar{P}_i), \quad i = 1, \ldots, s, \\ & \dot{\bar{P}}_1 = -H_q(\bar{Q}_1, \bar{P}_1), \qquad \dot{\bar{P}}_s = -H_q(\bar{Q}_s, \bar{P}_s), \\ & \dot{\bar{P}}_i = -H_q(\bar{P}_i, \bar{Q}_i) - G^T(\bar{Q}_i)\bar{\Lambda}_i, \; 0 = g(\bar{Q}_i), \quad i = 2, \ldots, s-1. \end{aligned} \tag{2.8}$$

Note that the definitions of $\dot{\bar{P}}_1$ and $\dot{\bar{P}}_s$ above are different from other $\dot{\bar{P}}_i$ (in fact, $\dot{\bar{P}}_i = \dot{P}_i$ for $i \neq 1, s$ while there should be some corrections for $\dot{\bar{P}}_1$ and $\dot{\bar{P}}_s$ to define $\dot{P}_1, \dot{P}_s$). Moreover,

$\bar{p}_1$ and $\bar{p}_0$ are not p_1, p_0 in (2.1). They are different by some terms involving the corresponding Lagrange multipliers. See the proof of [20, Theorem 3.5.1] for the details. With the quantities defined in (2.8), one can define the discrete Lagrangian

$$L_h(q_0, q_1) = h \sum_{i=1}^{s} b_i L(\bar{Q}_i, \dot{\bar{Q}}_i), \tag{2.9}$$

where $L(q, \dot{q})$ is the Lagrangian for the time-continuous dynamics. The Euler-Lagrange equation for this discrete Lagrangian under the holonomic constraints $(q_0, q_1) \in \mathcal{Q} \times \mathcal{Q}$ reads

$$\begin{aligned} &p_0 = -\frac{\partial L_h}{\partial x}(q_0, q_1) + hG^T(q_0) \cdot \lambda_0, \qquad p_1 = \frac{\partial L_h}{\partial y}(q_0, q_1) - hG^T(q_1) \cdot \lambda_1, \\ &g(q_1) = 0, \qquad G(q_1) H_p(p_1, q_1) = 0. \end{aligned} \tag{2.10}$$

See [20, eqs. (3.5.2a-d)]. Note that though the Euler-Lagrange equations are derived by fixing q_0, q_1, one should regard p_0, q_0 as knowns and solve (p_1, q_1) dynamically. The good thing of this variational formulation is that many conservation properties can be derived via the discrete Noether theorem. See [20] and also section 3 below for more details on conservation properties and discrete Noether theorem. However, for quadratic invariants, the form (2.8), (2.9) is not convenient to use and we will propose another variational formulation below in section 3.

2.1. PRK schemes: Shake–Rattle and Lobatto IIIA-IIIB pairs

We first recall some famous PRK methods, including Shake–Rattle algorithm and Lobatto IIIA-IIIB pairs, which will be used to construct the parameterization α-PRK later. For typical separable Hamiltonian $H(p, q) = \frac{1}{2} p^T M^{-1} p + U(q)$, the traditional Shake method reads

$$\begin{aligned} &q_{n+1} - 2q_n + q_{n-1} = -h^2 M^{-1}(U_q(q_n) + G(q_n)^T \Lambda_n), \\ &0 = g(q_{n+1}). \end{aligned}$$

Then, the momentum is $p_n = M(q_{n+1} - q_{n-1})/(2h)$. The corresponding Hamiltonian formulation for the Shake method is

$$\begin{aligned} &p_{n+1/2} = p_n - \frac{h}{2}(U_q(q_n) + G(q_n)^T \Lambda_n), \\ &q_{n+1} = q_n + hM^{-1} p_{n+1/2}, \qquad g(q_{n+1}) = 0, \\ &p_{n+1} = p_{n+1/2} - \frac{h}{2}(U_q(q_{n+1}) + G(q_{n+1})^T \Lambda_{n+1}). \end{aligned}$$

Unfortunately, so-defined p_n may not satisfy the constraint. Anderson [2] proposed the Rattle algorithm. That is to determine p_{n+1} by using another multiplier μ_n which can be different from Λ_{n+1}:

$$p_{n+1} = p_{n+1/2} - \frac{h}{2}(U_q(q_{n+1}) + G(q_{n+1})^T \mu_n).$$

Then, one uses the condition $G(q_{n+1}) \cdot M^{-1} p_{n+1} = 0$ to determine μ_n and thus p_{n+1}. Clearly, this Shake–Rattle algorithm is one of the symplectic PRK method mentioned above. The more general form of Shake–Rattle for the general Hamiltonian system with holonomic constraints

reads

$$\begin{aligned} p_{n+1/2} &= p_n - \frac{h}{2}\left(\nabla_q H(p_{n+1/2}, q_n) + G^T(q_n)\Lambda_n\right), \\ q_{n+1} &= q_n + \frac{h}{2}(\nabla_p H(p_{n+1/2}, q_n) + \nabla_p H(p_{n+1/2}, q_{n+1})), \quad g(q_{n+1}) = 0, \\ p_{n+1} &= p_{n+1/2} - \frac{h}{2}(\nabla_q H(p_{n+1/2}, q_{n+1}) + G^T(q_{n+1})\Lambda_{n+1}), \\ & G(q_{n+1})\nabla_p H(p_{n+1}, q_{n+1}) = 0. \end{aligned} \tag{2.11}$$

It is proved that the Shake–Rattle algorithm is symmetric, symplectic and convergent of order two [16, sec VII.I]. A nice extension to higher order method is the Lobatto IIIA–IIIB pairs developed in [18]. This method combined with the projection step by the hidden constraint condition defined in the manifold $\mathcal{M}$ has the following merits:

(a) preserving the numerical solutions on the manifold $\mathcal{M}$ exactly;

(b) it is symmetric, symplectic and super convergent of order $2s-2$, where s is the stage of the PRK method.

In particular, for $s = 3$, the coefficients for Lobatto IIIA–IIIB pairs are given by

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{5}{24} & \frac{1}{3} & -\frac{1}{24} \\ 1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}, \qquad \begin{array}{c|ccc} 0 & \frac{1}{6} & -\frac{1}{6} & 0 \\ \frac{1}{2} & \frac{1}{6} & \frac{1}{3} & 0 \\ 1 & \frac{1}{6} & \frac{5}{6} & 0 \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}. \tag{2.12}$$

3. An Alternative Variational Formulation

In this section, we aim to study the quadratic invariants of the PRK schemes via the discrete Noether's theorem. For this purpose, we need to find some equivalent variational forms for the PRK schemes. However, the form in the work of Marsden and West (i.e. (2.8)-(2.9)) is not convenient, as it involves Lagrangian multipliers and there is nonlinearity. Instead, we will propose an alternative formulation so that the symmetry can be studied better.

It is known that symplectic PRK schemes for Hamiltonian systems without constraints can conserve quadratic invariants of the form

$$I(p, q) = q^T D p, \tag{3.1}$$

where D is some fixed matrix ([16, sec VI.2.2]). Naturally, one is curious whether there is an analogue for Hamiltonian systems with holonomic constraints. Clearly, due to the constraint $g(q) = 0$, the quadratic invariants must be some particular forms. Instead, motivated by Noether's theorem [3, 22], we will consider that

$$\mathfrak{D} := \left\{ D : g\left(e^{sD} q\right) = g(q), \quad L\left(e^{sD} q, e^{sD} \dot{q}\right) = L(q, \dot{q}), \text{ for all } s \in \mathbb{R} \right\}, \tag{3.2}$$

Clearly, according to Noether's theorem we have the following.

Lemma 3.1. *For any $D \in \mathfrak{D}$, the quantity $q^T D p$ is a first integral of the Hamiltonian system with holonomic constraints.*

We now aim to show that the symplectic PRK schemes will conserve all the quadratic invariants of the form $q^T D p$ for $D \in \mathfrak{D}$.

Theorem 3.1. *The symplectic PRK schemes for Hamiltonian system with holonomic constraints defined in* (2.1) *conserve all quadratic invariants of the form*

$$I(p,q) = q^T D p, \quad D \in \mathfrak{D}. \tag{3.3}$$

To do this, we first recall the discrete Noether's theorem for variational integrators.

Lemma 3.2 (Discrete Noether's theorem). *Assume the discrete Lagrangian $L_h(q_0,q_1)$ is invariant under a one-parameter group of transformation $\{\mathfrak{g}_s : s \in \mathbb{R}\}$: $L_h\left(\mathfrak{g}_s(q_0),\mathfrak{g}_s(q_1)\right) = L_h(q_0,q_1)$ for all $s \in \mathbb{R}$ and (q_0,q_1). Then the corresponding variational integrators for Lagrangian systems have the first integral in the form of $p_{n+1}^T a(q_{n+1}) = p_n^T a(q_n)$, where $a(q) = \frac{d}{ds}\mathfrak{g}_s(q)|_{s=0}$ is the generator for the group. Furthermore, when there are holonomic constraints, besides the conditions above, if moreover $\{\mathfrak{g}_s : s \in \mathbb{R}\}$ leaves the constraints manifold $\mathcal{Q}$ invariant, then the claim still holds.*

The first part can be found in [16, sec VI.6]. The second part has been remarked in [20, sec. 3.4.2]. For the convenience, we provide a direct verification here.

Proof. [Proof of the second part of Lemma 3.2] Taking derivative on s and setting $s = 0$ in $L_h\left(\mathfrak{g}_s(q_0),\mathfrak{g}_s(q_1)\right) = L_h(q_0,q_1)$, one has

$$a(q_0)\cdot\frac{\partial L_h}{\partial x}(q_0,q_1) + a(q_1)\cdot\frac{\partial L_h}{\partial y}(q_0,q_1) = 0.$$

Since $\{\mathfrak{g}_s : s \in \mathbb{R}\}$ leaves the constraints manifold invariant, we have $G(q)a(q) = 0$ implies that $a(q)\cdot G^T(q)\lambda = 0$ for all λ. Using (2.10), one easily finds $p_1^T a(q_1) = p_0^T a(q_0)$. □

Below, we propose an alternative variational formulation for the PRK schemes that appears different from (2.8), (2.9). This formulation is suitable for verifying the conditions in the discrete Noether's theorem.

Proposition 3.1. *The discrete Lagrangian for the symplectic PRK methods* ((2.1) *with conditions* (2.2), (2.3)) *can be defined as*

$$L_h(q_0,q_1) = \operatorname{ext}_{\{\dot{Q}_i\}} h\sum_{i=1}^{s} b_i L(Q_i,\dot{Q}_i), \quad (q_0,q_1) \in \mathbb{R}^d\times\mathbb{R}^d, \tag{3.4}$$

subject to constraints

$$g(Q_i) = 0, \qquad i = 2,\dots,s-1, \tag{3.5}$$

$$q_1 = q_0 + h\sum_{j=1}^{s} b_j\dot{Q}_j. \tag{3.6}$$

Above, $Q_i = q_0 + h\sum_{j=1}^{s} a_{ij}\dot{Q}_j$, $i = 2,\dots,s-1$ and "ext" means extremizing.

Remark 3.1. Note that L_h is defined in $\mathbb{R}^d\times\mathbb{R}^d$ instead of $\mathcal{Q}\times\mathcal{Q}$ (i.e., q_0, q_1 do not have to be in $\mathcal{Q}$). Moreover, there are no Q_1, Q_s above.

Proof. [Proof of Proposition 3.1]

Step 1. First of all, we note that the discrete Lagrangian $L_h(q_0, q_1)$ is well-defined. We consider the augmented Langrangian for the extremization problem

$$\bar{L}(\{\dot{Q}_i\}, \{\Lambda_i\}, \lambda) := h\sum_{i=1}^{s} b_i L(Q_i, \dot{Q}_i) - \sum_{i=2}^{s-1} g(Q_i)^T (b_i \Lambda_i) - h^{-1}\lambda(q_0 + h\sum_{j=1}^{s} b_j \dot{Q}_j - q_1).$$

Note that we have built in the constraint $g(Q_i) = 0$ using the multiplier $b_i\Lambda_i$, and the constraint for q_0, q_1 using the multiplier $h^{-1}\lambda$. Since $b_i \neq 0$ and $h \neq 0$, this will not change anything. Taking the first variational gives the corresponding Euler-Lagrange equations, i.e., the necessary conditions for the functional to obtain the extreme value (see for example [20, sec. 3.3, page 431]):

$$\begin{aligned} &\left(\sum_{i=1}^{s} b_i \frac{\partial L}{\partial q}(Q_i, \dot{Q}_i) h a_{ij}\right) + b_j \frac{\partial L}{\partial \dot{q}}(Q_j, \dot{Q}_j) = \sum_{i=2}^{s-1} b_i h a_{ij} G^T(Q_i)\Lambda_i + b_j \lambda, \\ &g(Q_i) = 0,\ i = 2, \ldots, s-1, \quad q_1 = q_0 + h\sum_{j=1}^{s} b_j \dot{Q}_j. \end{aligned} \tag{3.7}$$

These $sd + (s-2)m + d$ equations in (3.7) can yield the solutions $(\{\dot{Q}_j\}_{j=1}^{s}, \{\Lambda_i\}_{i=2}^{s-1}, \lambda)$ for h sufficiently small. Hence, $L_h(q_0, q_1)$ is well-defined. Here we are solving $\dot{Q}_i$ in terms of q_0, q_1 for any (q_0, q_1) in $\mathbb{R}^d \times \mathbb{R}^d$, not just for $(q_0, q_1) \in \mathcal{Q} \times \mathcal{Q}$. With this observation, we can take differentiation on $q_\ell, \ell = 0, 1$ for the constraint (3.6) to find

$$h\sum_{j=1}^{s} b_j \frac{\partial \dot{Q}_j}{\partial q_0} = -I, \quad h\sum_{j=1}^{s} b_j \frac{\partial \dot{Q}_j}{\partial q_1} = I, \tag{3.8}$$

and for the constraints (3.5) to find

$$h\left(\sum_{j=1}^{s} a_{ij} \frac{\partial \dot{Q}_j}{\partial q_0}\right) G^T(Q_i) = -G^T(Q_i), \quad h\left(\sum_{j=1}^{s} a_{ij} \frac{\partial \dot{Q}_j}{\partial q_1}\right) G^T(Q_i) = 0. \tag{3.9}$$

Note that here we used the convention $\frac{\partial \dot{Q}_j}{\partial q_0} := \nabla_{q_0} \dot{Q}_j$, and $\left(\frac{\partial \dot{Q}_j}{\partial q_0}\right)_{\ell,m} = \frac{\partial \dot{Q}_j^{(m)}}{\partial q_0^{(\ell)}}$. The reason to do this is that we have made $\frac{\partial L}{\partial q}$ a column vector.

Step 2. Now that $\{\dot{Q}_j\}_{j=1}^{s}$ are solved in terms of (q_0, q_1), we may write out the explicit expressions of p_i in the Euler-Lagrange equations for the discrete Lagrangian as in (2.10). By the first equation in (2.10), one has

$$\begin{aligned} p_0 &= -\left(h\sum_{i=1}^{s} b_i \left[I + h\sum_{j=1}^{s} a_{ij} \frac{\partial \dot{Q}_j}{\partial q_0}\right] \frac{\partial L}{\partial q}(Q_i, \dot{Q}_i) + h\sum_{i=1}^{s} b_i \frac{\partial \dot{Q}_i}{\partial q_0} \frac{\partial L}{\partial \dot{q}}(Q_i, \dot{Q}_i)\right) + hG^T(q_0)\cdot\lambda_0 \\ &= -h\sum_{i=1}^{s} b_i \frac{\partial L}{\partial q}(Q_i, \dot{Q}_i) - h\sum_{j=1}^{s} \frac{\partial \dot{Q}_j}{\partial q_0}\left[\sum_{i=2}^{s-1} h b_i a_{ij} G^T(Q_i)\Lambda_i + b_j\lambda\right] + hG^T(q_0)\cdot\lambda_0 \\ &= -h\sum_{i=1}^{s} b_i \frac{\partial L}{\partial q}(Q_i, \dot{Q}_i) + h\sum_{i=2}^{s-1} b_i G^T(Q_i)\Lambda_i + \lambda + hG^T(q_0)\cdot\lambda_0. \end{aligned}$$

Above, the second equality follows from (3.7) while last inequality follows from (3.8) and (3.9). Similarly, we can compute by the second equation in (2.10) that

$$\begin{aligned} p_1 &= h\sum_{i=1}^{s} b_i h \sum_{j=1}^{s} a_{ij}\frac{\partial \dot{Q}_j}{\partial q_1}\frac{\partial L}{\partial q}(Q_i,\dot{Q}_i) + h\sum_{i=1}^{s} b_i \frac{\partial \dot{Q}_i}{\partial q_1}\frac{\partial L}{\partial \dot{q}}(Q_i,\dot{Q}_i) - hG^T(q_1)\cdot\lambda_1 \\ &= h\sum_{j=1}^{s}\frac{\partial \dot{Q}_j}{\partial q_1}\left[\sum_{i=2}^{s-1} hb_i a_{ij} G^T(Q_i)\Lambda_i + b_j\lambda\right] - hG^T(q_1)\cdot\lambda_1 \\ &= \lambda - hG^T(q_1)\cdot\lambda_1. \end{aligned}$$

Defining that $\Lambda_1 := \lambda_0/b_1, \Lambda_s := \lambda_1/b_s$, one has

$$p_1 = p_0 + h\sum_{i=1}^{s} b_i \frac{\partial L}{\partial q}(Q_i,\dot{Q}_i) - h\sum_{i=1}^{s} b_i G^T(Q_i)\Lambda_i. \tag{3.10}$$

Step 3. We verify that the Euler-Lagrange equations (2.10) given by so-defined discrete Lagrangian is equivalent to the symplectic PRK methods with constraints. Recall that the (continuous) Hamiltonian is related to Lagrangian by $H(p,q) = p^T\dot{q} - L(q,\dot{q}),\ \ p = \frac{\partial L}{\partial \dot{q}}$, where $\dot{q} = \dot{q}(p,q)$ is determined by the second equation. It can be computed that

$$\dot{q} = \frac{\partial H(p,q)}{\partial p}, \qquad \frac{\partial H(p,q)}{\partial q} = -\frac{\partial L(q,\dot{q})}{\partial q}.$$

Hence, we have

$$Q_i = q_0 + h\sum_{j=1}^{s} a_{ij} H_p(P_j,Q_j), \quad q_1 = q_0 + h\sum_{i=1}^{s} b_i H_p(P_i,Q_i), \tag{3.11}$$

$$p_1 = p_0 - h\sum_{i=1}^{s} b_i H_q(P_i,Q_i) - h\sum_{i=1}^{s} b_i G^T(Q_i)\Lambda_i, \tag{3.12}$$

where $P_i = \frac{\partial L(Q_i,\dot{Q}_i)}{\partial \dot{Q}_i}$. The first equation in (3.7) can then be rewritten as

$$\sum_{i=1}^{s} hb_i a_{ij}(-H_q(P_i,Q_i)) + b_j P_j = \sum_{i=2}^{s-1} b_i h a_{ij} G^T(Q_i)\Lambda_i + b_j[p_1 + hb_s G^T(q_1)\cdot\Lambda_s].$$

Using (3.12), we then have

$$P_j = p_0 - h\sum_{i=1}^{s}[b_i - b_i a_{ij}/b_j]H_q(P_i,Q_i) - \sum_{i=2}^{s-1}[b_i - b_i a_{ij}/b_j]G^T(Q_i)\Lambda_i - hb_1 G^T(Q_1)\cdot\Lambda_1. \tag{3.13}$$

Using the condition $a_{1j} = 0, a_{sj} = b_j$, this is further simplified to

$$P_j = p_0 - h\sum_{i=1}^{s}[b_i - b_i a_{ij}/b_j]H_q(P_i,Q_i) - \sum_{i=1}^{s}[b_i - b_i a_{ij}/b_j]G^T(Q_i)\Lambda_i. \tag{3.14}$$

Defining $\hat{a}_{ji} = b_i - b_i a_{ij}/b_j$, one has the desired form for P_j.

Eventually, we find (3.11), (3.12), (3.14) and (3.5)–(3.6) then form a complete system that is the same as the symplectic PRK method. □

Lastly, we verify Theorem 3.1.

Proof. [Proof of Theorem 3.1] The constraint condition is obvious. We verify that

$$L_h(e^{sD}q_0, e^{sD}q_1) = L_h(q_0, q_1). \tag{3.15}$$

This is in fact a direct corollary of Proposition 3.1. Since e^{sD} is a linear group, then for any (q_0, q_1) and any $\{\dot{Q}_j\}_{j=1}^s$, we have a corresponding sequence of data $\{\bar{\dot{Q}}_j\}_{j=1}^s := \{e^{sD}\dot{Q}_j\}_{j=1}^s$ for $(e^{sD}q_0, e^{sD}q_1)$. Correspondingly the new Q_i (denoted by $\bar{Q}_i$) is given by

$$\bar{Q}_i = e^{sD}q_0 + h\sum_{j=1}^{s} a_{ij}e^{sD}\dot{Q}_j = e^{sD}Q_i,$$

by the linearity of $e^{sD} : \mathbb{R}^d \to \mathbb{R}^d$. Since for the continuous Lagrangian one has $L(e^{sD}Q_i, e^{sD}\dot{Q}_i) = L(Q_i, \dot{Q}_i)$, we find the sums to extremize in (3.4) have the same value at the corresponding data. Hence, their extrema must be the same and thus (3.15) follows. Applying the discrete Noether's theorem (Lemma 3.2), we obtain the desired result. □

4. Energy and Quadratic Invariants Preserving Methods

In this section, we propose methods that preserve the energy and quadratic invariants for Hamiltonian systems with constraints based on some parametric PRK schemes, following the spirit of [8, 29]. Recall that the following conditions guarantee that the s-stage PRK method is symplectic and preserves the quadratic invariants:

$$\begin{aligned}&\text{The symplecticity and quadratic invariants: } b_i = \hat{b}_i,\ b_i\hat{a}_{ij} + \hat{b}_j a_{ji} = b_i\hat{b}_j,\ i,j = 1, ..., s.\\ &\text{For the constraints: } a_{1j} = 0,\ a_{sj} = b_j, \text{or equivalently, } \hat{a}_{is} = 0,\quad \hat{a}_{i1} = b_1,\ i = 1, \ldots, s.\end{aligned} \tag{4.1}$$

These schemes do not in general preserve the Hamiltonian (energy). In fact, such methods conserve the symplectic properties and Hamiltonian energy for constant stepsize $h > 0$ has been proven not to exist in general [9, 14]. The key observation now is that the conditions imposed above cannot determine $\left(c, A, b; \hat{A}, \hat{b}\right)$ totally, so there is actually some freedom to choose these parameters, and thus possibly to preserve the energy.

Inspired by [8, 29], we are motivated to construct α-PRK methods. It is desired that the methods are symplectic and quadratic invariants preserving when the parameter α is fixed, and also the energy can be preserved if α is adjusted suitably. However, the particular construction technique developed in [8,29] is not feasible here in general. In fact, the key in the construction of α-PRK methods in the two papers is the so called W-transformation, which allows us to express the symplectic condition in a very compact form with the help of matrix X_G, where the three diagonal anti-symmetric matrix X_G is the W-transformation matrix of Gauss collocation method. Thus, one can parameterize the transformed matrix so that it remains to satisfy the same conditions as usual symplectic RK or PRK methods, and then obtain the parameterized α-PRK method by inverse W-transformation. For example, the 2-stage and 3-stage α-PRK methods based on Lobatto IIIA-IIIB pairs are given by [29]

$$\begin{array}{c|cc} 0 & \frac{1}{6}\alpha & -\frac{1}{6}\alpha \\ 1 & \frac{1}{2}-\frac{1}{6}\alpha & \frac{1}{2}+\frac{1}{6}\alpha \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}, \qquad \begin{array}{c|cc} 0 & \frac{1}{2}-\frac{1}{6}\alpha & \frac{1}{6}\alpha \\ 1 & \frac{1}{2}+\frac{1}{6}\alpha & -\frac{1}{6}\alpha \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}. \tag{4.2}$$

$$\begin{array}{c|ccc} 0 & \frac{1}{5}\alpha & -\frac{2}{5}\alpha & \frac{1}{5}\alpha \\ \frac{1}{2} & \frac{5}{24}-\frac{1}{15}\alpha & \frac{1}{3}+\frac{2}{15}\alpha & -\frac{1}{24}-\frac{1}{15}\alpha \\ 1 & \frac{1}{6}+\frac{1}{5}\alpha & \frac{2}{3}-\frac{2}{5}\alpha & \frac{1}{6}-\frac{1}{5}\alpha \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}, \qquad \begin{array}{c|ccc} 0 & \frac{1}{6}-\frac{1}{5}\alpha & -\frac{1}{6}+\frac{2}{5}\alpha & -\frac{1}{5}\alpha \\ \frac{1}{2} & \frac{1}{6}+\frac{1}{15}\alpha & \frac{1}{3}-\frac{2}{15}\alpha & \frac{1}{15}\alpha \\ 1 & \frac{1}{6}-\frac{1}{5}\alpha & \frac{5}{6}+\frac{2}{5}\alpha & -\frac{1}{5}\alpha \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}. \tag{4.3}$$

We can see that although the method keeps symplecticity and quadratic invariants, it generally does not satisfy the constraint conditions $a_{1j} = 0, a_{sj} = b_j$, so its numerical solution cannot be guaranteed to fall on the manifold $\mathcal{M}$.

In this article, we introduce another new class of parametric α-PRK methods. According to (4.1), we focus only on (A, b). Note that the first and last rows of A are fixed and depend on b while the other rows of A can be determined in a great freedom. Since the energy $H(p, q)$ is a scalar, we can let these coefficients change depending on a scalar $\alpha \in \mathbb{R}$ in a particular chosen way. We hope to choose α such that the conditions (4.1) are satisfied. Of course, due to the degrees of freedom, such a choice may not be unique. In this work, we just choose some particular parametrization to illustrate the ideas, and we are not aiming to find the optimal choice of parametrization. Currently, it is unclear to us what criterion can be used to determine which one is optimal. Let's first take a closer look at classic examples, and then introduce the energy and quadratic invariants preserving methods.

4.1. Some parametric PRK methods based on existing methods

4.1.1. α-Rattle

In this section, we aim to propose a method based on the Shake-Rattle algorithm in section 2.1. As known, this method is a two–stage method with order 2. If we perturb b, the order can be reduced. Since $s = 2$, with the conditions (4.1), there is only one degree of freedom left for choosing the parameters. In particular, we let

$$b_1 = \frac{1}{2} + \alpha, \quad b_2 = \frac{1}{2} - \alpha, \quad \alpha \in \mathbb{R}. \tag{4.4}$$

Then, the matrix $A(\alpha)$-$\widehat{A}(\alpha)$ is fully determined, and the α-PRK, which we call α-Rattle, in the form Butcher table is given:

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & \frac{1}{2}+\alpha & \frac{1}{2}-\alpha \\ \hline & \frac{1}{2}+\alpha & \frac{1}{2}-\alpha \end{array}, \qquad \begin{array}{c|cc} \frac{1}{2}+\alpha & \frac{1}{2}+\alpha & 0 \\ \frac{1}{2}+\alpha & \frac{1}{2}+\alpha & 0 \\ \hline & \frac{1}{2}+\alpha & \frac{1}{2}-\alpha \end{array}. \tag{4.5}$$

We can see that this new α-PRK method is different from the previous method given in (4.2). For fixed α, it not only can preserve the symplecticity and quadratic invariants, but also can guarantee the numerical solutions to fall on the manifold $\mathcal{M}$. When we adjust α each step, the method can preserve energy and quadratic invariants, and also to guarantee the numerical solutions to fall on the manifold $\mathcal{M}$.

We write out the details of the α-Rattle method below for convenience:

$$\begin{cases} P_1 = p_0 + h(1/2+\alpha)\left(-H_q(P_1, Q_1) - G^T(Q_1)\Lambda_1\right), \\ P_2 = P_1, \\ Q_1 = q_0, \\ Q_2 = q_0 + h\left((\frac{1}{2}+\alpha)H_p(P_1, Q_1) + (\frac{1}{2}-\alpha)H_p(P_2, Q_2)\right), \\ g(Q_1) = g(Q_2) = 0, \end{cases} \tag{4.6}$$

The numerical solution (p_1, q_1) is then solved by

$$\begin{cases} q_1 = Q_2, \\ \ell_1 = -H_q(P_1, Q_1) - G^T(Q_1)\Lambda_1, \\ \ell_2 = -H_q(P_2, Q_2) - G^T(Q_2)\Lambda_2, \\ p_1 = p_0 + h\left((\frac{1}{2}+\alpha)\ell_1 + (\frac{1}{2}-\alpha)\ell_2\right), \\ 0 = G(q_1)H_p(p_1, q_1). \end{cases} \tag{4.7}$$

The system (4.6) can be reduced to that

$$\begin{cases} P = p_0 - h(1/2+\alpha)H_q(P, q_0) - hG^T(q_0)\lambda_1, \\ q_1 = q_0 + h\left((\frac{1}{2}+\alpha)H_p(P, q_0) + (\frac{1}{2}-\alpha)H_p(P, q_1)\right), \\ 0 = g(q_1), \end{cases} \tag{4.8}$$

where $\lambda_1 := (1/2+\alpha)\Lambda_1$. There are three unknowns in this system. Then, one can solve (p_1, λ_2) by

$$\begin{cases} p_1 = p_0 - h(\frac{1}{2}+\alpha)H_q(P, q_0) - h(\frac{1}{2}-\alpha)H_q(P, q_1) - hG^T(q_0)\lambda_1 - hG^T(q_1)\lambda_2, \\ 0 = G(q_1)H_p(p_1, q_1), \end{cases} \tag{4.9}$$

where $\lambda_2 := (1/2-\alpha)\Lambda_2$.

4.1.2. α-PRK III methods

We now construct the α-PRK III methods from Lobatto IIIA or IIIB methods. For unconstrained Hamiltonian systems, this method has been used by Sun [27] to construct symplectic PRK method. However, as we pointed out earlier, this method generally does not conserve the Hamiltonian energy. The general Runge-Kutta method with parameters (c, A, b) for non-autonomous equations $\dot{y} = f(t, y)$ is given by

$$\begin{aligned} y_1 &= y_0 + h\sum_{j=1}^{s} b_j f(t_0 + c_j h, k_j), \\ k_i &= y_0 + h\sum_{j=1}^{s} a_{ij} f(t_0 + c_j h, k_j), \quad i = 1, \ldots, s. \end{aligned}$$

The classical $B(p), C(\eta)$ and $D(\zeta)$ conditions for the RK method with parameters (c, A, b) are given by

$$\begin{aligned} B(p): &\quad \sum_{i=1}^{s} b_i c_i^{q-1} = \frac{1}{q} && q = 1, \ldots, p; \\ C(\eta): &\quad \sum_{j=1}^{s} a_{ij} c_j^{q-1} = \frac{c_i^q}{q} && i = 1, \ldots, s,\ q = 1, \ldots, \eta; \\ D(\zeta): &\quad \sum_{i=1}^{s} b_i c_i^{q-1} a_{ij} = \frac{b_j}{q}(1 - c_j^q) && i = 1, \ldots, s,\ q = 1, \ldots, \zeta. \end{aligned} \tag{4.10}$$

See [17, IV.5, pp71] for more details on the $B(p), C(\eta)$ and $D(\zeta)$ assumptions for RK methods.

Theorem 4.1 ([27]). *Suppose that an s-stage RK method (c, A, b) with distinct abscissae c_i and $b_i \neq 0$ satisfies $B(p), C(\eta)$ and $D(\zeta)$. Then the PRK method generated by $(c_i, a_{ij}, \hat{a}_{ij} = b_j(1 - \frac{a_{ji}}{b_i}), b_i)$ is symplectic and of order $q = \min(p, 2\eta + 2, 2\zeta + 2, \eta + \zeta + 1)$ for Hamiltonian systems.*

As a remark, the equations considered in this work are autonomous and the parameters c do not appear in the scheme. However, the conditions $B(p), C(\eta), D(\zeta)$ still make sense: one may find the parameters c from $C(\eta)$ condition and then require $B(p), D(\zeta)$ to hold.

Here we construct several specific parameterized α-PRK III methods for Hamiltonian systems with holonomic constraints. One method to parameterize the Lobatto IIIA or IIIB methods is to keep b being constant at first but to change a_{i2} in some suitable ways.

Taking $s = 3$, this strategy leads to the following 3-stage parameterized α-Lobatto IIIA–III$\widehat{A}$

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{5}{24} - \alpha & \frac{1}{3} - \alpha & 2\alpha - \frac{1}{24} \\ 1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}, \qquad \begin{array}{c|ccc} 0 & \frac{1}{6} & 4\alpha - \frac{1}{6} & 0 \\ \frac{1}{2} & \frac{1}{6} & \frac{1}{3} + \frac{2}{3}\alpha & 0 \\ 1 & \frac{1}{6} & \frac{5}{6} - 8\alpha & 0 \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}. \tag{4.11}$$

Or the 3-stage parameterized α-Lobatto III$\widehat{B}$-IIIB

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{5}{24} - \frac{\alpha}{2} & \frac{1}{3} + \alpha & -\frac{1}{24} - \frac{\alpha}{2} \\ 1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}, \qquad \begin{array}{c|ccc} 0 & \frac{1}{6} & 2\alpha - \frac{1}{6} & 0 \\ \frac{1}{2} & \frac{1}{6} & \frac{1}{3} - \alpha & 0 \\ 1 & \frac{1}{6} & \frac{5}{6} + 2\alpha & 0 \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}. \tag{4.12}$$

One can check that all the α-PRK III methods used in (4.11)-(4.12) satisfy that $B(2)$ and $C(1)$. Hence, those four α-PRK methods have second order accuracy according to Theorem 4.1. We can construct general s-stage α-PRK methods based on IIIA-IIIB methods in the same way. Note that those methods are different from the previous α-PRK based on W-transformation method given in (4.3). When $\alpha = 0$, all the α-PRK methods presented in (4.3), (4.11)-(4.12) are reduced to the classical Lobatto IIIA-IIIB pairs.

4.2. Energy and quadratic invariants preserving methods

As we can see from the above example, we can first parameterize the coefficients $b(\alpha), A(\alpha)$, and then determine the entire α-PRK method according to the conditions (4.1). This then gives some parametric PRK methods, based on which we can construct the desired energy preserving methods.

4.2.1. The general method and properties

With the parametric PRK methods, we propose the energy and quadratic invariants preserving α-PRK methods as follows:

Algorithm 4.1 (Energy and quadratic invariant preserving methods).

1: Choose a particular form of functions $b = b(\alpha)$, and $A = A(\alpha)$ such that there exists an interval $I \subset \mathbb{R}$ satisfying

- For all $1 \leq i \leq s$, $b_i(\alpha) \neq 0$ for all most all $\alpha \in I$; $\sum_i b_i(\alpha) = 1$.

- $a_{1j}(\alpha) = 0$, $a_{sj}(\alpha) = b_j(\alpha)$ for all $1 \le j \le s$ and all $\alpha \in I$.
- Determine $\widehat{b}$ and $\widehat{A}$ by relation (4.1).

2: Pick computational time $T > 0$; time step $h > 0$. Let $N = \lceil T/h \rceil$. Pick initial data (p_0, q_0).
3: **For** n in $1 : N$ **do**
Let $(p_n(\alpha), q_n(\alpha))$ be given by (2.1) with coefficients above and initial data (p_{n-1}, q_{n-1}).
Choose $\alpha^* \in I$ such that $H(p_1(\alpha^*), q_1(\alpha^*)) = H(p_0, q_0)$.
Let $(p_n, q_n) = (p_n(\alpha^*), q_n(\alpha^*))$.
EndFor

Remark 4.1. For the general s-stage ($s \ge 3$) RK methods, due to the increase of degrees of freedom, the parameterization methods is not unique, and there may be many other methods.

We now explore the properties of the new methods.

Theorem 4.2. *If the method in Algorithm* 4.1 *has a solution, then the energy* $H(p_n, q_n)$ *is a constant. Moreover, for all the quadratic invariant* $q_n^T D p_n$ *is also a constant.*

Proof. The energy constant is obvious by the method. For the quadratic invariant, we note that Theorem 3.1 tells us that for any α, $q_n^T(\alpha) D p_n(\alpha) = q_0 D p_0$. Hence, the claims follow. We skip the details. □

Here, as that for parametric RK methods for unconstrained Hamiltonian systems, let us point out the difference between the conservation of quadratic invariants and symplecticity regarding parametric PRK methods. As we have seen, for PRK methods with fixed coefficients, (4.1) guarantees the symplecticity and conservation of quadratic invariants. In fact, for the classical Hamiltonian system, as we remarked in footnote 1, for an irreducible RK method with fixed coefficients, the sufficient and necessary condition of symplecticity and quadratic invariants-preserving is given by the same requirement $b_i a_{i,j} + b_j a_{j,i} = b_i b_j, i, j = 1, 2, ..., s$. Now, if we apply the method for all initial data (p_0, q_0) (all trajectories), the method given by Theorem 4.2 may not be symplectic although (4.1) is satisfied. The reason is that the coefficients in the method depend on the initial data now, and thus $dp_n \wedge dq_n$ may not be equal to $dp_0 \wedge dq_0$. Compared to the fact that symplecticity involves the differential of numerical solutions, the quadratic invariants depend only on the values of the numerical solutions. The conservation of quadratic invariants still holds by relations (4.1). Based on the discussion here, our method can be applied in two possible cases.

- We apply the method for all trajectories so that the energy and quadratic invariants are preserved for all trajectories. However, the method may not be symplectic though.
- We fix down the coefficients obtained by a particular trajectory. Then, the method is symplectic, preserves the quadratic invariants, and preserves the energy for the chosen trajectory.

4.2.2. Existence of the numerical solutions and order of the methods

The methods in Algorithm 4.1 depend crucially on the solvability of

$$\mu(\alpha, h) := H(p_1(\alpha, h), q_1(\alpha, h)) - H(p_0, q_0) = 0, \tag{4.13}$$

for small enough $h > 0$ and some given consistent initial values $(p_0, q_0) \in \mathcal{Q} \times \mathcal{Q}$. Clearly, $\mu(\alpha, h)$ is the error measuring the error for energy. As $h \to 0^+$, $\mu(\alpha, h) \to 0$ for all α. We assume the order of the energy satisfies the following.

Assumption 4.1. We assume the method for $\alpha = 0$ is a special base method that satisfies the following.

1. $\mu(\alpha, h)$ is analytic in a neighborhood of $(0, 0)$.
2. The order of energy approximation is higher for $\alpha = 0$ than other α values near 0. In other words, there exist r, r_1 with $r \geq r_1 > 1$ such that

$$\lim_{h\to 0^+} \frac{1}{h^r}\mu(0, h) \neq 0, \qquad \lim_{h\to 0^+} \frac{1}{h^{r_1}}\mu(\alpha, h) \neq 0. \tag{4.14}$$

Remark 4.2. To understand the second item in Assumption 4.1, we note that

$$\mu(\alpha, h) = H(p_1(\alpha, h), q_1(\alpha, h)) - H(p(h), q(h)),$$

where $(p(t), q(t))$ is the exact solution of the Hamiltonian system with initial data (p_0, q_0). Hence, μ is in fact the numerical error of the energy for the scheme. The second item in Assumption 4.1 is the convergence order of the energy, which is often $O(h^{\beta+1})$ if the method has a convergence order β. In other words, equation (4.14) implies that the order of energy for $\alpha = 0$ is $r - 1$ while the order of energy for α near 0 is $r_1 - 1$.

By the analyticity, one has in a neighborhood of $(0, 0)$ that

$$\mu(\alpha, h) = \sum_{\ell\geq 0, m>1} c_{\ell,m}\alpha^\ell h^m.$$

Since μ cannot be identically zero, there must some ℓ, m such that $c_{\ell,m} \neq 0$. Hence, there always exists some $r(\alpha) > 0$ such that $\lim_{h\to 0^+} \mu(\alpha, h)/h^{r(\alpha)}$ exists and is nonzero. Hence, the second item in Assumption 4.1 implies that

$$\mu(\alpha, h) = \left[c_{0,r}h^r + \sum_{m>r} c_{0,m}h^m\right] + c_{kr_1}\alpha^k h^{r_1} + \cdots, \qquad k > 0, r \geq r_1 > 1. \tag{4.15}$$

We further assume that the dependence in α is not degenerate, and without los of generalization in (4.15) for $k = 1$. If $k \neq 1$, we may set $\tilde{\alpha} = \alpha^k$. Of course, in terms of $(\tilde{\alpha}, h)$, the analyticity of μ may break down. However, as soon as μ is C^1 in $\tilde{\alpha}$ and h, the claim below still holds. Provided $k = 1$, we can prove that the method can give a sequence of numerical solutions, as below.

Theorem 4.3. *Suppose Assumption* 4.1 *holds and r, r_1 are the numbers as in Assumption* 4.1. *If it holds that*

$$\lim_{h\to 0^+} \frac{1}{h^{r_1}}\frac{\partial\mu}{\partial\alpha}(0, 0) \neq 0, \tag{4.16}$$

then the equation (4.13) *has a solution* α^* *for* h *sufficiently small, and this solution can be written as*

$$\alpha^*(h) = \eta(h)h^{r-r_1} \tag{4.17}$$

for some smooth function $\eta(\cdot)$*, with* $\lim_{h\to 0^+}\eta(h) \neq 0$*.*

Proof. The proof can be done by the implicit function theorem, following similar approach as in [8]. Define a new variable $\eta = h^{-(r-r_1)}\alpha$. Then,

$$\tilde{\mu}(\eta, h) = h^{-r}\mu(h^{(r-r_1)}\eta, h).$$

By the assumptions, $\tilde{\mu}$ is analytic in a neighborhood of $(0, 0)$. Moreover, it follows from (4.16) that $\frac{\partial\tilde{\mu}}{\partial\eta}(0, 0) \neq 0$. Clearly, $\tilde{\mu} = 0$ implies $\mu = 0$. By implicit function theorem, $\tilde{\mu} = 0$ implicitly defines a smooth function $\eta = \eta(h)$ for $h \in J$, where J is a small interval containing 0. By Assumption 4.1, it is not hard to see (depending on $c_{0,r}$ and c_{1,r_1} in (4.15)) $\eta(0) \neq 0$. The claims then follow if we define $\alpha^* = h^{r-r_1}\eta$.

With the relation $\alpha^* = \eta(h)h^{r-r_1}$, the convergence order of the method given in Algorithm 4.1 is in fact the same as that for $\alpha = 0$. This means that the order of convergence can be preserved. We in fact have the following claim.

Corollary 4.1. *Suppose that for all* $\alpha \neq 0$ *near* 0*, the order of PRK is* $r_1 - 1$ *and that the order of PRK scheme for* $\alpha = 0$ *is* $r - 1$*. If the conditions in Theorem* 4.3 *hold, then the order of convergence for the method given in Algorithm* 1 *is equal to* $r - 1$*.*

Proof. By the assumptions,

$$\|p_1(\alpha, h) - p(h)\| = \eta_1(\alpha, h)h^{r_1}, \qquad \|q_1(\alpha, h) - q(h)\| = \eta_2(\alpha, h)h^{r_1},$$

where $(p(h), q(h))$ are the exact solutions for the Hamiltonian system with initial data (p_0, q_0). Here, $\eta_1(\alpha, h)$ and $\eta_2(\alpha, h)$ are bounded smooth functions. Then, it is easy to see $|\eta_i(\alpha, h) - \eta_i(0, h)| \leq C|\alpha|$ for $i = 1, 2$. Hence, with $\alpha = \alpha^*$,

$$\|p_1(\alpha, h) - p_1(0, h)\| \leq Ch^{r_1}h^{r-r_1} = Ch^r.$$

The same is true for q_1. By the assumption on the accuracy for $\alpha = 0$, the claim follows. □

As a direct application of the Theorem 4.3 and Corollary 4.1, we in the next try to find more explicit conditions corresponding to the condition in Theorem 4.3 to hold (namely $\lim_{h\to 0^+} h^{-r_1}\partial_\alpha\mu \neq 0$) and determine r_1 for the α-Rattle algorithm described in section 4.1.1. We first of all assume the following.

Assumption 4.2. *The matrix* $G(q)$ *is of rank* m *for all* q*, and* $H_{pp}(p, q)$ *is invertible for all* (p, q)*.*

Clearly, the first is reasonable as we assume the m holonomic constraints are independent. Below, we perform the discussion with Assumption 4.2. Motivated by the condition in Theorem 4.3, we define the operator

$$\mathcal{D}_s f := \lim_{h\to 0^+}\Big[h^{-s}\partial_\alpha f(\alpha, h)|_{\alpha=0}\Big]. \tag{4.18}$$

Since $\lim_{h\to 0^+} p_1(0,h) = p_0$ and $\lim_{h\to 0^+} q_1(0,h) = q_0$, one has for $s \geq 1$ that

$$\mathcal{D}_s\mu = (\mathcal{D}_s p_1)\cdot H_p(p_0,q_0) + (\mathcal{D}_s q_1)\cdot H_q(p_0,q_0). \tag{4.19}$$

Now, we aim to find the minimum s such that $\mathcal{D}_s\mu \neq 0$. First consider $s = 1$. By (4.8) and $P(0,h) \to p_0$, one has $\mathcal{D}_1 P = -H_q(p_0,q_0) - \frac{1}{2}(\mathcal{D}_0 P)\cdot H_{pq}(p_0,q_0) - G^T(q_0)\cdot \mathcal{D}_0\lambda_1$. Clearly, $\mathcal{D}_0 P = 0$. Hence, $\mathcal{D}_1 P = -H_q(p_0,q_0) - G^T(q_0)\cdot\mathcal{D}_0\lambda_1$. In a similar fashion,

$$\begin{aligned}
\mathcal{D}_1 q_1 &= H_p(p_0,q_0) - H_p(p_0,q_0) + \frac{1}{2}[\mathcal{D}_0 P\cdot H_{pp}(p_0,q_0) + \mathcal{D}_0 P H_{pp}(p_0,q_0) + \mathcal{D}_0 q_1 H_{qp}(p_0,q_0)] = 0,\\
\mathcal{D}_1 p_1 &= [-H_q(p_0,q_0) + H_q(p_0,q_0)] - G^T(q_0)\mathcal{D}_0(\lambda_1+\lambda_2) - \mathcal{D}_0 q_1\cdot\nabla_{qq}g(q_0)\cdot\lim_{h\to 0^+}\lambda_2(0,h)\\
&= -G^T(q_0)\mathcal{D}_0(\lambda_1+\lambda_2).
\end{aligned}$$

By the constraint of p_1 in (4.9), $0 = \mathcal{D}_1 q_1 \otimes H_p(p_0,q_0) : \nabla^2 g(q_0) + G(q_0)\cdot[\mathcal{D}_1 p_1\cdot H_{pp}(p_0,q_0)] = G(q_0)\cdot[\mathcal{D}_1 p_1\cdot H_{pp}(p_0,q_0)]$. This means $0 = G(q_0)H_{pp}(p_0,q_0)G^T(q_0)\mathcal{D}_0(\lambda_1+\lambda_2)$. Since the m constraints are independent and H_{pp} is invertible, $GH_{pp}G^T$ is invertible and thus $\mathcal{D}_0(\lambda_1+\lambda_2) = 0$. Hence, $\mathcal{D}_1 p_1 = 0$.

Now, we move to $s = 2$. By the q_1 equation in (4.8),

$$\begin{aligned}
\mathcal{D}_2 q_1 &= \lim_{h\to 0^+} h^{-1}[H_p(P,q_0) - H_p(P,q_1)] + \mathcal{D}_1 P\cdot H_{pp}(p_0,q_0) + \frac{1}{2}\mathcal{D}_1 q_1\cdot H_{qp}(p_0,q_0)\\
&= -H_p(p_0,q_0)\cdot H_{qp}(p_0,q_0) - [H_q(p_0,q_0) + G^T(q_0)\cdot\mathcal{D}_0\lambda_1]\cdot H_{pp}(p_0,q_0).
\end{aligned}$$

By the constraint in (4.8), one has $G(q_0)\mathcal{D}_2 q_1 = 0$. Using this, one can determine $\mathcal{D}_0\lambda_1 = -\mathcal{D}_0\lambda_2$. Similarly, we have

$$\begin{aligned}
\mathcal{D}_2 p_1 =& \lim_{h\to 0^+} h^{-1}(H_q(P,q_1) - H_q(P,q_0)) - \mathcal{D}_1 P\cdot H_{pq}(p_0,q_0) - \frac{1}{2}\mathcal{D}_1 q_1\cdot H_{qq}\\
&- G^T(q_0)\mathcal{D}_1[\lambda_1+\lambda_2] - \mathcal{D}_1 q_1\cdot\nabla_2 g(q_0)\cdot\lim_{h\to 0^+}\lambda_2\\
=& H_p(p_0,q_0)\cdot H_{qq}(p_0,q_0) + [H_q(p_0,q_0) + G^T(q_0)\mathcal{D}_0\lambda_1]\cdot H_{pq}(p_0,q_0) - G^T(q_0)\mathcal{D}_1[\lambda_1+\lambda_2].
\end{aligned}$$

Moreover, By the constraint of p_1 in (4.9), we have

$$0 = H_p(p_0,q_0)\otimes\mathcal{D}_2 q_1 : \nabla_{qq}g(q_0) + (\mathcal{D}_2 p_1\cdot H_{pp}(p_0,q_0) + \mathcal{D}_2 q_1\cdot H_{qp}(p_0,q_0))\cdot\nabla_q g(q_0).$$

With this, one can determine $\mathcal{D}_1(\lambda_1+\lambda_2)$. Hence, we can find that

$$\mathcal{D}_2\mu = H_p\otimes H_p : H_{qq} - H_q\otimes H_q : H_{pp} + R, \tag{4.20}$$

where $R := [G^T\mathcal{D}_0\lambda_1]\otimes H_p : H_{pq} - H_p G^T\mathcal{D}_1[\lambda_1+\lambda_2] - [G^T\mathcal{D}_0\lambda_1]\otimes H_q : H_{pp}$. Every term in R involves G, while the first two terms in $\mathcal{D}_2\mu$ do not depend on G. Hence, $\mathcal{D}_2\mu \neq 0$ for all most all (p,q). It is possible that at some special points, this can be zero.

Remark 4.3. For a more straightforward derivation, one may take derivatives on α in (4.8)-(4.9) and then expand the quantities like $\partial_\alpha P, \partial_\alpha p_1$ etc in terms of powers of h. Then compare the coefficients, one can derive the same formulas.

To summarize, we expect that for almost all (p_0,q_0), $\lim_{h\to 0^+}\frac{1}{h^2}\frac{\partial\mu(0,h)}{\partial\alpha} \neq 0$. This coincides with the fact the method for $\alpha \neq 0$ is first order. Hence, the method should be second order by Corollary 4.1. We know the order of convergence for $\alpha = 0$ is two or $r = 3$. Hence, mostly, we will have $\alpha^* = O(h)$. It could be possible that at some special points, $\lim_{h\to 0^+}\frac{1}{h^2}\frac{\partial\mu(0,h)}{\partial\alpha} = 0$. For these points, there could still be solutions for α^* but one may have larger $\alpha^* \gg h$, as we need to look into higher orders.

5. Numerical Experiments

In this section, we present numerical examples to verify our theoretical findings. We verify that the method constructed in this paper can accurately conserve the quadratic invariants and manifold constraints of the system, and at the same time, the appropriate parameters α^* can be selected to make the system energy conservation at each step. As far as we know, this is the first time that there is a numerical method for a constrained Hamiltonian systems that can hold all three quantities at once. We will also verify the order of convergence of the parameterized method and prove that the parameter perturbation will not decrease the order of convergence of the numerical solutions. All the experiments in this paper are implemented using Julia with Version 1.4.2 and Packages: NLsolve v4.4.0.

5.1. Spherical pendulum

Consider the spherical pendulum with Hamiltonian $H(p,q) = \frac{1}{2}(p_1^2 + p_2^2 + p_3^2) + q_3$ and constraint $g(q) = (q_1^2 + q_2^2 + q_3^2) - 1$, so that

$$H_p(p,q) = \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}, \; H_q(p,q) = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \; G^T(q) = 2 \begin{bmatrix} q_1 \\ q_2 \\ q_3 \end{bmatrix}. \tag{5.1}$$

For this example, the Lagrangian

$$L(Q, \dot{Q}) = \frac{1}{2}|\dot{Q}|^2 - Q_3,$$

is invariant under rotations about z axis. In particular, taking D_1 to be a 2×2 anti-symmetric matrix and setting

$$D := \begin{bmatrix} D_1 & 0 \\ 0 & 0 \end{bmatrix}. \tag{5.2}$$

Then, using $D^T = -D$, and $(e^{sD}v)_3 = v_3$, it can be verified easily that

$$g(e^{sD}q) = q^T e^{sD^T} e^{sD} q - 1 = q^T q - 1 = 0, \quad L(e^{sD}\dot{q}, e^{sD}q) = \frac{1}{2}|e^{sD}\dot{q}|^2 - (e^{sD}q)_3 = L(\dot{q}, q).$$

Hence, the quantity $I(p,q) = q^T Dp$ is invariant under this Hamiltonian dynamics by Lemma 3.2. In particular, this implies that the third component of the angular momentum $L(p,q) = q \times p$ is conservative. Physically, the forces (force due to the constraint which points along the radius of the sphere, the gravity), q and z-axis are coplanar, so z-component of the torque is zero. Thus, the z-component of the angular moment is conserved. We will verify through numerical experiments in this example that the parameterized method we constructed can preserve both the Hamilton function and L_3.

We take the initial value $q_0 = (0, \sin(0.1), -\cos(0.1)), p_0 = (0.06, 0, 0)$ for the simulations. In Fig. 5.2, we present the third component of the angular momentum $L(p,q)$. From which we can see that both the standard Rattle and Lobatto IIIA-IIIB methods and the parameterized methods constructed in this paper can preserve this quadratic invariants to machine precision, that is up to 10^{-16}.

In Fig. 5.3, we show the results for the chosen parameters α and computed Hamiltonians for the α-Rattle in (4.8)-(4.9) and α-PRK III method in (4.11). Clearly, the standard symplectic

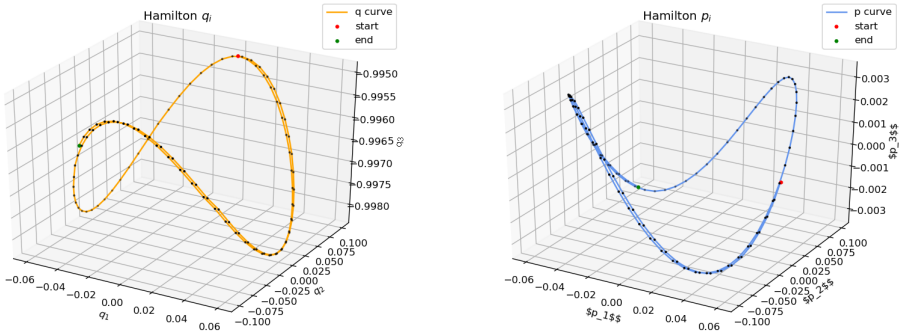


Fig. 5.1. Numerical solutions.

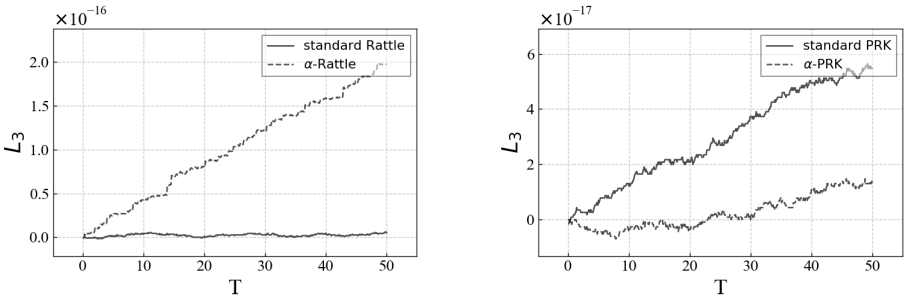
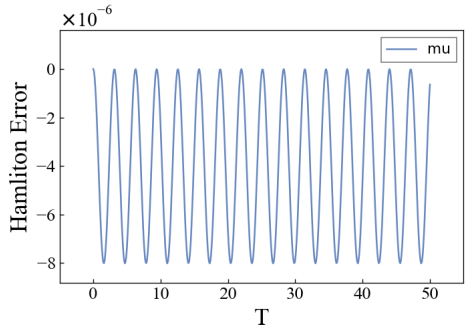


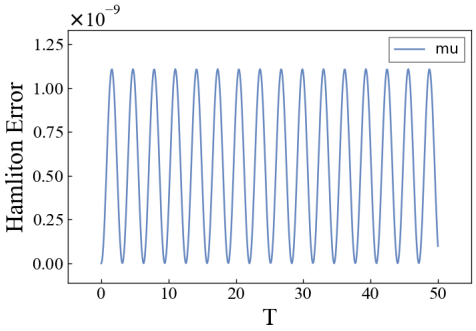
Fig. 5.2. The errors in the third component of the angular momentum for standard Rattle and Lobatto IIIA-IIB methods and the α-Rattle and α-PRK III methods.

methods (i.e. Rattle and Lobatto IIIA-IIIB methods) have energy error range from 10^{-9} to 10^{-6}, while the parameterized symplectic methods can make the energy conservation in the sense of that the energy error reach the machine accuracy. At each step, we can find parameters $\alpha^* = \alpha(h, y_n)$ that achieve energy conservation. We can see from (c) in Fig. 5.3 that the parameter is small in most cases for α-Rattle method, but it may take a slightly larger value at a very few points, and such an exceptional points may lower the order of the parameterized methods.

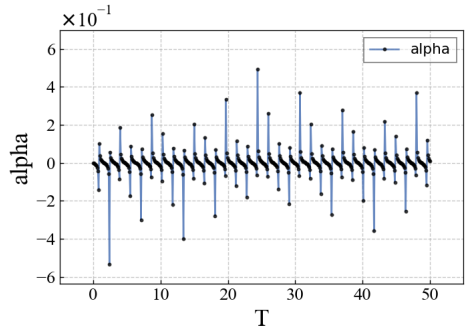
In Tables 5.1 and 5.2 we give the specific order of convergence for the α-Rattle method. We can see that the order of the numerical solutions shown in Table 5.1 is completely consistent with the standard algorithm of second order when computed on $[0, 0.5]$, while the order shown in Table 5.2 is slightly reduced when we computed on $[0, 1]$. We found that there is some α that is big as shown in Fig. 5.3 (c) between $t = 0.5$ and $t = 1$, and this seems to reduce the computational accuracy as commented above. We are not clear with the deeper reason for this. Maybe, the conditions in Theorem 4.3 was violated at some point, or maybe the nonlinear system was not solved with high accuracy as commented below in Remark 5.1. For the 3-stage α-PRK method, we can see from (e) in Fig. 5.3 that the parameter is uniform small, about $O(10^{-5})$. As shown in Table 5.3, the convergence order of α-PRK III method is preserved exactly as the standard 3-stage PRK method, i.e., forth order.



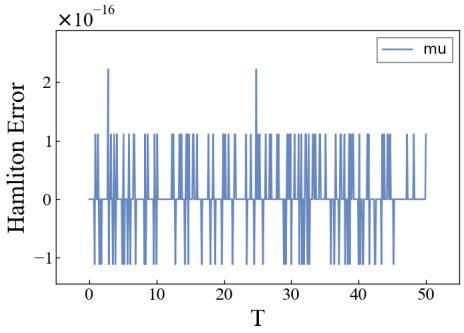
(a) Energy errors for standard Rattle method.



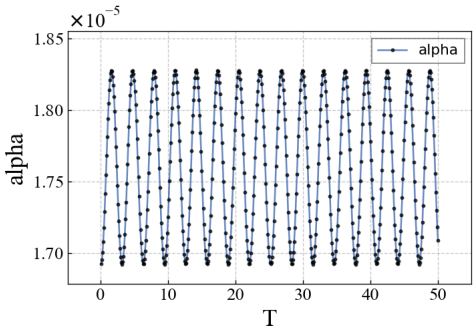
(b) Energy errors for standard Lobatto IIIA-IIIB method.



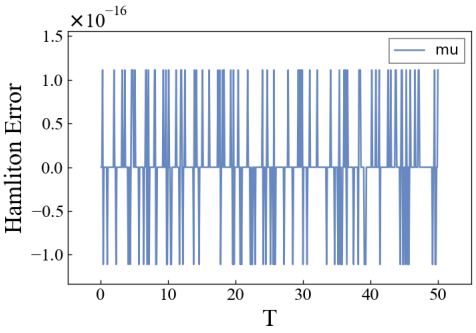
(c) α^* for α-Rattle method.



(d) Energy errors for α-Rattle method.



(e) α^* for α-PRK III method.



(f) Energy errors for α-PRK III method.

Fig. 5.3. α^* and energy errors with $h = 0.1$.

Remark 5.1. In the specific implementation of the parameterized methods presented in this article, it is very important to accurately solve the corresponding nonlinear system of equations like (4.6)-(4.8). For example, most of the nonlinear equations solvers have an accuracy from $O(10^{-8})$ to $O(10^{-12})$, which cannot reach the machine accuracy, so it is possible that the solution accuracy of the nonlinear system is not enough, which leads to the same energy error range from $O(10^{-8})$ to $O(10^{-12})$, and the searched parameters α^* might not be very good. One may try to improve the accuracy of nonlinear equations by giving a good initial value during the

Table 5.1: The errors e_p, e_q and the orders at $T = 0.5$ for the α-Rattle method for Example 1.

h	e_p	order	e_q	order
0.25	3.3643e-4	-	3.5220e-4	-
0.125	8.6813e-5	1.9543	8.9671e-5	1.9737
0.0625	2.1895e-5	1.9872	2.2535e-5	1.9924
0.03125	5.4863e-6	1.9967	5.6416e-6	1.9980
0.015625	1.7323e-6	1.9992	1.4108e-6	1.9995

Table 5.2: The errors e_p, e_q and the orders at $T = 1$ for the α-Rattle method for Example 1.

h	e_p	order	e_q	order
0.1	1.1216e-4	-	1.0774e-4	-
0.05	4.5419e-5	1.3042	4.8323e-5	1.1569
0.025	1.5315e-5	1.5683	2.0176e-5	1.2600
0.0125	1.6383e-6	3.2247	1.5628e-6	3.6905
0.00625	5.7032e-7	1.5226	5.9045e-7	1.4043

Table 5.3: The errors e_p, e_q and the orders at $T = 1$ for the α-PRK III method for Example 1.

h	e_p	order	e_q	order
0.25	4.0025e-7	-	4.7611e-7	-
0.125	2.5089e-8	3.9957	2.9843e-8	3.9958
0.0625	1.5692e-9	3.9989	1.8665e-9	3.9989
0.03125	9.8091e-11	3.9998	1.1666e-10	3.9998
0.015625	5.9634e-12	4.0399	6.9571e-12	4.0677

iteration. For example, use the numerical results of the standard PRK methods as the initial value in the iteration of the nonlinear equations for the corresponding parameterized methods. For future work, one may introduce some correction field or augmented variables to make the nonlinear system more stable to solve.

5.2. Satellites system

We consider a closed-loop rotating triangular tethered satellites system, consisting of three satellites (considered as mass-points) of masses $m_i, i = 1, 2, 3$, joined by inextensible, tight, and massless tethers, of lengths $L_i, i = 1, 2, 3$, respectively. For sake of simplicity, we assume unit masses and lengths, and normalize the gravity constant. Consequently, if $q_i := (x_i, y_i, z_i)^T \in \mathbb{R}^3, i = 1, 2, 3$, are the positions of the three satellites, the constraints $0 = g(q)$ are given by

$$\begin{cases} g_1(q) = (q_1 - q_2)^T(q_1 - q_2) - 1 = 0, \\ g_2(q) = (q_2 - q_3)^T(q_2 - q_3) - 1 = 0, \\ g_3(q) = (q_3 - q_1)^T(q_3 - q_1) - 1 = 0. \end{cases} \tag{5.3}$$

The Hamiltonian is specified by $H(p, q) = \sum_{i=1}^{3} \left(\frac{1}{2} p_i^T p_i - \frac{1}{\sqrt{q_i^T q_i}} \right)$. Hence, we have that

$$H_p = p = \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}, \qquad H_q = f(q) := \begin{bmatrix} (q_1^T q_1)^{-\frac{3}{2}} q_1 \\ (q_2^T q_2)^{-\frac{3}{2}} q_2 \\ (q_3^T q_3)^{-\frac{3}{2}} q_3 \end{bmatrix},$$

$$G^T(q) = 2\begin{bmatrix} q_1 - q_2 & 0 & q_1 - q_3 \\ q_2 - q_1 & q_2 - q_3 & 0 \\ 0 & q_3 - q_2 & q_3 - q_1 \end{bmatrix}. \tag{5.4}$$

For the simulation, we choose the consistent initial values given by

$$q_1(0) = \begin{bmatrix} 0 \\ \frac{1}{2} \\ z_0 \end{bmatrix}, \quad q_2(0) = \begin{bmatrix} 0 \\ -\frac{1}{2} \\ z_0 \end{bmatrix}, \quad q_3(0) = \begin{bmatrix} 0 \\ 0 \\ z_0 - \frac{\sqrt{3}}{2} \end{bmatrix},$$

$$p_1(0) = p_2(0) = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \quad p_3(0) = \begin{bmatrix} v_0 \\ 0 \\ 0 \end{bmatrix}.$$

where $z_0 = 20$ and v_0 is such that the initial Hamiltonian is zero. This provides a configuration in which the first two satellites remain parallel to each other, moving in the planes $y = 1/2$ and $y = -1/2$, respectively, and the third one moves around the tether joining the first two, in the plane $y = 0$.

Table 5.4: The errors e_p, $e_q$and the orders at $T = 1$ for the α-Rattle method for Example 2.

h	e_p	order	e_q	order
0.25	1.2290e-3	-	1.9300e-3	-
0.125	3.0460e-4	2.0125	4.7835e-4	2.1247
0.0625	7.59745e-5	2.0033	1.1931e-4	2.0033
0.03125	1.8968e-5	2.0018	2.9789e-5	2.0018
0.015625	4.7270e-6	2.0046	7.4235e-6	2.0046

Table 5.5: The errors e_p, $e_q$and the orders at $T = 1$ for the α-PRK III method for Example 2.

h	e_p	order	e_q	order
0.25	1.2299e-6	-	1.9307e-6	-
0.125	7.1884e-8	4.0967	1.1284e-7	4.0967
0.0625	3.0717e-9	4.5485	4.8219e-9	4.5485
0.03125	9.7230e-11	4.9815	1.5263e-10	4.9815
0.015625	6.4283e-12	3.9188	1.0091e-11	3.9188

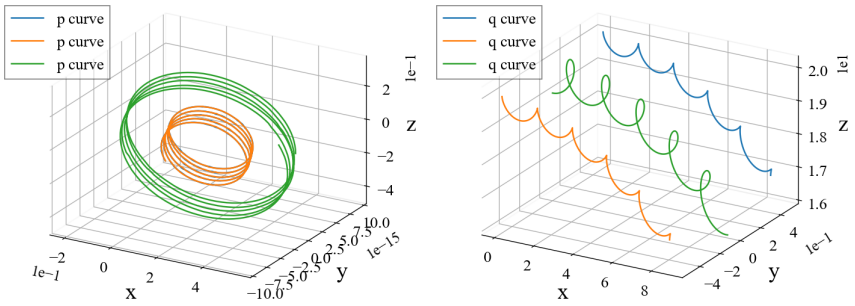
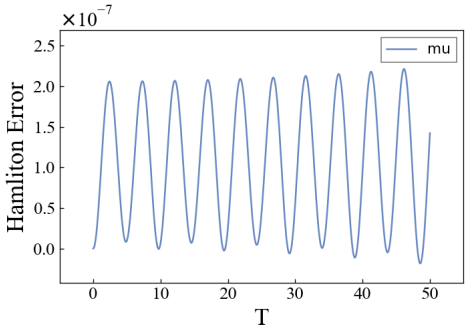
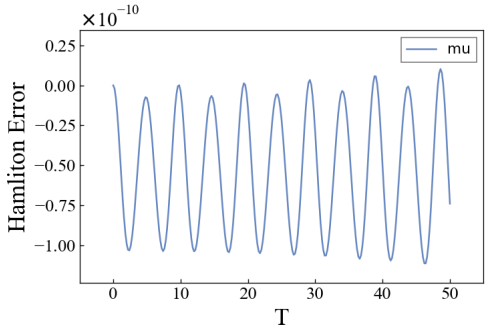


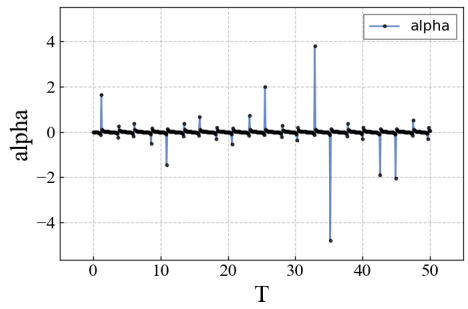
Fig. 5.4. Numerical solutions obtained by α-Rattle method with $h = 0.1$ for Example 2.



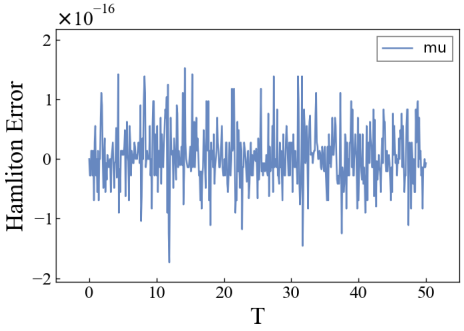
(a) Energy errors for Rattle method with $h = 0.1$.



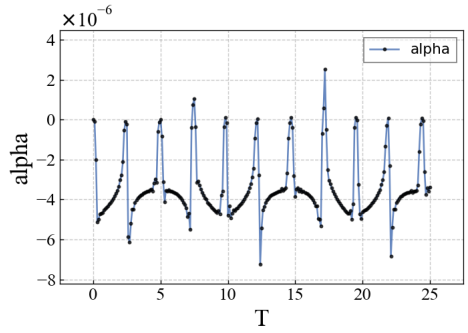
(b) Energy errors for Lobatto IIIA-IIIB method with $h = 0.2$.



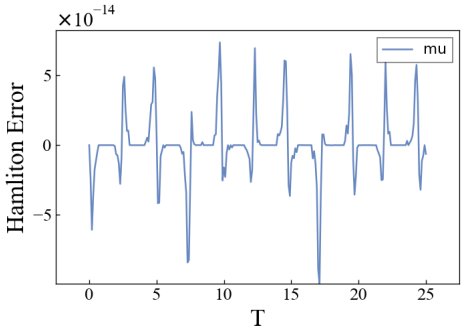
(c) α^* for α-Rattle method with $h = 0.1$.



(d) Energy errors for α-Rattle method with $h = 0.1$.



(e) α^* for α-PRK III method with $h = 0.2$.



(f) Energy errors forα-PRK III method with $h = 0.2$.

Fig. 5.5. α^* and energy errors for Example 2.

For this more complex example, our numerical results are similar to the first example. The numerical results for Example 2 are plotted in Fig. 5.4 and Fig. 5.5. The standard symplectic PRK methods have energy errors, but the parameterized methods can preserves energy to machine accuracy. At each step, we can find the parameter values that make the energy conserved. Meanwhile, as shown in Tables 5.4 and 5.5, the order of convergence of the two parameterized methods can be completely consistent with the standard methods. By comparison, it is found that α-PRK III methods are often superior to the α-Rattle method, and the parameter values of α-PRK III methods are usually uniformly small, while α-Rattle method may have a few points with large α^* values.

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