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Discrete Hamiltonian variational integrators

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We derive a variational characterization of the exact discrete Hamiltonian, which is a Type II generating function for the exact flow of a Hamiltonian system, by considering a Legendre transformation of Jacobi's solution of the Hamilton–Jacobi equation. This provides an exact correspondence between continuous and discrete Hamiltonian mechanics, which arise from the continuous- and discrete-time Hamilton's variational principle on phase space, respectively. The variational characterization of the exact discrete Hamiltonian naturally leads to a class of generalized Galerkin Hamiltonian variational integrators that includes the symplectic partitioned Runge–Kutta methods. This extends the framework of variational integrators to Hamiltonian systems with degenerate Hamiltonians, for which the standard theory of Lagrangian variational integrators cannot be applied. We also characterize the group invariance properties of discrete Hamiltonians that lead to a discrete Noether's theorem.

Keywords: geometric numerical integration; geometric mechanics; symplectic integrators; variational integrators; Hamiltonian mechanics.

1. Introduction

1.1 *Discrete mechanics*

Discrete-time analogues of Lagrangian and Hamiltonian mechanics, which are derived from discrete variational principles, yield a class of geometric numerical integrators (Hairer *et al.*, 2006) referred to as variational integrators (Marsden & West, 2001; Lall & West, 2006). The discrete variational approach to constructing numerical integrators is of interest as they automatically yield methods that are symplectic, and, by a backward error analysis, exhibit bounded energy errors for exponentially long times (see, for example, Hairer, 1994). When the discrete Lagrangian or Hamiltonian is group invariant, they will yield numerical methods that are momentum preserving.

Discrete Hamiltonian mechanics can be derived from discrete Lagrangian mechanics by relaxing the discrete second-order curve condition. The dual formulation of this constrained optimization problem yields discrete Hamiltonian mechanics (Lall & West, 2006). Alternatively, the second-order curve condition can be imposed using Lagrange multipliers, and this corresponds to the discrete Hamilton–Pontryagin principle (Leok & Ohsawa, 2008).

In contrast to the prior literature on discrete Hamiltonian mechanics, which typically start from the Lagrangian setting, we will focus on constructing Hamiltonian variational integrators from the Hamiltonian point of view, without recourse to the Lagrangian formulation. When the Hamiltonian is hyperregular, it is possible to obtain the corresponding Lagrangian function, adopt the Galerkin construction of Lagrangian variational integrators to obtain a discrete Lagrangian and then perform a discrete Legendre transformation to obtain a discrete Hamiltonian. This is described in the following diagram.

$$\begin{array}{ccc} H(q,p) & \xrightarrow{\quad \mathbb{F}H \quad} & L(q,\dot{q}) \\ \Big\downarrow & & \Big\downarrow \\ H_d^+(q_0,p_1) & \xleftarrow[\quad \mathbb{F}L_d \quad]{} & L_d(q_0,q_1) \end{array}$$

The goal of this paper is to directly express the discrete Hamiltonian in terms of the continuous Hamiltonian, so that the diagram above commutes when the Hamiltonian is hyperregular. An added benefit is that such an approach would remain valid even if the Hamiltonian is degenerate, as is the case for point vortices (see Newton, 2001, p. 22), and no corresponding Lagrangian formulation exists.

The Galerkin construction for Lagrangian variational integrators is attractive since it provides a general framework for constructing a large class of symplectic methods based on suitable choices of finite-dimensional approximation spaces and numerical quadrature formulas. Our approach allows one to apply the Galerkin construction of variational integrators to Hamiltonian systems directly and may potentially generalize to variational integrators for multisymplectic Hamiltonian partial differential equations (PDEs) (Marsden *et al.*, 1999; Bridges & Reich, 2001; Lew *et al.*, 2003).

Discrete Lagrangian mechanics is expressed in terms of a discrete Lagrangian, which can be viewed as a Type I generating function of a symplectic map, and discrete Hamiltonian mechanics is naturally expressed in terms of discrete Hamiltonians (Lall & West, 2006), which are either Type II or III generating functions. The discrete Hamiltonian perspective allows one to avoid some of the technical difficulties associated with the singularity associated with Type I generating functions at time $t = 0$ (see Marsden, 1992, p. 177).

EXAMPLE 1.1. To illustrate the difficulties associated with degenerate Hamiltonians consider

$$H(q, p) = qp,$$

with the Legendre transformation given by $\mathbb{F}H\colon T^*Q \to TQ$, $(q, p) \mapsto (q, \partial H/\partial p) = (q, q)$. Clearly, in this situation, the Legendre transformation is not invertible. Furthermore, the associated Lagrangian is identically zero, that is, $L(q, \dot{q}) = p\dot{q} - H(q, p)|_{\dot{q}=\partial H/\partial p} = p\dot{q} - qp|_{\dot{q}=q} \equiv 0$.

The associated Hamilton's equations are given by $\dot{q} = \partial H/\partial p = q$ and $\dot{p} = -\partial H/\partial q = -p$, with exact solution $q(t) = q(0)\exp(t)$ and $p(t) = p(0)\exp(-t)$. This exact solution is, in general, incompatible with the (q_0, q_1) boundary conditions associated with Type I generating functions, but it is compatible with the (q_0, p_1) boundary conditions associated with Type II generating functions.

In view of this example, our discussion of discrete Hamiltonian mechanics will be expressed directly in terms of continuous Hamiltonians and Type II generating functions.

1.2 *Main results*

We provide a characterization of the Type II generating function that generates the exact flow of Hamilton's equations and derive the corresponding Type II Hamilton–Jacobi equation that it satisfies. By considering a discrete Type II Hamilton's variational principle in phase space, we derive the discrete Hamilton's equations in terms of a discrete Hamiltonian. We provide a variational characterization of the exact discrete Hamiltonian that, when substituted into the discrete Hamilton's equations, generates samples of the exact continuous solution of Hamilton's equations. Also, we introduce a discrete Type II Hamilton–Jacobi equation.

From the variational characterization of the exact discrete Hamiltonian, we introduce a generalized Galerkin approximation from both the Hamiltonian and the Lagrangian viewpoints and show that they are equivalent when the Hamiltonian is hyperregular. In addition, we provide a systematic means of implementing these methods as symplectic-partitioned Runge–Kutta (SPRK) methods. We also establish the invariance properties of the discrete Hamiltonian that yield a discrete Noether's theorem. Galerkin discrete Hamiltonians derived from group-invariant interpolatory functions satisfy these invariance properties and therefore preserve momentum.

1.3 *Outline of the paper*

In Section 2 we present the Type II analogues of Hamilton's phase space variational principle and the Hamilton–Jacobi equation, and we consider the discrete-time analogues of these in Section 3. In Section 4 we develop generalized Galerkin Hamiltonian and Lagrangian variational integrators and consider their implementation as SPRK methods. In Section 5 we establish a discrete Noether's theorem and provide a discrete Hamiltonian that preserves momentum. In Section 6 we present numerical experiments where we apply two Galerkin Hamiltonian variational integrators to a degenerate Hamiltonian system and the harmonic oscillator.

2. Variational formulation of Hamiltonian mechanics

2.1 *Hamilton's variational principle for Hamiltonian and Lagrangian mechanics*

Consider an n-dimensional configuration manifold Q with associated tangent space TQ and phase space T^*Q. We introduce the generalized coordinates $q = (q^1, q^2, \ldots, q^n)$ on Q and $(q, p) = (q^1, q^2, \ldots, q^n, p_1, p_2, \ldots, p_n)$ on T^*Q. Given a Hamiltonian $H\colon T^*Q \to \mathbb{R}$, Hamilton's phase space variational principle states that

$$\delta \int_0^T [p\dot{q} - H(q, p)]\mathrm{d}t = 0$$

for fixed $q(0)$ and $q(T)$. This is equivalent to Hamilton's canonical equations

$$\dot{q} = \frac{\partial H}{\partial p}(q, p), \qquad \dot{p} = -\frac{\partial H}{\partial q}(q, p). \tag{2.1}$$

If the Hamiltonian is hyperregular, then there is a corresponding Lagrangian $L\colon TQ \to \mathbb{R}$ given by

$$L(q, \dot{q}) = \operatorname*{ext}_p \; p\dot{q} - H(q, p) = \left. p\dot{q} - H(q, p)\right|_{\dot{q}=\partial H/\partial p},$$

where ext_p denotes the extremum over p. Then Hamilton's phase space principle is equivalent to Hamilton's principle

$$\delta \int_0^T L(q, \dot{q}) \mathrm{d}t = 0$$

for fixed $q(0)$ and $q(T)$. The exact discrete Lagrangian is then given by

$$L_d^{\text{exact}}(q_0, q_1) = \underset{\substack{q \in C^2([0,h],Q) \\ q(0)=q_0, q(h)=q_1}}{\text{ext}} \int_0^h L(q(t), \dot{q}(t)) \mathrm{d}t = \underset{\substack{(q,p) \in C^2([0,h],T^*Q) \\ q(0)=q_0, q(h)=q_1}}{\text{ext}} \int_0^h p\dot{q} - H(q, p) \mathrm{d}t,$$

which corresponds to Jacobi's solution of the Hamilton–Jacobi equation. The usual characterization of the exact discrete Lagrangian involves evaluating the action integral on a curve q that satisfies the boundary conditions at the end points and the Euler–Lagrange equations in the interior.; However, as we will see, the variational characterization above naturally leads to the construction of Galerkin variational integrators.

2.2 *Type II Hamilton's variational principle in phase space*

The boundary conditions associated with both Hamilton's principle and Hamilton's phase space variational principle are naturally related to Type I generating functions since they specify the positions at the initial and final times. We will introduce a version of Hamilton's phase space principle for fixed boundary conditions $q(0)$, and $p(T)$ boundary conditions, that correspond to a Type II generating function, and we will refer to this as the Type II Hamilton's variational principle in phase space. As would be expected this will give a characterization of the exact discrete Hamiltonian. Taking the Legendre transformation of the Jacobi solution of the Hamilton–Jacobi equation leads us to consider the functional $\mathfrak{S}\colon C^2([0, T], T^*Q) \to \mathbb{R}$ given by

$$\mathfrak{S}(q(\cdot), p(\cdot)) = p(T)q(T) - \int_0^T [p\dot{q} - H(q(t), p(t))] \mathrm{d}t. \tag{2.2}$$

LEMMA 2.1. Consider the functional $\mathfrak{S}(q(\cdot), p(\cdot))$ given by (2.2). The condition that $\mathfrak{S}(q(\cdot), p(\cdot))$ is stationary with respect to the boundary conditions $\delta q(0) = 0$ and $\delta p(T) = 0$ is equivalent to $(q(\cdot), p(\cdot))$ satisfying Hamilton's canonical equations (2.1).

Proof. Direct computation of the variation of $\mathfrak{S}$ over the path space $C^2([0, T], T^*Q)$ yields

$$\begin{aligned}\delta\mathfrak{S} &= q(T)\delta p(T) + p(T)\delta q(T) \\ &\quad - \int_0^T \left[\dot{q}(t)\delta p(t) + p(t)\delta\dot{q}(t) - \frac{\partial H}{\partial q}(q(t), p(t))\delta q(t) - \frac{\partial H}{\partial p}(q(t), p(t))\delta p(t)\right] \mathrm{d}t.\end{aligned}$$

By using integration by parts and the boundary conditions $\delta q(0) = 0$ and $\delta p(T) = 0$, we obtain

$$\begin{aligned}\delta\mathfrak{S} &= q(T)\delta p(T) + p(T)\delta q(T) - p(T)\delta q(T) + p(0)\delta q(0) \\ &\quad + \int_0^T \left[\left(\dot{p}(t) + \frac{\partial H}{\partial q}(q(t), p(t))\right)\delta q(t) - \left(\dot{q}(t) - \frac{\partial H}{\partial p}(q(t), p(t))\right)\delta p(t)\right] \mathrm{d}t \\ &= \int_0^T \left[\left(\dot{p}(t) + \frac{\partial H}{\partial q}(q(t), p(t))\right)\delta q(t) - \left(\dot{q}(t) - \frac{\partial H}{\partial p}(q(t), p(t))\right)\delta p(t)\right] \mathrm{d}t. \qquad (2.3)\end{aligned}$$

If (q, p) satisfies Hamilton's equations (2.1), then the integrand vanishes and $\delta\mathfrak{S} = 0$. Conversely, if we assume that $\delta\mathfrak{S} = 0$ for any $\delta q(0) = 0$ and $\delta p(T) = 0$, then from (2.2) we obtain

$$\delta\mathfrak{S} = \int_0^T \left[\left(\dot p(t) + \frac{\partial H}{\partial q}(q(t), p(t))\right)\delta q(t) - \left(\dot q(t) - \frac{\partial H}{\partial p}(q(t), p(t))\right)\delta p(t)\right]\mathrm{d}t = 0,$$

and, by the fundamental theorem of calculus of variations (Arnoĺd, 1989), we recover Hamilton's equations

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

The above lemma states that the integral curve $(q(\cdot), p(\cdot))$ of Hamilton's equations extremizes the action functional $\mathfrak{S}(q(\cdot), p(\cdot))$ given in (2.2) for fixed boundary conditions $q(0)$ and $p(T)$. We now introduce the function $\mathscr{S}(q_0, p_T)$, which is given by the extremal value of the action functional $\mathfrak{S}$ over the family of curves satisfying the boundary conditions $q(0) = q_0$ and $p(T) = p_T$, namely,

$$\mathscr{S}(q_0, p_T) = \underset{\substack{(q,p)\in C^2([0,T],T^*Q)\\ q(0)=q_0,\, p(T)=p_T}}{\operatorname{ext}} \mathfrak{S}(q(\cdot), p(\cdot)) = \underset{\substack{(q,p)\in C^2([0,T],T^*Q)\\ q(0)=q_0,\, p(T)=p_T}}{\operatorname{ext}} p_T q_T - \int_0^T [p\dot q - H(q, p)]\mathrm{d}t. \tag{2.4}$$

The next theorem describes how $\mathscr{S}(q_0, p_T)$ generates the flow of Hamilton's equations.

THEOREM 2.2. Given the function $\mathscr{S}(q_0, p_T)$ defined by (2.4), the exact time-T flow map of Hamilton's equations $(q_0, p_0) \mapsto (q_T, p_T)$ is implicitly given by the following relation:

$$q_T = D_2\mathscr{S}(q_0, p_T), \quad p_0 = D_1\mathscr{S}(q_0, p_T). \tag{2.5}$$

In particular, $\mathscr{S}(q_0, p_T)$ is a Type II generating function that generates the exact flow of Hamilton's equations.

Proof. We directly compute

$$\begin{aligned}
&\frac{\partial\mathscr{S}}{\partial q_0}(q_0, p_T)\\
&= \frac{\partial q_T}{\partial q_0}p_T - \int_0^T \left[\frac{\partial p(t)}{\partial q_0}\dot q(t) + \frac{\partial \dot q(t)}{\partial q_0}p(t) - \frac{\partial q(t)}{\partial q_0}\frac{\partial H}{\partial q}(q, p) - \frac{\partial p(t)}{\partial q_0}\frac{\partial H}{\partial p}(q, p)\right]\mathrm{d}t\\
&= \frac{\partial q_T}{\partial q_0}p_T - \frac{\partial q_T}{\partial q_0}p_T + \frac{\partial q_0}{\partial q_0}p_0 - \int_0^T \left[\frac{\partial p(t)}{\partial q_0}\left(\dot q - \frac{\partial H}{\partial p}(q, p)\right) - \frac{\partial q(t)}{\partial q_0}\left(\dot p + \frac{\partial H}{\partial q}(q, p)\right)\right]\mathrm{d}t\\
&= p_0 - \int_0^T \left[\frac{\partial p(t)}{\partial q_0}\left(\dot q - \frac{\partial H}{\partial p}(q, p)\right) - \frac{\partial q(t)}{\partial q_0}\left(\dot p + \frac{\partial H}{\partial q}(q, p)\right)\right]\mathrm{d}t,
\end{aligned}$$

where we have used integration by parts. By Lemma 2.1, the extremum of $\mathfrak{S}$ is achieved when the curve (q, p) satisfies Hamilton's equations. Consequently, the integrand in the above equation vanishes, giving $p_0 = \frac{\partial\mathscr{S}}{\partial q_0}(q_0, p_T)$. Similarly, by using integration by parts and restricting ourselves to the curves

(q, p) that satisfy Hamilton's equations, we obtain

$$\begin{aligned}\frac{\partial \mathscr{S}}{\partial p_T}(q_0, p_T) &= \frac{\partial p_T}{\partial p_T} q_T + \frac{\partial q_T}{\partial p_T} p_T - \int_0^T \left[\frac{\partial p(t)}{\partial p_T}\dot{q}(t) + \frac{\partial \dot{q}(t)}{\partial p_T} p(t) - \frac{\partial q(t)}{\partial p_T}\frac{\partial H}{\partial q}(q, p) - \frac{\partial p(t)}{\partial p_T}\frac{\partial H}{\partial p}(q, p)\right] \mathrm{d}t \\ &= q_T + \frac{\partial q_T}{\partial p_T} p_T - \frac{\partial q_T}{\partial p_T} p_T + \frac{\partial q_0}{\partial p_T} p_0 - \int_0^T \left[\frac{\partial p(t)}{\partial p_T}\left(\dot{q} - \frac{\partial H}{\partial p}(q, p)\right) - \frac{\partial q(t)}{\partial p_T}\left(\dot{p} + \frac{\partial H}{\partial q}(q, p)\right)\right] \mathrm{d}t \\ &= q_T. \end{aligned}$$

□

2.3 *Type II Hamilton–Jacobi equation*

Let us explicitly consider $\mathscr{S}(q_0, p_T)$ as a function of the time T, and we denote this by $\mathscr{S}_T(q_0, p_T)$. Theorem 2.2 states that the Type II generating function $\mathscr{S}_T(q_0, p_T)$ generates the exact time-T flow map of Hamilton's equations, and consequently it has to be related by the Legendre transformation to the Jacobi solution of the Hamilton–Jacobi equation, which is the Type I generating function for the same flow map. Consequently, we expect that the function $\mathscr{S}_T(q_0, p_T)$ satisfies a Type II analogue of the Hamilton–Jacobi equation that we derive in the following proposition.

PROPOSITION 2.3. Let

$$S_2(q_0, p, t) \equiv \mathscr{S}_t(q_0, p) = \underset{\substack{(q,p)\in C^2([0,t],T^*Q) \\ q(0)=q_0,\, p(t)=p}}{\operatorname{ext}} \left(p(t)q(t) - \int_0^t [p(s)\dot{q}(s) - H(q(s), p(s))]\mathrm{d}s\right). \tag{2.6}$$

Then the function $S_2(q_0, p, t)$ satisfies the *Type II Hamilton–Jacobi equation*

$$\frac{\partial S_2(q_0, p, t)}{\partial t} = H\left(\frac{\partial S_2}{\partial p}, p\right). \tag{2.7}$$

Proof. From the definition of $S_2(q_0, p, t)$, the curve that extremizes the functional connects the fixed initial point (q_0, p_0) with the arbitrary final point (q, p) at time t. Computing the time derivative of $S_2(q_0, p, t)$ yields

$$\frac{\mathrm{d}S_2}{\mathrm{d}t} = \dot{p}(t)q(t) + p(t)\dot{q}(t) - p(t)\dot{q}(t) + H(q(t), p(t)). \tag{2.8}$$

On the other hand,

$$\frac{\mathrm{d}S_2}{\mathrm{d}t} = \dot{p}(t)\frac{\partial S_2}{\partial p} + \frac{\partial S_2}{\partial t}. \tag{2.9}$$

Equating (2.8) and (2.9) and applying (2.5) yields

$$\frac{\partial S_2}{\partial t} = \dot{p}(t)q(t) + H(q(t), p(t)) - \dot{p}(t)\frac{\partial S_2}{\partial p} = H(q(t), p(t)) = H\left(\frac{\partial S_2}{\partial p}, p\right). \tag{2.10}$$

□

The Type II Hamilton–Jacobi equation also appears on page 201 of Hairer *et al.* (2006) and in de León *et al.* (2007). However, this equation has generally been used in the construction of symplectic integrators based on Type II generating functions by considering a series expansion of S_2 in powers of t, substituting the series into the Type II Hamilton–Jacobi equation and truncating. Then, a term-by-term comparison allows one to determine the coefficients in the series expansion of S_2, from which one constructs a symplectic map that approximates the exact flow map (de Vogelaére, 1956; Ruth, 1983; Feng, 1986; Channell & Scovel, 1990).

However, approximating Jacobi's solution in the Lagrangian formulation or the exact discrete right Hamiltonian $\mathscr{S}(q_0, p_T)$ in (2.4) in terms of their variational characterization provides an elegant method for constructing symplectic integrators. In particular, this naturally leads to the generalized Galerkin framework for constructing discrete Lagrangians and discrete Hamiltonians, which we will explore in the rest of the paper.

In Section 3 we will also present a discrete analogue of the Type II Hamilton–Jacobi equation, which can be viewed as a composition theorem that expresses the discrete Hamiltonian for a given time interval in terms of discrete Hamiltonians for the subintervals. This can be viewed as the Type II analogue of the discrete Hamilton–Jacobi equation that was introduced in Elnatanov & Schiff (1996).

3. Discrete variational Hamiltonian mechanics

3.1 *Discrete Type II Hamilton's variational principle in phase space*

The Lagrangian formulation of discrete variational mechanics is based on a discretization of Hamilton's principle, and a comprehensive review of this approach is given in Marsden & West (2001). The Hamiltonian analogue of discrete variational mechanics was introduced in Lall & West (2006), wherein discrete Lagrangian mechanics was viewed as the primal formulation of a constrained discrete optimization problem, where the constraints are given by the discrete analogue of the second-order curve condition, and dual formulation of this yields discrete Hamiltonian variational mechanics. An analogous approach is based on the discrete Hamilton–Pontryagin variational principle (Leok & Ohsawa, 2008), in which the discrete Hamilton's principle is augmented with a Lagrange multiplier term that enforces the discrete second-order curve condition.

We begin by introducing a partition of the time interval $[0, T]$ with the discrete times $0 = t_0 < t_1 < \cdots < t_N = T$ and a discrete curve in T^*Q, denoted by $\{(q_k, p_k)\}_{k=0}^N$, where $q_k \approx q(t_k)$, and $p_k \approx p(t_k)$. Our discrete variational principle will be formulated in terms of a discrete Hamiltonian $H_d^+(q_k, p_{k+1})$, which is an approximation of the Type II generating function given in (2.4), as follows:

$$H_d^+(q_k, p_{k+1}) \approx \underset{\substack{(q,p)\in C^2([t_k,t_{k+1}],T^*Q)\\ q(t_k)=q_k,\, p(t_{k+1})=p_{k+1}}}{\operatorname{ext}} p(t_{k+1})q(t_{k+1}) - \int_{t_k}^{t_{k+1}} [p\dot{q} - H(q,p)]\mathrm{d}t. \tag{3.1}$$

As we saw in Section 2, the curve in phase space with fixed boundary conditions (q_0, p_T) that extremizes the functional (2.2),

$$\mathfrak{S}(q(\cdot), p(\cdot)) = p(T)q(T) - \int_0^T [p\dot{q} - H(q(t), p(t))]\mathrm{d}t,$$

satisfies Hamilton's canonical equations. Consequently, we can formulate discrete variational Hamiltonian mechanics in terms of a discrete analogue of this functional, which is given by

$$\begin{aligned}\mathfrak{S}_d(\{(q_k, p_k)\}_{k=0}^N) &= p_N q_N - \sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} [p\dot{q} - H(q(t), p(t))]\mathrm{d}t \\ &= p_N q_N - \sum_{k=0}^{N-1} [p_{k+1}q_{k+1} - H_d^+(q_k, p_{k+1})].\end{aligned} \tag{3.2}$$

Then the *Type II discrete Hamilton's phase space variational principle* states that

$$\delta\mathfrak{S}_d(\{(q_k, p_k)\}_{k=0}^N) = 0$$

for discrete curves in T^*Q with fixed (q_0, p_N) boundary conditions.

LEMMA 3.1. The Type II discrete Hamilton's phase space variational principle is equivalent to the discrete right Hamilton's equations

$$\begin{aligned} q_k &= D_2 H_d^+(q_{k-1}, p_k), \quad k = 1, \ldots, N-1, \\ p_k &= D_1 H_d^+(q_k, p_{k+1}), \quad k = 1, \ldots, N-1, \end{aligned} \tag{3.3}$$

where $H_d^+(q_k, p_{k+1})$ is defined in (3.1).

Proof. We compute the variation of $\mathfrak{S}_d$ as follows:

$$\begin{aligned} \delta\mathfrak{S}_d &= \delta\left(p_N q_N - \sum_{k=0}^{N-1}(p_{k+1}q_{k+1} - H_d^+(q_k, p_{k+1}))\right) \\ &= \delta\left(-\sum_{k=0}^{N-2} p_{k+1}q_{k+1} + \sum_{k=0}^{N-1} H_d^+(q_k, p_{k+1})\right) \\ &= -\sum_{k=0}^{N-2}(q_{k+1}\delta p_{k+1} + p_{k+1}\delta q_{k+1}) + \sum_{k=0}^{N-1}(D_1 H_d^+(q_k, p_{k+1})\delta q_k + D_2 H_d^+(q_k, p_{k+1})\delta p_{k+1}) \\ &= -\sum_{k=1}^{N-1}(q_k\delta p_k + p_k\delta q_k) + \sum_{k=1}^{N-1} D_1 H_d^+(q_k, p_{k+1})\delta q_k + D_1 H_d^+(q_0, p_1)\delta q_0 \\ &\quad + \sum_{k=1}^{N-1} D_2 H_d^+(q_{k-1}, p_k)\delta p_k + D_2 H_d^+(q_{N-1}, p_N)\delta p_N \\ &= -\sum_{k=1}^{N-1}(q_k - D_2 H_d^+(q_{k-1}, p_k))\delta p_k - \sum_{k=1}^{N-1}(p_k - D_1 H_d^+(q_k, p_{k+1}))\delta q_k \\ &\quad + D_1 H_d^+(q_0, p_1)\delta q_0 + D_2 H_d^+(q_{N-1}, p_N)\delta p_N, \end{aligned}$$

where we have re-indexed the sum, which is the discrete analogue of integration by parts. Using the fact that (q_0, p_N) are fixed, which implies that $\delta q_0 = 0$ and $\delta p_N = 0$, the above equation reduces to

$$\delta\mathfrak{S}_d = -\sum_{k=1}^{N-1}(q_k - D_2 H_d^+(q_{k-1}, p_k))\delta p_k - \sum_{k=1}^{N-1}(p_k - D_1 H_d^+(q_k, p_{k+1}))\delta q_k. \tag{3.4}$$

Clearly, if the discrete right Hamilton's equations $q_k = D_2 H_d^+(q_{k-1}, p_k)$ and $p_k = D_1 H_d^+(q_k, p_{k+1})$ are satisfied, then the functional is stationary. Conversely, if the functional is stationary, then a discrete analogue of the fundamental theorem of the calculus of variations yields the discrete right Hamilton's equations. □

The above lemma states that the discrete-time solution trajectory of the discrete right Hamilton's equations (3.3) extremizes the discrete functional (3.2) for fixed q_0 and p_N. However, it does not indicate how the discrete solution is related to p_0 and q_N. Note that the discrete solution trajectory that renders $\mathfrak{S}_d(\{(q_k, p_k)\}_{k=0}^N)$ stationary depends on the boundary conditions q_0 and p_N. Consequently, we can introduce the function $\mathscr{S}_d$ that is given by the extremal value of the discrete functional $\mathfrak{S}_d$ as a function of the boundary conditions $q(t_0)$ and $p(t_N)$ and is explicitly given by

$$\begin{aligned}\mathscr{S}_d(q(t_0), p(t_N)) &= \operatorname*{ext}_{\substack{(q_k,p_k)\in T^*Q\\ q_0=q(t_0),\, p_N=p(t_N)}} \mathfrak{S}_d(\{(q_k, p_k)\}_{k=0}^N)\\ &= \operatorname*{ext}_{\substack{(q_k,p_k)\in T^*Q\\ q_0=q(t_0),\, p_N=p(t_N)}} p_N q_N - \sum_{k=0}^{N-1}(p_{k+1}q_{k+1} - H_d^+(q_k, p_{k+1})).\end{aligned} \tag{3.5}$$

Then, using a similar approach to the proof of Theorem 2.2, we compute the derivatives of $\mathscr{S}_d(q_0, p_N)$ with respect to q_0 and p_N. By re-indexing the sum, which is the discrete analogue of integration by parts, we obtain

$$\begin{aligned}\frac{\partial \mathscr{S}_d}{\partial q_0}(q_0, p_N) &= \frac{\partial}{\partial q_0}\left(-\sum_{k=0}^{N-2} p_{k+1}q_{k+1} + \sum_{k=0}^{N-1} H_d^+(q_k, p_{k+1})\right)\\ &= -\sum_{k=1}^{N-1}\frac{\partial p_k}{\partial q_0}(q_k - D_2H_d^+(q_{k-1}, p_k))\\ &\quad -\sum_{k=1}^{N-1}\frac{\partial q_k}{\partial q_0}(p_k - D_1H_d^+(q_k, p_{k+1})) + D_1H_d^+(q_0, p_1).\end{aligned}$$

By Lemma 3.1, the extremum of $\mathfrak{S}_d$ is obtained if the discrete curve satisfies the discrete right Hamilton's equations (3.3). Thus, by the definition of $\mathscr{S}_d(q_0, p_N)$, the above equation reduces to

$$D_1\mathscr{S}_d(q_0, p_N) = D_1H_d^+(q_0, p_1). \tag{3.6}$$

A similar argument yields

$$\begin{aligned}&\frac{\partial \mathscr{S}_d}{\partial p_N}(q_0, p_N) \qquad (3.7)\\ &\quad = \frac{\partial}{\partial p_N}\left(-\sum_{k=0}^{N-2} p_{k+1}q_{k+1} + \sum_{k=0}^{N-1} H_d^+(q_k, p_{k+1})\right)\\ &\quad = -\sum_{k=1}^{N-1}\frac{\partial p_k}{\partial p_N}(q_k - D_2H_d^+(q_{k-1}, p_k)) - \sum_{k=1}^{N-1}\frac{\partial q_k}{\partial p_N}(p_k - D_1H_d^+(q_k, p_{k+1})) + D_2H_d^+(q_{N-1}, p_N)\\ &\quad = D_2H_d^+(q_{N-1}, p_N).\end{aligned}$$

Recall that the exact discrete Hamiltonian $\mathscr{S}(q_0, p_T)$ defined in (2.4) is a Type II generating function of the symplectic map implicitly defined by the relation (2.5) that is, the exact flow map of the continuous Hamilton's equations. To be consistent with this, we require that $\mathscr{S}_d(q_0, p_N)$ satisfies the relation (2.5), which is to say

$$q_N = D_2\mathscr{S}_d(q_0, p_N), \qquad p_0 = D_1\mathscr{S}_d(q_0, p_N). \tag{3.8}$$

Comparing (3.6) and (3.7) to (3.8), we obtain

$$q_N = D_2 H_d^+(q_{N-1}, p_N), \quad p_0 = D_1 H_d^+(q_0, p_1). \tag{3.9}$$

Then, by combining (3.3) and (3.9), we obtain the complete set of discrete right Hamilton's equations

$$q_{k+1} = D_2 H_d^+(q_k, p_{k+1}), \quad k = 0, 1, \dots, N-1, \tag{3.10a}$$
$$p_k = D_1 H_d^+(q_k, p_{k+1}), \quad k = 0, 1, \dots, N-1. \tag{3.10b}$$

It is easy to see that

$$\begin{aligned} 0 &= \mathrm{d}\mathrm{d}H_d^+(q_k, p_{k+1}) = \mathrm{d}(D_1 H_d^+(q_k, p_{k+1})\mathrm{d}q_k + D_2 H_d^+(q_k, p_{k+1})\mathrm{d}p_{k+1}) \\ &= \mathrm{d}(p_k \mathrm{d}q_k + q_{k+1}\mathrm{d}p_{k+1}) = \mathrm{d}p_k \wedge \mathrm{d}q_k - \mathrm{d}p_{k+1} \wedge \mathrm{d}q_{k+1} \end{aligned}$$

for $k = 0, \dots, N-1$. Then, successively applying the above equation gives

$$\mathrm{d}p_0 \wedge \mathrm{d}q_0 = \mathrm{d}p_1 \wedge \mathrm{d}q_1 = \cdots = \mathrm{d}p_{N-1} \wedge \mathrm{d}q_{N-1} = \mathrm{d}p_N \wedge \mathrm{d}q_N.$$

This implies that the map from the initial state (q_0, p_0) to the final state (q_N, p_N) defined by (3.8) is sympletic since it is the composition of the N symplectic maps $(q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$, where $k = 0, \dots, N-1$, given in (3.10). Alternatively, one can directly prove the symplecticity of the map $(q_0, p_0) \mapsto (q_N, p_N)$ by using (3.8) to compute $0 = \mathrm{d}^2\mathscr{S}_\mathrm{d}(q_0, p_N) = \mathrm{d}p_0 \wedge \mathrm{d}q_0 - \mathrm{d}p_N \wedge \mathrm{d}q_N$. Given initial conditions q_0 and p_0, and under the regularity assumption $\left|\frac{\partial^2 H_d^+}{\partial q_k \partial p_{k+1}}(q_k, p_{k+1})\right| \neq 0$, we can solve (3.10b) to obtain p_1, and then substitute p_1 into (3.10a) to get q_1. By repeatedly applying this process, we obtain the discrete solution trajectory $\{(q_k, p_k)\}_{k=1}^N$.

3.2 *Discrete Type II Hamilton–Jacobi equation*

A discrete analogue of the Hamilton–Jacobi equation was first introduced in Elnatanov & Schiff (1996), and the connections to discrete Hamiltonian mechanics and discrete optimal control theory were explored in Ohsawa *et al.* (2009). In essence, the discrete Hamilton–Jacobi equation therein can be viewed as a composition theorem that relates the discrete Hamiltonians that generate the maps over subintervals to the discrete Lagrangian that generates the map over the entire time interval.

We will adopt the derivation of the discrete Hamilton–Jacobi equation in Ohsawa *et al.* (2009), which is based on introducing a discrete analogue of Jacobi's solution to the setting of Type II generating functions.

THEOREM 3.2. Consider the discrete extremum function (3.5) that is given as follows:

$$\mathscr{S}_d^k(p_k) = p_k q_k - \sum_{l=0}^{k-1} [p_{l+1} q_{l+1} - H_d^+(q_l, p_{l+1})], \tag{3.11}$$

which can be obtained from the discrete functional (3.2) by evaluating it along a solution of the right discrete Hamilton's equations (3.10). Each $\mathscr{S}_d^k(p_k)$ is viewed as a function of the momentum p_k at the discrete end time t_k. Then these satisfy the discrete Type II Hamilton–Jacobi equation

$$\mathscr{S}_d^{k+1}(p_{k+1}) - \mathscr{S}_d^k(p_k) = H_d^+(D\mathscr{S}_d^k(p_k), p_{k+1}) - p_k \cdot D\mathscr{S}_d^k(p_k). \tag{3.12}$$

Proof. From equation (3.11) we have

$$\mathscr{S}_d^{k+1}(p_{k+1}) - \mathscr{S}_d^k(p_k) = H_d^+(q_k, p_{k+1}) - p_k \cdot q_k, \tag{3.13}$$

where q_k is considered to be a function of p_k and p_{k+1}, that is, $q_k = q_k(p_k, p_{k+1})$. Taking the derivative of both sides with respect to p_k, we have

$$-D\mathscr{S}_d^k(p_k) = -q_k + \frac{\partial q_k}{\partial p_k} \cdot [D_1 H_d^+(q_k, p_{k+1}) - p_k].$$

However, the terms in the brackets vanish because the right discrete Hamilton's equations (3.10) are assumed to be satisfied. Thus we have

$$q_k = D\mathscr{S}_d^k(p_k). \tag{3.14}$$

Substituting this into (3.13) gives (3.12). □

3.3 *Summary of discrete and continuous results*

We have introduced the continuous and discrete variational formulations of Hamiltonian mechanics in a parallel fashion, and the correspondence between the two is summarized in Fig. 1. Similarly, the correspondence between the continuous and discrete Type II Hamilton–Jacobi equations is summarized in Table 1.

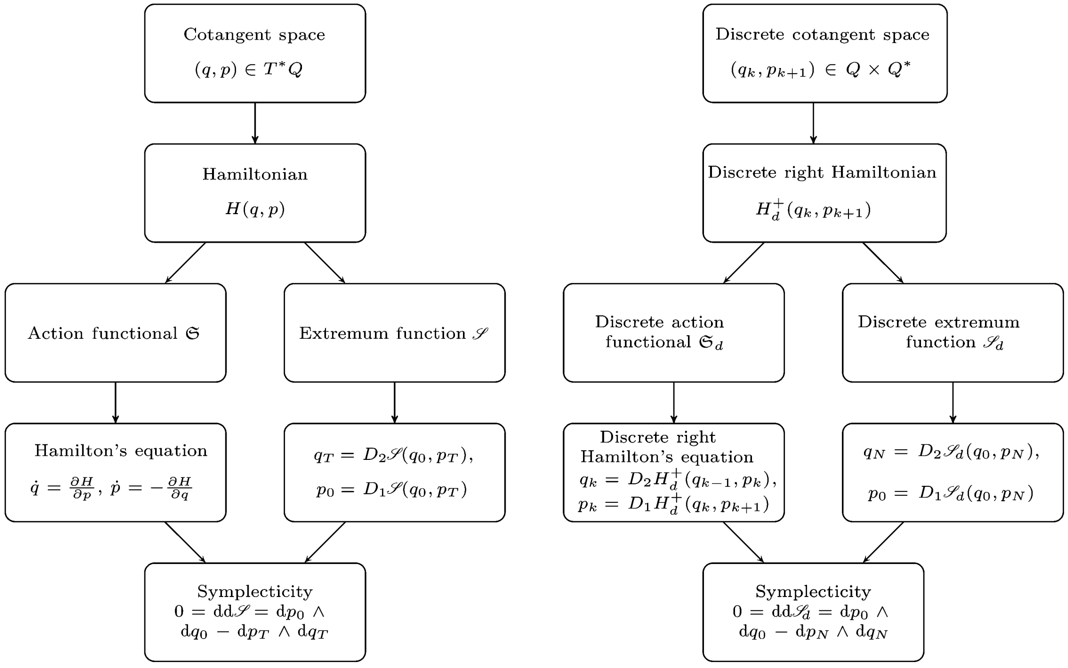

FIG. 1. The continuous and discrete *Type II Hamilton's phase space variational principle*. In the continuous case the variation of the action functional $\mathfrak{S}$ over the space of curves gives Hamilton's equations, and the derivatives of the extremum functional $\mathscr{S}$ with respect to the boundary points yield the exact flow map of Hamilton's equations. In the discrete case the variation of the discrete action functional $\mathfrak{S}_d$ over the space of discrete curves gives the discrete right Hamilton's equations, and the derivatives of the extremum functional $\mathscr{S}_d$ with respect to the boundary points yield the symplectic map from the initial state to the final state.

TABLE 1. *Correspondence between ingredients in the continuous and discrete Type II Hamilton–Jacobi theories.* $\mathbb{N}_0$ *is the set of non-negative integers and* $\mathbb{R}_{\geqslant 0}$ *is the set of non-negative real numbers*

Continuous	Discrete
$(p, t) \in Q^* \times \mathbb{R}_{\geqslant 0}$	$(p_k, k) \in Q^* \times \mathbb{N}_0$
$\dot{q} = \partial H/\partial p$	$q_{k+1} = D_2 H_d^+(q_k, p_{k+1})$
$\dot{p} = -\partial H/\partial q$	$p_k = D_1 H_d^+(q_k, p_{k+1})$
$S_2(p, t)$	$\mathscr{S}_d^k(p_k)$
$\equiv p(t)q(t) - \int_0^t [p(s)\dot{q}(s) - H(q(s), p(s))]\mathrm{d}s$	$\equiv p_k q_k - \sum_{l=0}^{k-1}[p_{l+1}q_{l+1} - H_d^+(q_l, p_{l+1})]$
$\mathrm{d}S_2 = \frac{\partial S_2}{\partial p}\mathrm{d}p + \frac{\partial S_2}{\partial t}\mathrm{d}t$	$\mathscr{S}_d^{k+1}(p_{k+1}) - \mathscr{S}_d^k(p_k)$
$q\,\mathrm{d}p + H(q, p)\mathrm{d}t$	$H_d^+(q_k, p_{k+1}) - p_k \cdot q_k$
$\frac{\partial S_2}{\partial t} = H\left(\frac{\partial S_2}{\partial p}, p\right)$	$\mathscr{S}_d^{k+1}(p_{k+1}) - \mathscr{S}_d^k(p_k) = H_d^+(D\mathscr{S}_d^k(p_k), p_{k+1}) - p_k \cdot D\mathscr{S}_d^k(p_k)$

4. Galerkin Hamiltonian variational integrators

4.1 *Exact discrete Hamiltonian*

The exact discrete Hamiltonian $H^+_{d,\mathrm{exact}}(q_0, p_1)$ and the discrete right Hamilton's equations (3.10) generate a discrete solution curve $\{q_k, p_k\}_{k=0}^N$ that samples the exact solution $(q(\cdot), p(\cdot))$ of the continuous Hamilton's equations for the continuous Hamiltonian $H(q, p)$, that is, $q_k = q(t_k)$ and $p_k = p(t_k)$.

By comparing the definition (3.1) of a discrete right Hamiltonian function $H_d^+(q_0, p_1)$ on $[0, h]$ and the corresponding discrete Hamiltonian flow in (3.10) to the definition (2.4) of the extremal function on $[0, T]$ and corresponding symplectic map given by (2.5), and applying Theorem 2.2, it is clear that the discrete right Hamiltonian function on $[0, h]$, given by

$$H^+_{d,\mathrm{exact}}(q_0, p_1) = \underset{\substack{(q,p)\in C^2([0,T],T^*Q)\\ q(t_0)=q_0,\, p(t_1)=p_1}}{\mathrm{ext}} p_1 q_1 - \int_0^h [p(t)\dot{q}(t) - H(q(t), p(t))]\mathrm{d}t, \tag{4.1}$$

is an exact discrete right Hamiltonian function on $[0, h]$.

4.2 *Galerkin discrete Hamiltonian*

In general, the exact discrete Hamiltonian is not computable since it requires one to evaluate the functional $\mathfrak{S}(q(\cdot), p(\cdot))$ given in (2.2) on a solution curve of Hamilton's equations that satisfies the given boundary conditions (q_0, p_1). However, the variational characterization of the exact discrete Hamiltonian naturally leads to computable approximations based on Galerkin techniques. In practice, one replaces the path space $C^2([0, T], T^*Q)$, which is an infinite-dimensional function space, with a finite-dimensional function space and uses numerical quadrature to approximate the integral.

Let $\{\psi_i(\tau)\}_{i=1}^s$, where $\tau \in [0, 1]$, be a set of basis functions for an s-dimensional function space C_d^s. We also choose a numerical quadrature formula with quadrature weights b_i and quadrature points c_i, that is, $\int_0^1 f(x)\mathrm{d}x \approx \sum_{j=1}^s b_i f(c_i)$. From these basis functions and the numerical quadrature formula, we will systematically construct a generalized Galerkin Hamiltonian variational integrator in the following manner.

1. Use the basis functions ψ_i to approximate the velocity $\dot{q}$ over the interval $[0, h]$ as follows:

$$\dot{q}_d(\tau h) = \sum_{i=1}^s V^i \psi_i(\tau).$$

2. Integrate $\dot{q}_d(\rho)$ over $[0, \tau h]$ to obtain the following approximation for the position q:

$$q_d(\tau h) = q_d(0) + \int_0^{\tau h} \sum_{i=1}^s V^i \psi_i(\rho)\mathrm{d}(\rho h) = q_0 + h\sum_{i=1}^s V^i \int_0^{\tau} \psi_i(\rho)\mathrm{d}\rho,$$

where we have applied the boundary condition $q_d(0) = q_0$. Applying the boundary condition $q_d(h) = q_1$ yields

$$q_1 = q_d(h) = q_0 + h\sum_{i=1}^s V^i \int_0^1 \psi_i(\rho)\mathrm{d}\rho \equiv q_0 + h\sum_{i=1}^s B_i V^i,$$

where $B_i = \int_0^1 \psi_i(\tau)\mathrm{d}\tau$. Furthermore, we introduce the internal stages

$$Q^i \equiv q_d(c_i h) = q_0 + h\sum_{j=1}^s V^j \int_0^{c_i} \psi_j(\tau)\mathrm{d}\tau \equiv q_0 + h\sum_{j=1}^s A_{ij} V^j,$$

where $A_{ij} = \int_0^{c_i} \psi_j(\tau)\mathrm{d}\tau$.

3. Let $P^i = p(c_i h)$. Use the numerical quadrature formula (b_i, c_i) and the finite-dimensional function space C_d^s to construct $H_d^+(q_0, p_1)$ as follows:

$$H_d^+(q_0, p_1) \approx \underset{\substack{(q,p)\in C^2([0,T],T^*Q)\\ q(t_0)=q_0,\, p(t_1)=p_1}}{\operatorname{ext}} p_1 q_1 - \int_0^h [p(t)\dot{q}(t) - H(q(t), p(t))]\mathrm{d}t,$$

$$\begin{aligned} H_d^+(q_0, p_1) &= \underset{q_d\in C_d^s([0,h],Q),\, P_i\in Q^*}{\operatorname{ext}} \left\{ p_1 q_d(h) - h\sum_{i=1}^s b_i [p(c_i h)\dot{q}_d(c_i h) \right.\\ &\qquad \left. - H(q_d(c_i h), p(c_i h))] \right\} \\ &= \underset{V^i, P^i}{\operatorname{ext}} \left\{ p_1\left(q_0 + h\sum_{i=1}^s B_i V^i\right) - h\sum_{i=1}^s b_i \left[P^i \sum_{j=1}^s V^j \psi_j(c_i) \right.\right.\\ &\qquad \left.\left. -H\left(q_0 + h\sum_{j=1}^s A_{ij}V^j, P^i\right)\right]\right\} \\ &\equiv \underset{V^i, P^i}{\operatorname{ext}} K(q_0, V^i, P^i, p_1). \end{aligned} \tag{4.2}$$

In order to obtain an expression for $H_d^+(q_0, p_1)$ we first compute the stationarity conditions for $K(q_0, V^i, P^i, p_1)$ under the fixed boundary condition (q_0, p_1) as follows:

$$0 = \frac{\partial K(q_0, V^i, P^i, p_1)}{\partial V^j} = hp_1 B_j - h\sum_{i=1}^{s} b_i \left(P^i \psi_j(c_i) - hA_{ij}\frac{\partial H}{\partial q}(Q^i, P^i)\right), \quad j = 1, \ldots, s, \tag{4.3a}$$

$$0 = \frac{\partial K(q_0, V^i, P^i, p_1)}{\partial P^j} = hb_j\left(\sum_{i=1}^{s} \psi_i(c_j)V^i - \frac{\partial H}{\partial p}(Q^j, P^j)\right), \qquad j = 1, \ldots, s. \tag{4.3b}$$

4. By solving the $2s$ stationarity conditions (4.3), we can express the parameters V^i and P^i in terms of q_0 and p_1, that is, $V^i = V^i(q_0, p_1)$ and $P^i = P^i(q_0, p_1)$. Then the symplectic map $(q_0, p_0) \mapsto (q_1, p_1)$ can be expressed in terms of the internal stages as follows:

$$\begin{aligned} p_0 &= \frac{\partial H_d^+(q_0, p_1)}{\partial q_0} = \frac{\partial K(q_0, V^i(q_0, p_1), P^i(q_0, p_1), p_1)}{\partial q_0} \\ &= \frac{\partial K}{\partial q_0} + \frac{\partial K}{\partial V^i}\frac{\partial V^i}{\partial q_0} + \frac{\partial K}{\partial P^i}\frac{\partial P^i}{\partial q_0} = \frac{\partial K}{\partial q_0} \\ &= p_1 + h\sum_{i=1}^{s} b_i \frac{\partial H}{\partial q}(Q^i, P^i). \end{aligned} \tag{4.4}$$

Similarly, we obtain

$$\begin{aligned} q_1 &= \frac{\partial H_d^+(q_0, p_1)}{\partial p_1} = \frac{\partial K(q_0, V^i(q_0, p_1), P^i(q_0, p_1), p_1)}{\partial p_1} \\ &= \frac{\partial K}{\partial V^i}\frac{\partial V^i}{\partial p_1} + \frac{\partial K}{\partial P^i}\frac{\partial P^i}{\partial p_1} + \frac{\partial K}{\partial p_1} = \frac{\partial K}{\partial p_1} \\ &= q_0 + h\sum_{i=1}^{s} B_i V^i. \end{aligned} \tag{4.5}$$

Without loss of generality, we assume that the quadrature weights $b_i \neq 0$. Then the stationarity condition (4.3b) reduces to

$$\sum_{i=1}^{s} \psi_i(c_j)V^i - \frac{\partial H}{\partial p}(Q^j, P^j) = 0.$$

Moreover, by substituting (4.4) into the stationarity condition (4.3a), we obtain

$$\sum_{i=1}^{s} b_i P^i \psi_j(c_i) - p_0 B_j + h\sum_{i=1}^{s}(b_i B_j - b_i A_{ij})\frac{\partial H}{\partial q}(Q^i, P^i) = 0.$$

In summary, the above procedure gives a systematic way of constructing a generalized Galerkin Hamiltonian variational integrator, which can be rewritten in the following compact form:

$$q_1 = q_0 + h\sum_{i=1}^{s} B_i V^i, \tag{4.6a}$$

$$p_1 = p_0 - h\sum_{i=1}^{s} b_i \frac{\partial H}{\partial q}(Q^i, P^i), \tag{4.6b}$$

$$Q^i = q_0 + h\sum_{j=1}^{s} A_{ij} V^j, \qquad i = 1, \dots, s, \tag{4.6c}$$

$$0 = \sum_{i=1}^{s} b_i P^i \psi_j(c_i) - p_0 B_j + h\sum_{i=1}^{s}(b_i B_j - b_i A_{ij})\frac{\partial H}{\partial q}(Q^i, P^i), \quad j = 1, \dots, s, \tag{4.6d}$$

$$0 = \sum_{i=1}^{s} \psi_i(c_j) V^i - \frac{\partial H}{\partial p}(Q^j, P^j), \qquad j = 1, \dots, s, \tag{4.6e}$$

where (b_i, c_i) are the quadrature weights and quadrature points and $B_i = \int_0^1 \psi_i(\tau)\mathrm{d}\tau$ and $A_{ij} = \int_0^{c_i} \psi_j(\tau)\mathrm{d}\tau$.

This is the general form of a Galerkin Hamiltonian variational integrator. Issues of solvability, convergence and accuracy depend on the specific Hamiltonian system and the choice of finite-dimensional function space C_d^s and numerical quadrature formula (b_i, c_i). We will not perform an in-depth analysis here, but we will illustrate how our proposed framework is related to the discrete Lagrangian-based methods given in Marsden & West (2001) and page 209 of Hairer *et al.* (2006).

4.3 *Galerkin variational integrators from the Lagrangian point of view*

In this subsection we investigate the generalized Galerkin variational integrators from the Lagrangian point of view when the Hamiltonian function is hyperregular. In this case the exact discrete right Hamiltonian function is related by the Legendre transformation to the exact discrete Lagrangian function, that is,

$$\begin{aligned} L_d^{\mathrm{exact}}(q_0, q_1) &= \operatorname*{ext}_{\substack{q \in C^2([0,h],Q) \\ q(0)=q_0, q(h)=q_1}} \int_0^h L(q(t), \dot{q}(t))\mathrm{d}t \\ &= \operatorname*{ext}_{\substack{(q,p) \in C^2([0,h],T^*Q) \\ q(0)=q_0, q(h)=q_1}} \int_0^h p\dot{q} - H(q, p)\mathrm{d}t \\ &= p_1 q_1 - H^+_{d,\mathrm{exact}}(q_0, p_1)\Big|_{q_1 = D_2 H^+_{d,\mathrm{exact}}(q_0,p_1)}. \end{aligned} \tag{4.7}$$

We wish to see how Galerkin variational integrators that are derived from the Hamiltonian and Lagrangian viewpoints are related. In order for the comparison to make sense, we will approximate the exact discrete Lagrangian using the same basis functions and numerical quadrature formula as in the Hamiltonian formulation. As before, let $\{\psi_i(\tau)\}_{i=1}^s$, where $\tau \in [0, 1]$, be a set of basis functions for an

s-dimensional function space C_d^s and choose a numerical quadrature formula with quadrature weights b_i and quadrature points c_i. From these basis functions and the numerical quadrature formula, we will systematically construct a generalized Galerkin Lagrangian variational integrator in the following manner.

1. Use the basis functions ψ_i to approximate the velocity $\dot{q}$ over the interval $[0, h]$ as follows:

$$\dot{q}_d(\tau h) = \sum_{i=1}^{s} V^i \psi_i(\tau).$$

2. Integrate $\dot{q}_d(\rho)$ over $[0, \tau h]$ to obtain the following approximation for the position q:

$$q_d(\tau h) = q_d(0) + \int_0^{\tau h} \sum_{i=1}^{s} V^i \psi_i(\rho)\mathrm{d}(\rho h) = q_0 + h \sum_{i=1}^{s} V^i \int_0^{\tau} \psi_i(\rho)\mathrm{d}\rho,$$

where we have applied the boundary condition $q_d(0) = q_0$. In the discrete Lagrangian framework the boundary conditions are given by (q_0, q_1), and so we will use a Lagrange multiplier to enforce the boundary condition $q_d(h) = q_1$ as follows:

$$q_1 = q_d(h) = q_0 + h \sum_{i=1}^{s} V^i \int_0^1 \psi_i(\rho)\mathrm{d}\rho \equiv q_0 + h \sum_{i=1}^{s} B_i V^i,$$

where $B_i = \int_0^1 \psi_i(\tau)\mathrm{d}\tau$. Furthermore, we introduce the internal stages

$$Q^i \equiv q_d(c_i h) = q_0 + h \sum_{j=1}^{s} V^j \int_0^{c_i} \psi_j(\tau)\mathrm{d}\tau \equiv q_0 + h \sum_{j=1}^{s} A_{ij} V^j, \tag{4.8}$$

where $A_{ij} = \int_0^{c_i} \psi_j(\tau)\mathrm{d}\tau$, and their velocities

$$\dot{Q}^i \equiv \dot{q}_d(c_i h) = \sum_{j=1}^{s} \psi_j(c_i) V^j. \tag{4.9}$$

3. Use the numerical quadrature formula (b_i, c_i) and the finite-dimensional function space C_d^s to construct $L_d(q_0, q_1)$ as follows:

$$L_d(q_0, q_1) \approx \operatorname*{ext}_{\substack{q \in C^2([0,h], Q), \lambda \\ q(0) = q_0}} \left[\int_0^h L(q(t), \dot{q}(t)) dt \right] + \lambda(q_1 - q(h)),$$

$$\begin{aligned} L_d(q_0, q_1) &= \operatorname*{ext}_{\substack{q_d \in C_d^s([0,h], Q), \lambda \\ q(0) = q_0}} \left[h \sum_{i=1}^{s} b_i L(q_d(c_i h), \dot{q}_d(c_i h)) \right] + \lambda(q_1 - q_d(h)) \\ &= \operatorname*{ext}_{V^i, \lambda} \left\{ \left[h \sum_{i=1}^{s} b_i L\left(q_0 + h \sum_{j=1}^{s} A_{ij} V^j, \sum_{j=1}^{s} V^j \psi_j(c_i) \right) \right] \right. \end{aligned}$$

$$+\lambda\left(q_1 - q_0 - h\sum_{i=1}^{s} B_i V^i\right)\Bigg\}$$

$$\equiv \operatorname*{ext}_{V^i,\lambda} K(q_0, V^i, \lambda, q_1). \tag{4.10}$$

To obtain an expression for $L_d(q_0, q_1)$ we compute the stationarity conditions for $K(q_0, V^i, \lambda, q_1)$ under the fixed boundary condition (q_0, q_1) as follows:

$$\begin{aligned} 0 &= \frac{\partial K(q_0, V^i, \lambda, q_1)}{\partial V^j} \\ &= h\sum_{i=1}^{s} b_i\left(\frac{\partial L}{\partial q}(Q^i, \dot{Q}^i) h A_{ij} + \frac{\partial L}{\partial \dot{q}}(Q^i, \dot{Q}^i)\psi_j(c_i)\right) - h\lambda B_j, \quad j = 1, \ldots, s, \end{aligned} \tag{4.11a}$$

$$0 = \frac{\partial K(q_0, V^i, \lambda, q_1)}{\partial \lambda} = q_1 - q_0 - h\sum_{i=1}^{s} B_i V^i. \tag{4.11b}$$

4. By solving the $2s$ stationarity equations (4.11) we can express the parameters V^i and λ in terms of q_0 and q_1, that is, $V^i = V^i(q_0, q_1)$ and $\lambda = \lambda(q_0, q_1)$. Then the symplectic map $(q_0, p_0) \mapsto (q_1, p_1)$ can be expressed in terms of the internal stages and the Lagrange multiplier as follows:

$$\begin{aligned} p_0 &= -\frac{\partial L_d(q_0, q_1)}{\partial q_0} = -\left(\frac{\partial K(q_0, V^i(q_0, p_1), \lambda(q_0, p_1), q_1)}{\partial q_0}\right) \\ &= -\left(\frac{\partial K}{\partial q_0} + \frac{\partial K}{\partial V^i}\frac{\partial V^i}{\partial q_0} + \frac{\partial K}{\partial \lambda}\frac{\partial \lambda}{\partial q_0}\right) = -\frac{\partial K}{\partial q_0} \\ &= -h\sum_{i=1}^{s} b_i \frac{\partial L}{\partial q}(Q^i, \dot{Q}^i) + \lambda. \end{aligned} \tag{4.12}$$

Similarly, we obtain

$$\begin{aligned} p_1 &= \frac{\partial L_d(q_0, q_1)}{\partial q_1} = \frac{\partial K(q_0, V^i(q_0, p_1), \lambda(q_0, p_1), q_1)}{\partial q_1} \\ &= \frac{\partial K}{\partial q_1} + \frac{\partial K}{\partial V^i}\frac{\partial V^i}{\partial q_1} + + \frac{\partial K}{\partial \lambda}\frac{\partial \lambda}{\partial q_1} = \frac{\partial K}{\partial q_1} \\ &= \lambda. \end{aligned} \tag{4.13}$$

By combining (4.12) and (4.13) we obtain

$$p_1 = p_0 + h\sum_{i=1}^{s} b_i \frac{\partial L}{\partial q}(Q^i, \dot{Q}^i).$$

Substituting this into the stationarity condition (4.11a) yields

$$\sum_{i=1}^{s} b_i \frac{\partial L}{\partial \dot{q}}(Q^i, \dot{Q}^i)\psi_j(c_i) - p_0 B_j - h\sum_{i=1}^{s}(b_i B_j - b_i A_{ij})\frac{\partial L}{\partial q}(Q^i, \dot{Q}^i) = 0.$$

In summary, the above procedure gives a systematic way of constructing a generalized Galerkin Lagrangian variational integrator, which can be written in the following compact form:

$$q_1 = q_0 + h\sum_{i=1}^{s} B_i V^i, \tag{4.14a}$$

$$p_1 = p_0 + h\sum_{i=1}^{s} b_i \frac{\partial L}{\partial q}(Q^i, \dot{Q}^i), \tag{4.14b}$$

$$Q^i = q_0 + h\sum_{j=1}^{s} A_{ij} V^j, \quad i = 1, \dots, s, \tag{4.14c}$$

$$0 = \sum_{i=1}^{s} b_i \frac{\partial L}{\partial \dot{q}}(Q^i, \dot{Q}^i)\psi_j(c_i) - p_0 B_j - h\sum_{i=1}^{s}(b_i B_j - b_i A_{ij})\frac{\partial L}{\partial q}(Q^i, \dot{Q}^i), \quad j = 1, \dots, s, \tag{4.14d}$$

$$0 = \sum_{i=1}^{s} \psi_i(c_j) V^i - \dot{Q}^j, \quad j = 1, \dots, s, \tag{4.14e}$$

where (b_i, c_i) are the quadrature weights and quadrature points and $B_i = \int_0^1 \psi_i(\tau)\mathrm{d}\tau$ and $A_{ij} = \int_0^{c_i} \psi_j(\tau)\mathrm{d}\tau$.

As expected, this is equivalent to the generalized Galerkin Hamiltonian variational integrator, as the following proposition indicates.

PROPOSITION 4.1. If the continuous Hamiltonian $H(q, p)$ is hyperregular and we construct a Lagrangian $L(q, \dot{q})$ by the Legendre transformation, then the generalized Galerkin Hamiltonian variational integrator (4.6) and the generalized Galerkin Lagrangian variational integrator (4.14), associated with the same choice of basis functions ψ^i and numerical quadrature formula (b_i, c_i), are equivalent.

Proof. Since we chose the same basis functions and numerical quadrature formula for both methods, the approximations for q_1 and Q^i are the same in both methods, as can be seen by comparing (4.6a) to (4.14a) and (4.6c) to (4.14c). Since we assumed that the Lagrangian and Hamiltonian are related by $L(q, \dot{q}) = p\dot{q} - H(q, p)$, subject to the Legendre transformation $\dot{q} = \partial H/\partial p(q, p)$, we consider p to be a function of $(q, \dot{q})$ and compute

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

Since these identities have to hold at the internal stages, we have that

$$\frac{\partial H}{\partial p}(Q^i, P^i) = \dot{Q}^i,$$
$$\frac{\partial H}{\partial q}(Q^i, P^i) = \frac{\partial L}{\partial q}(Q^i, \dot{Q}^i),$$
$$P^i = \frac{\partial L}{\partial \dot{q}}(Q^i, \dot{Q}^i)$$

for $i = 1, \ldots, s$. Clearly, substituting these identities into (4.6b), (4.6d) and (4.6e) yields (4.14b), (4.14d) and (4.14e). Thus the two systems of equations (4.6) and (4.14) are equivalent once the Legendre transformation and the identities relating the continuous Lagrangian and Hamiltonian are taken into account. □

4.4 *Variational integrators and SPRK methods*

In this subsection we consider a special class of Galerkin variational integrators and demonstrate that they can be implemented as SPRK methods.

Let $C_d^s([0, 1], Q)$ be an s-dimensional function space and consider a set of basis functions $\psi_i(\tau)$ on $[0, 1]$ and a set of control points where c_i, $i = 1, \ldots, s$. We would like to construct a new set of basis functions $\phi_i(\tau)$ that span the same function space and satisfies $\phi_i(c_j) = \delta_{ij}$, where δ_{ij} is the Kronecker delta. This is possible whenever the matrix

$$M = \begin{bmatrix} \psi_1(c_1) & \psi_1(c_2) & \cdots & \psi_1(c_s) \\ \psi_2(c_1) & \psi_2(c_2) & \cdots & \psi_2(c_s) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_s(c_1) & \psi_s(c_2) & \cdots & \psi_s(c_s) \end{bmatrix} \tag{4.15}$$

is invertible. In particular, let $\psi(\cdot) = [\psi_1(\cdot), \ldots, \psi_s(\cdot)]^{\mathrm{T}}$ and construct a new set of basis functions $\phi(\cdot) = [\phi_1(\cdot), \ldots, \phi_s(\cdot)]^{\mathrm{T}}$ by $\phi(\cdot) = M^{-1}\psi(\cdot)$. It is easy to see that $\phi_i(c_j) = \delta_{ij}$ since

$$\begin{bmatrix} \phi_1(c_1) & \phi_1(c_2) & \cdots & \phi_1(c_s) \\ \phi_2(c_1) & \phi_2(c_2) & \cdots & \phi_2(c_s) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_s(c_1) & \phi_s(c_2) & \cdots & \phi_s(c_s) \end{bmatrix} = M^{-1}M = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}. \tag{4.16}$$

We can construct a numerical quadrature formula that is exact on the span of the basis functions $\psi_i(\tau)$ as follows. Since $\phi_i(c_j) = \delta_{ij}$, we can interpolate any function $f(\tau)$ on $[0, 1]$ at the control points c_i by taking $\bar{f}(\tau) = \sum_{i=1}^{s} f(c_i)\phi_i(\tau)$. Then we obtain the following quadrature formula:

$$\int_0^1 f(\tau)\mathrm{d}\tau \approx \int_0^1 \bar{f}(\tau)\mathrm{d}\tau = \int_0^1 \sum_{i=1}^{s} f(c_i)\phi_i(\tau)\mathrm{d}\tau = \sum_{i=1}^{s} f(c_i)\left[\int_0^1 \phi_i(\tau)\mathrm{d}\tau\right] \equiv \sum_{i=1}^{s} b_i f(c_i), \tag{4.17}$$

where $b_i = \int_0^1 \phi_i(\tau)\mathrm{d}\tau$ are the quadrature weights. By construction, the above quadrature formula is exact for any function in the s-dimensional function space $C_d^s([0, 1], Q)$. Now, if we apply this quadrature formula with the quadrature points c_i, then we obtain a Galerkin variational integrator that can be implemented as an SPRK method.

THEOREM 4.2. Given any set of basis functions $\psi(\cdot) = [\psi_1(\cdot), \ldots, \psi_s(\cdot)]^{\mathrm{T}}$ that span $C_d^s([0, 1], Q)$, consider the quadrature formula given in (4.17). Then the associated generalized Galerkin Hamiltonian variational integrator (4.6), which is expressed in terms of the discrete right Hamiltonian function (4.2), can be implemented by the following s-stage SPRK method applied to Hamilton's equations (2.1):

$$q_1 = q_0 + h \sum_{i=1}^{s} b_i \frac{\partial H}{\partial p}(Q^i, P^i), \tag{4.18a}$$

$$p_1 = p_0 - h \sum_{i=1}^{s} b_i \frac{\partial H}{\partial q}(Q^i, P^i), \tag{4.18b}$$

$$Q^i = q_0 + h \sum_{j=1}^{s} a_{ij} \frac{\partial H}{\partial p}(Q^j, P^j), \quad i = 1, \ldots, s, \tag{4.18c}$$

$$P^i = p_0 - h \sum_{j=1}^{s} \tilde{a}_{ij} \frac{\partial H}{\partial q}(Q^j, P^j), \quad i = 1, \ldots, s, \tag{4.18d}$$

where $b_i = \int_0^1 \phi_i(\tau)\mathrm{d}\tau \neq 0$, $a_{ij} = \int_0^{c_i} \phi_j(\tau)\mathrm{d}\tau$ and $\tilde{a}_{ij} = \frac{b_i b_j - b_j a_{ji}}{b_i}$. The basis functions satisfy $\phi_i(c_j) = \delta_{ij}$ and are given by $\phi(\cdot) = M^{-1}\psi(\cdot)$, where $\phi(\cdot) = [\phi_1(\cdot), \ldots, \phi_s(\cdot)]^{\mathrm{T}}$ and M is defined in (4.15).

Proof. The new basis functions $\phi(\tau)$ are constructed from the original basis functions $\psi(\tau)$ by the relationship $\phi(\cdot) = M^{-1}\psi(\cdot)$. Thus $\psi(\cdot) = M\phi(\cdot)$, and, in particular, $\psi_i(\tau) = \sum_{j=1}^{s} \psi_i(c_j)\phi_j(\tau)$. By substituting this into $B_i = \int_0^1 \psi_i(\tau)\mathrm{d}\tau$, equation (4.6a) becomes

$$\begin{aligned}
q_1 &= q_0 + h \sum_{i=1}^{s} B_i V^i \\
&= q_0 + h \sum_{i=1}^{s} V^i \int_0^1 \sum_{j=1}^{s} \psi_i(c_j)\phi_j(\tau)\mathrm{d}\tau \\
&= q_0 + h \sum_{j=1}^{s} \sum_{i=1}^{s} \psi_i(c_j) V^i \int_0^1 \phi_j(\tau)\mathrm{d}\tau \\
&= q_0 + h \sum_{j=1}^{s} \frac{\partial H}{\partial p}(Q^j, P^j) \int_0^1 \phi_j(\tau)\mathrm{d}\tau \\
&\equiv q_0 + h \sum_{j=1}^{s} b_j \frac{\partial H}{\partial p}(Q^j, P^j),
\end{aligned}$$

where we have used equation (4.6e) to go from the third equality to the fourth one. Similarly, by substituting $\psi_k(\tau) = \sum_{j=1}^{s} \psi_k(c_j)\phi_j(\tau)$ into $A_{ik} = \int_0^{c_i} \psi_k(\tau)\mathrm{d}\tau$ and using equation (4.6e), equation (4.6c) becomes

$$\begin{aligned}
Q^i &= q_0 + h \sum_{k=1}^{s} A_{ik} V^k \\
&= q_0 + h \sum_{k=1}^{s} V^k \int_0^{c_i} \sum_{j=1}^{s} \psi_k(c_j)\phi_j(\tau)\mathrm{d}\tau
\end{aligned}$$

$$= q_0 + h \sum_{j=1}^{s} \frac{\partial H}{\partial p}(Q^j, P^j) \int_0^{c_i} \phi_j(\tau) \mathrm{d}\tau$$

$$\equiv q_0 + h \sum_{j=1}^{s} a_{ij} \frac{\partial H}{\partial p}(Q^j, P^j),$$

where $a_{ij} = \int_0^{c_i} \phi_j(\tau)\mathrm{d}\tau$. Note that equation (4.6b) has the same form as (4.18b), and so we only have to recover equation (4.18d). Let $E^{\psi} = [E_1^{\psi}, \ldots, E_s^{\psi}]^{\mathrm{T}}$, where $E_j^{\psi} \equiv \sum_{i=1}^{s} b_i P^i \psi_j(c_i) - p_0 B_j + h \sum_{i=1}^{s} (b_i B_j - b_i A_{ij}) \frac{\partial H}{\partial q}(Q^i, P^i) = 0$, which corresponds to (4.6d). By substituting

$$B_i = \int_0^1 \psi_i(\tau)\mathrm{d}\tau = \int_0^1 \sum_{j=1}^{s} \psi_i(c_j)\phi_j(\tau)\mathrm{d}\tau$$

and $b_i = \int_0^1 \phi_i(\tau)\mathrm{d}\tau$ into E_j^{ψ}, we obtain

$$\begin{aligned}
0 = E_j^{\psi} &= \sum_{i=1}^{s} b_i P^i \psi_j(c_i) - p_0 B_j + h \sum_{i=1}^{s} (b_i B_j - b_i A_{ij}) \frac{\partial H}{\partial q}(Q^i, P^i) \\
&= \sum_{i=1}^{s} b_i P^i \psi_j(c_i) - p_0 \int_0^1 \psi_j(\tau)\mathrm{d}\tau + h \sum_{i=1}^{s} \left(b_i \int_0^1 \psi_j(\tau)\mathrm{d}\tau - b_i \int_0^{c_i} \psi_j(\tau)\mathrm{d}\tau \right) \frac{\partial H}{\partial q}(Q^i, P^i) \\
&= \sum_{i=1}^{s} b_i P^i \psi_j(c_i) - p_0 \int_0^1 \sum_{i=1}^{s} \psi_j(c_i)\phi_i(\tau)\mathrm{d}\tau \\
&\quad + h \sum_{i=1}^{s} \left(b_i \int_0^1 \sum_{k=1}^{s} \psi_j(c_k)\phi_k(\tau)\mathrm{d}\tau - b_i \int_0^{c_i} \sum_{k=1}^{s} \psi_j(c_k)\phi_k(\tau)\mathrm{d}\tau \right) \frac{\partial H}{\partial q}(Q^i, P^i) \\
&= \sum_{i=1}^{s} \psi_j(c_i) \left(b_i P^i - b_i p_0 + h \sum_{k=1}^{s} (b_i b_k - b_k a_{ki}) \frac{\partial H}{\partial q}(Q^k, P^k) \right).
\end{aligned}$$

We have swapped the role of the indices i and k in the second-to-last line to obtain the final equality. Let $E^{\phi} = [E_1^{\phi}, \ldots, E_s^{\phi}]^{\mathrm{T}}$, where $E_i^{\phi} \equiv b_i P^i - b_i p_0 + h \sum_{k=1}^{s} (b_i b_k - b_k a_{ki}) \frac{\partial H}{\partial q}(Q^k, P^k)$. Then the above equation can be viewed as the jth component of the system of equations $M E^{\phi} \equiv E^{\psi} = 0$, where $M = [\psi_i(c_j)]$ is invertible. Therefore we have that $E^{\phi} = 0$, that is, $E_i^{\phi} = b_i P^i - b_i p_0 + h \sum_{k=1}^{s} (b_i b_k - b_k a_{ki}) \frac{\partial H}{\partial q}(Q^k, P^k) = 0$. Since $b_i \neq 0$, dividing by b_i and recalling that $\tilde{a}_{ij} = \frac{b_i b_j - b_j a_{ji}}{b_i}$ yields (4.18d). □

4.4.1 *Comparison with discrete Lagrangian SPRK methods.* Proposition 4.1 states that, for hyperregular Hamiltonians, if one chooses the same basis functions and quadrature formula, the the generalized Galerkin Hamiltonian variational integrator is equivalent to the generalized Galerkin Lagrangian variational integrator. Therefore the above theorem also applies in the Lagrangian setting. In particular, if one chooses the Lagrange polynomials associated with the quadrature nodes c_i as our choice of basis functions $\psi_i(\tau)$, then the coefficients of the SPRK method derived above agree with the method derived in Marsden & West (2001) using discrete Lagrangians. However, our approach remains valid in the case of degenerate Hamiltonians, for which it is impossible to obtain a Lagrangian and apply the method in Marsden & West (2001) to derive Hamiltonian variational integrators.

The derivation on page 209 of the book Hairer *et al.* (2006), which is analogous to the result in Suris (1990), generalizes the approach in Marsden & West (2001) by considering discrete Lagrangian SPRK methods without the restriction that the Runge–Kutta coefficients are obtained from integrals of Lagrange polynomials. It is, however, unclear how one should choose these coefficients. In contrast, our approach provides a systematic means of deriving the coefficients by an appropriate choice of basis functions and quadrature formula. Our discrete Hamiltonian method is expressed in terms of Type II generating functions and the continuous Hamiltonian, as opposed to the discrete Lagrangian approach based on Type I generating functions and the continuous Lagrangian.

4.4.2 *Discrete Hamiltonian associated with the Galerkin SPRK method.* For the SPRK method (4.18) described above we can explicitly compute the corresponding Type II generating function $H_d^+(q_0, p_1)$ given in (4.2) as follows:

$$\begin{aligned} H_d^+(q_0, p_1) &= p_1 q_d(h) - h\sum_{i=1}^{s} b_i[P^i \dot{q}_d(c_i h) - H(Q^i, P^i)] \\ &= p_1\left(q_0 + h\sum_{i=1}^{s} b_i \frac{\partial H}{\partial p}(Q^i, P^i)\right) - h\sum_{i=1}^{s} b_i \left[P^i \frac{\partial H}{\partial p}(Q^i, P^i) - H(Q^i, P^i)\right] \\ &= p_1 q_0 + h\sum_{i=1}^{s} b_i(p_1 - P^i)\frac{\partial H}{\partial p}(Q^i, P^i) + h\sum_{i=1}^{s} b_i H(Q^i, P^i) \\ &= p_1 q_0 - h^2 \sum_{i,j=1}^{s} b_i a_{ij}\frac{\partial H}{\partial q}(Q^i, P^i)\frac{\partial H}{\partial p}(Q^j, P^j) + h\sum_{i=1}^{s} b_i H(Q^i, P^i). \end{aligned} \tag{4.19}$$

This Type II generating function is consistent with the Type I generating function for SPRK methods that was given in Theorem 5.4 on page 198 of Hairer *et al.* (2006).

4.4.3 *Sufficient condition for consistency of the SPRK method.* If the constant function $f(x) = 1$ is in the finite-dimensional function space C_d^s, then, by interpolation, we have that $1 = \sum_{i=1}^{s} f(c_i)\phi_i(\tau) = \sum_{i=1}^{s} \phi_i(\tau)$. Thus $\sum_{i=1}^{s} b_i = \int_0^1 \sum_{i=1}^{s} \phi_i(\tau)\mathrm{d}\tau = 1$. Partitioned Runge–Kutta order theory (Butcher, 2008) states that the condition $\sum_{i=1}^{s} b_i = 1$ implies that the variational integrator (4.18) is at least first order. Therefore, to obtain a consistent method, it is sufficient that the constant function is in the span of the basis functions we choose. In particular, if we let $\psi_1(\tau) = 1$, then we ensure that our method is at least first order.

4.4.4 *Construction of the SPRK tableau.* Let the SPRK method (4.18) be denoted by the following tableau.

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array} \qquad \begin{array}{c|ccc} \tilde{c}_1 & \tilde{a}_{11} & \cdots & \tilde{a}_{1s} \\ \vdots & \vdots & & \vdots \\ \tilde{c}_s & \tilde{a}_{s1} & \cdots & \tilde{a}_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}$$

Based on the above generalized Galerkin method, the coefficients in the partitioned Runge–Kutta tableau can be constructed in the following systematic way.

ALGORITHM 4.3 (GENERALIZED GALERKIN HAMILTONIAN SPRK METHOD).

1. Choose a basis set $\psi_i(\tau)$, where $\tau \in [0, 1]$, $and i = 1, \ldots, s$, with $\psi_1(\tau) = 1$.
2. Choose quadrature points c_i, where $i = 1, \ldots, s$. Ensure that $M = [\psi_i(c_j)]$ is invertible.
3. Let the column vector $b = [b_1, b_2, \ldots, b_s]^{\mathrm{T}}$ contain the coefficients in the SPRK tableau. There are two ways to obtain b.

   (i) Compute $B_i = \int_0^1 \psi_i(\tau)\mathrm{d}\tau$ and let $B = [B_1, B_2, \ldots, B_s]^{\mathrm{T}}$. Then we have $b = M^{-1}B$.

   (ii) Compute a new basis set $\phi_i(\tau)$ by using the relation $\phi(\tau) = M^{-1}\psi(\tau)$, and then compute $b = [b_1, b_2, \ldots, b_s]^{\mathrm{T}}$ by $b_i = \int_0^1 \phi_i(\tau)\mathrm{d}\tau$.

4. Let the matrix $A^{\phi} = [a_{ij}]$ contain the coefficients of the SPRK tableau. As before, there are two ways to obtain A^{ϕ}.

   (i) Compute the coefficients $A^{\psi} = [A_{ij}]$, where $A_{ij} = \int_0^{c_i} \psi_j(\tau)\mathrm{d}\tau$. Then the matrix is given by $A^{\phi} = [a_{ij}] = A^{\psi}M^{-\mathrm{T}}$.

   (ii) Compute $A^{\phi} = [a_{ij}]$, where $a_{ij} = \int_0^{c_i} \phi_j(\tau)\mathrm{d}\tau$, directly by using the new basis functions $\phi(\cdot) = M^{-1}\psi(\cdot)$.

5. Compute the coefficients $\tilde{A}^{\phi} = [\tilde{a}_{ij}]$ by using $\tilde{a}_{ij} = \frac{b_i b_j - b_j a_{ji}}{b_i}$.

4.5 *Examples*

In this subsection we will consider four examples to illustrate the above procedure for constructing variational integrators.

EXAMPLE 4.4. We consider one-stage methods. Choose the basis function $\psi_1 = 1$. Then, for any quadrature point c_1, the matrix $M = [\psi_1(c_1)] = [1]$ is invertible.

(i) If $c_1 = 0$, then $b_1 = 1$, $a_{11} = 0$, and $\tilde{a}_{11} = 1$, which is the symplectic Euler method.
(ii) If $c_1 = \frac{1}{2}$, then $b_1 = 1$, $a_{11} = \frac{1}{2}$, and $\tilde{a}_{11} = \frac{1}{2}$, which is the midpoint rule.
(iii) If $c_1 = 1$, then $b_1 = 1$, $a_{11} = 1$, and $\tilde{a}_{11} = 0$, which is the adjoint symplectic Euler method.

EXAMPLE 4.5. Choose the basis functions $\psi_1 = 1$ and $\psi_2 = \cos(\pi\tau)$. If we choose the quadrature points $c_1 = 0$ and $c_2 = 1$, then we obtain

$$M = \begin{bmatrix} \psi_1(c_1) & \psi_1(c_2) \\ \psi_2(c_1) & \psi_2(c_2) \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \quad \text{and} \quad M^{-1} = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$

One can easily compute

$$B_1 = \int_0^1 \psi_1(\tau)\mathrm{d}\tau = 1, \quad B_2 = \int_0^1 \psi_1(\tau)\mathrm{d}\tau = 0.$$

Therefore we get $b = [b_1, b_2]^{\mathrm{T}} = M^{-1}B = [\frac{1}{2}, \frac{1}{2}]^{\mathrm{T}}$, which is the trapezoidal rule. We also compute

$$A^{\psi} = \begin{bmatrix} \int_0^{c_1} \psi_1(\tau)\mathrm{d}\tau & \int_0^{c_1} \psi_2(\tau)\mathrm{d}\tau \\ \int_0^{c_2} \psi_1(\tau)\mathrm{d}\tau & \int_0^{c_2} \psi_2(\tau)\mathrm{d}\tau \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}.$$

Therefore the matrix

$$A^{\phi} = \begin{bmatrix} \int_0^{c_1} \phi_1(\tau)\mathrm{d}\tau & \int_0^{c_1} \phi_2(\tau)\mathrm{d}\tau \\ \int_0^{c_2} \phi_1(\tau)\mathrm{d}\tau & \int_0^{c_2} \phi_2(\tau)\mathrm{d}\tau \end{bmatrix} = A^{\psi} M^{-\mathrm{T}} = \begin{bmatrix} 0 & 0 \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}.$$

By using the relationship $\tilde{a}_{ij} = \frac{b_i b_j - b_j a_{ji}}{b_i}$, one obtains

$$\tilde{A}^{\phi} = [\tilde{a}_{ij}] = \begin{bmatrix} 0 & 0 \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}.$$

Thus we obtain the Störmer–Verlet method. Interestingly, the Störmer–Verlet method is typically derived as a variational integrator by using linear interpolation, that is, $\psi_1 = 1$ *and* $\psi_2 = \tau$, and the trapezoidal rule.

EXAMPLE 4.6. If we choose the basis functions $\psi_1 = 1$, $\psi_2 = \cos(\pi\tau)$ and $\psi_3 = \sin(\pi\tau)$ and the quadrature points $c_1 = 0, c_2 = \frac{1}{2}$ and $c_3 = 1$, then we obtain a new method that is second-order accurate, and the coefficients of the SPRK method are given by

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{\pi} & \frac{\pi-4}{4\pi} \\ 1 & \frac{\pi-2}{2\pi} & \frac{2}{\pi} & \frac{\pi-2}{2\pi} \\ \hline & \frac{\pi-2}{2\pi} & \frac{2}{\pi} & \frac{\pi-2}{2\pi} \end{array} \qquad \begin{array}{c|ccc} \frac{\pi^2-2\pi-4}{2\pi^2-4\pi} & \frac{\pi-2}{2\pi} & \frac{\pi-4}{\pi^2-2\pi} & 0 \\ \frac{1}{2} & \frac{\pi-2}{2\pi} & \frac{1}{\pi} & 0 \\ \frac{\pi^2-2\pi+4}{2\pi^2-4\pi} & \frac{\pi-2}{2\pi} & \frac{1}{\pi-2} & 0 \\ \hline & \frac{\pi-2}{2\pi} & \frac{2}{\pi} & \frac{\pi-2}{2\pi} \end{array}$$

EXAMPLE 4.7. Chebyshev quadrature (see Hildebrand, 1974, p. 415) is designed to approximate weighted integrals of the form

$$\int_{-1}^{1} f(x)w(x)\mathrm{d}x = b\sum_{i=1}^{s} f(x_i) + E[f(x)]$$

by an equally weighted sum of the function values at the quadrature points x_i and an error term $E[f(x)]$. The weight b is chosen so that the quadrature is exact for $f(x) = 1$, that is, $b = \frac{1}{s}\int_{-1}^{1} w(x)\mathrm{d}x$. We are primarily interested in the case when the weight function $w(x) = 1$, in which case the quadrature formula becomes

$$\int_{-1}^{1} f(x)\mathrm{d}x = \frac{2}{s}\sum_{i=1}^{s} f(x_i) + E[f(x)],$$

where the quadrature points x_i are given by the roots of polynomials (see Hildebrand, 1974, p. 418), the first three of which are given by

$$G_0(x) = 1, \quad G_1(x) = x, \quad G_2(x) = \frac{1}{3}(3x^2 - 1), \quad G_3(x) = \frac{1}{2}(2x^3 - x). \tag{4.20}$$

The error term associated with the s-point formula is given by

$$E = \begin{cases} e_s \frac{f^{(s+1)}(\xi)}{(s+1)!} & s \text{ odd}, \\ e_s \frac{f^{(s+2)}(\xi)}{(s+2)!} & s \text{ even}, \end{cases} \quad \text{where } e_s = \begin{cases} \int_{-1}^{1} x G_s(x)\mathrm{d}x & s \text{ odd}, \\ \int_{-1}^{1} x^2 G_s(x)\mathrm{d}x & s \text{ even}. \end{cases}$$

The error term implies that the quadrature has degree of precision s for odd s and degree of precision $s+1$ for even s. Note that the roots x_i of the polynomials G_i are in the interval $[-1, 1]$, so that, after a change of coordinates, we obtain the quadrature points c_i in the interval $[0, 1]$ as follows, Then we use Lagrange polynomials associated with these quadrature points to construct variational integrators for $s = 1, 2, 3$ as follows.

(i) *One-stage, second-order method*

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array} \qquad \begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$

(ii) *Two-stage, fourth-order method*

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

(iii) *Three-stage, fourth-order method*

$$\begin{array}{c|ccc} \frac{1}{2}-\frac{\sqrt{2}}{4} & \frac{1}{6}+\frac{\sqrt{2}}{48} & \frac{1}{6}-\frac{\sqrt{2}}{6} & \frac{1}{6}-\frac{5\sqrt{2}}{48} \\ \frac{1}{2} & \frac{1}{6}+\frac{\sqrt{2}}{8} & \frac{1}{6} & \frac{1}{6}-\frac{\sqrt{2}}{8} \\ \frac{1}{2}+\frac{\sqrt{2}}{4} & \frac{1}{6}+\frac{5\sqrt{2}}{48} & \frac{1}{6}+\frac{\sqrt{2}}{6} & \frac{1}{6}-\frac{\sqrt{2}}{48} \\ \hline & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{array}$$

$$\begin{array}{c|ccc} \frac{1}{2}-\frac{\sqrt{2}}{4} & \frac{1}{6}-\frac{\sqrt{2}}{48} & \frac{1}{6}-\frac{\sqrt{2}}{8} & \frac{1}{6}-\frac{5\sqrt{2}}{48} \\ \frac{1}{2} & \frac{1}{6}+\frac{\sqrt{2}}{6} & \frac{1}{6} & \frac{1}{6}-\frac{\sqrt{2}}{6} \\ \frac{1}{2}+\frac{\sqrt{2}}{4} & \frac{1}{6}+\frac{5\sqrt{2}}{48} & \frac{1}{6}+\frac{\sqrt{2}}{8} & \frac{1}{6}+\frac{\sqrt{2}}{48} \\ \hline & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{array}$$

For $s = 1, 2$ we obtain the same methods as the ones obtained using Gauss–Legendre quadrature, namely, the midpoint rule and the two-stage, fourth-order method, respectively. For $s = 3$ we obtain a three-stage SPRK that is fourth order. The order of the SPRK methods above is determined using partitioned Runge–Kutta order theory (Butcher, 2008).

5. Momentum preservation and invariance of the discrete right Hamiltonian function

5.1 *Momentum maps*

First, we recall the definition of a momentum map defined on T^*Q given in Abraham & Marsden (1978).

DEFINITION 5.1. Let (P, ω) be a connected symplectic manifold and let $\Phi\colon G \times P \to P$ be a symplectic action of the Lie group G on P, that is, for each $g \in G$ the map $\Phi_g\colon P \to P;\ x \mapsto \Phi(g, x)$ is symplectic. We say that a map $J\colon P \to \mathfrak{g}^*$, where $\mathfrak{g}^*$ is a dual space of the Lie algebra $\mathfrak{g}$ of G, is a momentum map for the action Φ if, for every $\xi \in \mathfrak{g}$, we have $\mathrm{d}\hat{J}(\xi) = i_{\xi_P}\omega$, where $\hat{J}(\xi)\colon P \to \mathbb{R}$ is defined by $\hat{J}(\xi)(x) = J(x)\cdot\xi$ and ξ_P is the infinitesimal generator of the action corresponding to ξ. In other words, J is a momentum map provided that $X_{\hat{J}(\xi)} = \xi_P$ for all $\xi \in \mathfrak{g}$.

For our purposes, we are interested in the case where $P = T^*Q$ and $\omega = \mathrm{d}q^i \wedge \mathrm{d}p_i$ is the canonical symplectic two-form on T^*Q. This gives a momentum map of the form $J\colon T^*Q \to \mathfrak{g}^*$, and we now describe the construction given in Theorem 4.2.10 of Abraham & Marsden (1978). Note that ω is exact since $\omega = -\mathrm{d}\theta = -\mathrm{d}(p_i \mathrm{d}q^i)$. Consider an action Φ_g that leaves the Lagrange one-form θ invariant, that is, $\Phi_g^*\theta = \theta$ for all $g \in G$. Then the momentum map $J\colon T^*Q \to \mathfrak{g}^*$ is given by

$$J(x)\cdot\xi = i_{\xi_P}\theta(x). \tag{5.1}$$

We can show that this satisfies the definition of the momentum map given above by using the fact that Φ_g leaves the one-form θ invariant for all $g \in G$ and ξ_P is the infinitesimal generator of the action corresponding to ξ. This implies that the Lie derivative of θ along the vector field ξ_P vanishes, that is, $\pounds_{\xi_P}\theta = 0$ for all $\xi \in \mathfrak{g}$. By Cartan's magic formula, we have

$$0 = \pounds_{\xi_P}\theta = i_{\xi_P}\mathrm{d}\theta + \mathrm{d}i_{\xi_P}\theta.$$

Therefore $\mathrm{d}i_{\xi_P}\theta = -i_{\xi_P}\mathrm{d}\theta = i_{\xi_P}\omega$. Thus, $\hat{J}(\xi)(x) = i_{\xi_P}\theta$ satisfies the defining property, $\mathrm{d}\hat{J}(\xi) = i_{\xi_P}\omega$, of a momentum map. Then $J(x)\cdot\xi = \hat{J}(\xi)(x) = i_{\xi_P}\theta(x)$. Moreover, by Theorem 4.2.10 of Abraham & Marsden (1978), this momentum map is Ad*-equivariant.

Let $\Phi\colon G \times Q \to Q$ be an action of the Lie group G on Q. We will give the coordinate expression for the cotangent lifted action Φ^{T^*Q}. In coordinates, we denote $\Phi_{g^{-1}}\colon Q \to Q$ by $q^i = \Phi^i_{g^{-1}}(Q)$, and then its cotangent lifted action $\Phi^{T^*Q}\colon G \times T^*Q \to T^*Q$ is given by

$$\Phi^{T^*Q}(g,q,p) = T^*\Phi_{g^{-1}}(q,p) = \left(\Phi^i_g(q),\, p_j\frac{\partial q^j}{\partial \Phi^i_g(q)}\right), \tag{5.2}$$

where $T^*\Phi_{g^{-1}}$ means the cotangent lift of the action $\Phi_{g^{-1}}$.

In the following proposition we give the coordinate expression for the cotangent lifted action and show that it leaves the Lagrange one-form $\theta = p_i\,\mathrm{d}q^i$ invariant.

PROPOSITION 5.2. Given an action $\Phi\colon G \times Q$ of a Lie group G on Q, the cotangent lifted action $\Phi^{T^*Q}\colon G \times T^*Q \to T^*Q$ leaves the Lagrange one-form $\theta = p_i\,\mathrm{d}q^i$ invariant.

Proof. Given $g \in G$, let the cotangent lifted action of g on (q,p) be denoted by $(Q,P) = \Phi_g^{T^*Q}(q,p)$, the components of which are given by $Q^i = \Phi^i_g(q)$ and $P_i = p_j\frac{\partial q^j}{\partial \Phi^i_g(q)}$. Then a direct computation yields

$$P_i\,\mathrm{d}Q^i = P_i\,\mathrm{d}\Phi^i_g(q) = p_j\frac{\partial q^j}{\partial \Phi^i_g(q)}\frac{\partial \Phi^i_g(q)}{\partial q^j}\mathrm{d}q^j = p_j\,\mathrm{d}q^j. \tag{5.3}$$

This shows that $\Phi_g^{T^*Q}$ leaves the Lagrange one-form $p_i\,\mathrm{d}q^i$ invariant. □

Corresponding to the cotangent lift action Φ^{T^*Q}, for every $\xi \in \mathfrak{g}$ the momentum map $J\colon T^*Q \to \mathfrak{g}^*$ defined in (5.1) has the following explicit expression in coordinates:

$$J(\alpha_q)\cdot\xi = i_{\xi_P}(p_i\,\mathrm{d}q^i)(\alpha_q) = p\cdot\xi_Q(q) = p\cdot\left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0}\Phi_{\exp(\epsilon\xi)}(q^i), \tag{5.4}$$

where $\alpha_q = (q,p) \in T^*Q$.

5.2 *Discrete Noether's theorem*

In the discrete case, consider the one-step discrete flow map $F_{H_d^+}\colon (q_0, p_0) \mapsto (q_1, p_1)$ defined by the discrete right Hamilton's equations

$$p_0 = D_1 H_d^+(q_0, p_1), \quad q_1 = D_2 H_d^+(q_0, p_1). \tag{5.5}$$

We will show that if the generalized discrete Lagrangian $R_d(q_0, q_1, p_1) = p_1 q_1 - H_d^+(q_0, p_1)$ is invariant under the cotangent lifted action, then we have discrete momentum preservation, which is the discrete analogue of Noether's theorem for discrete Hamiltonian mechanics.

THEOREM 5.3. Let Φ^{T^*Q} be the cotangent lift action of the action Φ on the configuration manifold Q. If the generalized discrete Lagrangian $R_d(q_0, q_1, p_1) = p_1 q_1 - H_d^+(q_0, p_1)$ is invariant under the cotangent lifted action Φ^{T^*Q}, then the discrete flow map of the discrete right Hamilton's equations preserves the momentum map, that is, $F^*_{H_d^+} J = J$.

Proof. In coordinates, let $(q_0^\epsilon, p_0^\epsilon) := \Phi^{T^*Q}_{\exp(\epsilon\xi)}(q_0, p_0)$ and $(q_1^\epsilon, p_1^\epsilon) := \Phi^{T^*Q}_{\exp(\epsilon\xi)}(q_1, p_1)$. From the invariance of $p_1 q_1 - H_d^+(q_0, p_1)$ we have that

$$\begin{aligned}
0 &= \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} \{p_1^\epsilon q_1^\epsilon - H_d^+(q_0^\epsilon, p_1^\epsilon)\} \\
&= p_1 \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} q_1^\epsilon + q_1 \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} p_1^\epsilon - D_1 H_d^+(q_0, p_1) \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} q_0^\epsilon - D_2 H_d^+(q_0, p_1) \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} p_1^\epsilon \\
&= p_1 \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} q_1^\epsilon + q_1 \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} p_1^\epsilon - p_0 \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} q_0^\epsilon - q_1 \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} p_1^\epsilon \\
&= p_1 \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} \Phi_{\exp(\epsilon\xi)}(q_1) - p_0 \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} \Phi_{\exp(\epsilon\xi)}(q_0) \\
&= p_1 \cdot \xi_Q(q_1) - p_0 \cdot \xi_Q(q_0),
\end{aligned} \tag{5.6}$$

where we have used the discrete right Hamilton's equations (5.5) in going from the second to the third line, and $q_0^\epsilon = \Phi_{\exp(\epsilon\xi)}(q_0)$ and $q_1^\epsilon = \Phi_{\exp(\epsilon\xi)}(q_1)$ are used in going from the third to the fourth line. Then, by the definition of $F_{H_d^+}$ and J, (5.6) states that $F^*_{H_d^+} J = J$. □

5.3 *G-invariant generalized discrete Lagrangians from G-equivariant interpolants*

We now provide a systematic means of constructing a discrete Hamiltonian, so that the generalized discrete Lagrangian $R_d(q_0, q_1, p_1) = p_1 q_1 - H_d^+(q_0, p_1)$ is G-invariant, provided that the generalized Lagrangian $R(q, \dot{q}, p) = p\dot{q} - H(q, p)$ is G-invariant.

Our construction will be based on an interpolatory function $\varphi\colon Q^r \to C^2([0, h], Q)$ that is parameterized by $r + 1$ internal points $q^\nu \in Q$, defined at the times $0 = d_0 h < d_1 h < \cdots < d_r h \leqslant h$, that is, $\varphi(d_\eta h; \{q^\nu\}_{\nu=0}^r) = q^\eta$. We also use a numerical quadrature formula given by the quadrature weights b_i and the quadrature points c_i. We denote the momentum at the time $c_i h$ by p^i. Then we construct the following discrete Hamiltonian:

$$H_d^+(q_0, p_1) = \operatorname*{ext}_{\substack{q^\nu \in Q, p^i \in Q^* \\ q^0 = q_0}} \left[p_1 \cdot \varphi(h; \{q^\nu\}_{\nu=0}^r) - \sum_{i=1}^s b_i R(T\varphi(c_i h; \{q^\nu\}_{\nu=0}^r), p^i) \right], \tag{5.7}$$

where $R(q, \dot{q}, p) = p\dot{q} - H(q, p)$. An interpolatory function is G-equivariant if

$$\varphi(t; \{gq^\nu\}_{\nu=0}^r) = g\varphi(t; \{q^\nu\}_{\nu=0}^r).$$

Then a G-invariant discrete Hamiltonian can be obtained if we use G-equivariant interpolatory functions.

LEMMA 5.4. Let G be a Lie group acting on Q such that $gQ = Q$ for all $g \in G$. If the interpolatory function $\varphi(t; \{gq^\nu\}_{\nu=0}^r)$ is G-equivariant and the generalized Lagrangian $R : TQ \oplus T^*Q \to \mathbb{R}$,

$$R(q, \dot{q}, p) = p\dot{q} - H(q, p),$$

is G-invariant, then the generalized discrete Lagrangian $R_d : Q \times T^*Q \to \mathbb{R}$, given by

$$R_d(q_0, q_1, p_1) = p_1 q_1 - H_d^+(q_0, p_1),$$

where,

$$H_d^+(q_0, p_1) = \operatorname*{ext}_{\substack{q^\nu \in Q, p^i \in Q^* \\ q^0 = q_0}} \left[p_1 \cdot \varphi(h; \{q^\nu\}_{\nu=0}^r) - \sum_{i=1}^s b_i R(T\varphi(c_i h; \{q^\nu\}_{\nu=0}^r), p^i) \right],$$

is G-invariant.

Proof. To simplify the notation we denote the cotangent lifted action of G on Q by $\Phi_g^{T^*Q}(q, p) = (gq, gp)$. First, we note that

$$\begin{aligned} R_d(q_0, q_1, p_1) &= p_1 q_1 - \operatorname*{ext}_{\substack{q^\nu \in Q, p^i \in Q^* \\ q^0 = q_0}} \left[p_1 \cdot \varphi(h; \{q^\nu\}_{\nu=0}^r) - \sum_{i=1}^s b_i R(T\varphi(c_i h; \{q^\nu\}_{\nu=0}^r), p^i) \right] \\ &= \operatorname*{ext}_{\substack{q^\nu \in Q, p^i \in Q^* \\ q^0 = q_0}} \left[\sum_{i=1}^s b_i R(T\varphi(c_i h; \{q^\nu\}_{\nu=0}^r), p^i) \right]. \end{aligned}$$

Then

$$\begin{aligned} R_d(gq_0, gq_1, gp_1) &= \operatorname*{ext}_{\substack{\tilde{q}^\nu \in Q, \tilde{p}^i \in Q^* \\ \tilde{q}^0 = gq_0}} \left[\sum_{i=1}^s b_i R(T\varphi(c_i h; \{\tilde{q}^\nu\}_{\nu=0}^r), \tilde{p}^i) \right] \\ &= \operatorname*{ext}_{\substack{q^\nu \in g^{-1}Q, p^i \in g^{-1}Q^* \\ gq^0 = gq_0}} \left[\sum_{i=1}^s b_i R(T\varphi(c_i h; \{gq^\nu\}_{\nu=0}^r), gp^i) \right] \\ &= \operatorname*{ext}_{\substack{q^\nu \in Q, p^i \in Q^* \\ q^0 = q_0}} \left[\sum_{i=1}^s b_i R(TL_g \cdot T\varphi(c_i h; \{q^\nu\}_{\nu=0}^r), gp^i) \right] \\ &= \operatorname*{ext}_{\substack{q^\nu \in Q, p^i \in Q^* \\ q^0 = q_0}} \left[\sum_{i=1}^s b_i R(T\varphi(c_i h; \{q^\nu\}_{\nu=0}^r), p^i) \right] \\ &= R_d(q_0, q_1, p_1), \end{aligned}$$

where we have used the identification $\tilde{q}^\nu = gq^\nu$ in the second equality, the G-equivariance of the interpolatory function and the property that $gQ = Q$ in the third equality and the G-invariance of the generalized Lagrangian in the fourth equality. □

In view of Theorem 5.3 and Lemma 5.4, if we use a G-equivariant interpolatory function to construct a discrete Hamiltonian as given in (5.7), then the discrete flow given by the discrete right Hamilton's equations will preserve the momentum map $J : T^*Q \to \mathfrak{g}^*$.

5.4 *Natural charts and G-equivariant interpolants*

Following the approach of Marsden *et al.* (1999), we use the group exponential map at the identity, $\exp_e : \mathfrak{g} \to G$, to construct a G-equivariant interpolatory function and a higher-order discrete Lagrangian. As shown in Lemma 5.4, this construction yields a G-invariant generalized discrete Lagrangian if the generalized Lagrangian itself is G-invariant.

In a finite-dimensional Lie group G, $\exp_e$ is a local diffeomorphism, and thus there is an open neighbourhood $U \subset G$ of e such that $\exp_e^{-1} : U \to \mathfrak{u} \subset \mathfrak{g}$. When the group acts on the left we obtain a chart $\psi_g \colon L_g U \to \mathfrak{u}$ at $g \in G$ by

$$\psi_g = \exp_e^{-1} \circ L_{g^{-1}}.$$

LEMMA 5.5. The interpolatory function given by

$$\varphi(g^\nu; \tau h) = \psi_{g^0}^{-1}\left(\sum_{\nu=0}^{s} \psi_{g^0}(g^\nu)\tilde{l}_{\nu,s}(\tau)\right)$$

is G-equivariant.

Proof. we have

$$\begin{aligned}
\varphi(gg^\nu; \tau h) &= \psi_{(gg^0)}^{-1}\left(\sum_{\nu=0}^{s} \psi_{gg^0}(gg^\nu)\tilde{l}_{\nu,s}(\tau)\right)\\
&= L_{gg^0} \exp_e\left(\sum_{\nu=0}^{s} \exp_e^{-1}((gg^0)^{-1}(gg^\nu))\tilde{l}_{\nu,s}(\tau)\right)\\
&= L_g L_{g^0} \exp_e\left(\sum_{\nu=0}^{s} \exp_e^{-1}((g^0)^{-1}g^{-1}gg^\nu))\tilde{l}_{\nu,s}(\tau)\right)\\
&= L_g \psi_{g^0}^{-1}\left(\sum_{\nu=0}^{s} \exp_e^{-1} \circ L_{(g^0)^{-1}}(g^\nu)\tilde{l}_{\nu,s}(\tau)\right)\\
&= L_g \psi_{g^0}^{-1}\left(\sum_{\nu=0}^{s} \psi_{g^0}(g^\nu)\tilde{l}_{\nu,s}(\tau)\right)\\
&= L_g \varphi(g^\nu; \tau h).
\end{aligned}$$

□

This G-equivariant interpolatory function based on natural charts allows one to construct discrete Lie group Hamiltonian variational integrators that preserve the momentum map.

6. Numerical experiments

In this section we apply some of the SPRK methods derived in Section 4.5 to the model degenerate Hamiltonian system (Example 1.1) and the harmonic oscillator, and numerically verify the theoretical order of accuracy of these methods and consider the error behaviour for position, momentum and energy.

EXAMPLE 6.1. For the degenerate Hamiltonian $H = qp$, the associated Hamilton's equations are

$$\dot{q} = q, \quad \dot{p} = -p, \tag{6.1}$$

which have $q(t) = q_0 \exp(t)$ and $p(t) = p_0 \exp(-t)$ as the exact solution, where (q_0, p_0) is the initial value at time $t = 0$. We consider the methods derived in Example 4.7 and refer to the three-stage method as the Cheby4 method and refer to the two-stage method as the GauLe4 method since it can also be derived by using Gauss–Legendre quadrature. Here, the number 4 in Cheby4 and GauLe4 reflects the fact that both of these methods are fourth-order accurate.

By applying the Cheby4 method to (6.1) we obtain the following numerical scheme:

$$q_{n+1} = -\frac{h^3 + 10h^2 + 48h + 96}{h^3 - 10h^2 + 48h - 96} q_n, \quad p_{n+1} = -\frac{h^3 - 10h^2 + 48h - 96}{h^3 + 10h^2 + 48h + 96} p_n. \tag{6.2}$$

The GauLe4 method applied to equations (6.1) produces the scheme

$$q_{n+1} = \frac{h^2 + 6h + 12}{h^2 - 6h + 12} q_n, \quad p_{n+1} = \frac{h^2 - 6h + 12}{h^2 + 6h + 12} p_n. \tag{6.3}$$

Figure 2 presents the results of a numerical convergence study and provides a numerical verification of the fourth-order accuracy of the Cheby4 and GauLe4 methods. In Fig. 2 we chose the initial conditions $(q_0, p_0) = (2, 2)$ and the time interval $[0, 3]$. The global errors for the position (q) and momentum (p) components at six step sizes h are plotted on a log–log scale. The global error is given by

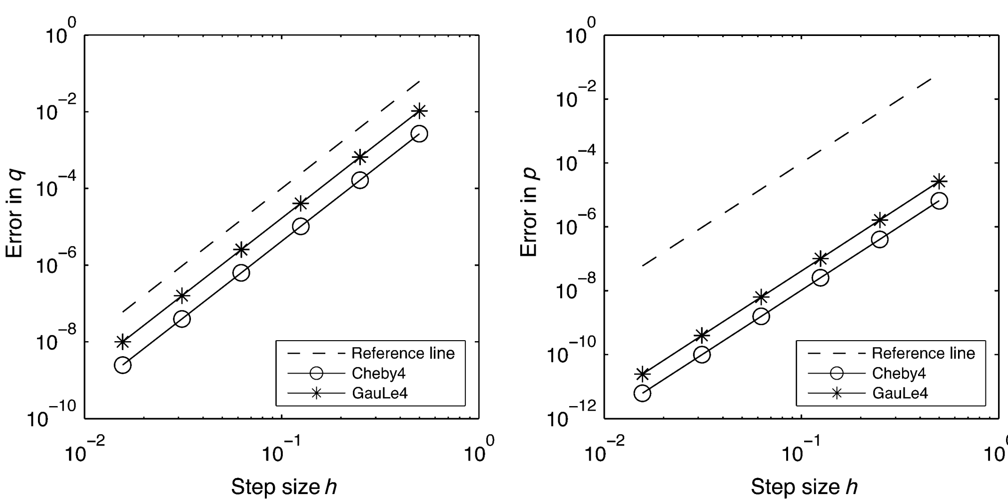

FIG. 2. Degenerate Hamiltonian example. Global errors for the position (q) and momentum (p) at six step sizes h for the GauLe4 and Cheby4 methods on a log–log scale.

the difference between the numerical solution and the exact solution at the end time $t = 3$. To show that the global errors in the position and momentum are fourth-order convergent, we have added a dashed reference line with slope 4 in each plot in Fig. 2. Clearly, the global error lines produced by the Cheby4 and GauLe4 methods are parallel to the reference line, which demonstrates that both the Cheby4 and the GauLe4 are fourth-order methods.

Furthermore, the errors produced by the Cheby4 method are smaller than the ones produced by the GauLe4 method in this example, even though they have the same order of accuracy. This can also be seen from Fig. 3, which compares the errors in the position and momentum for a fixed step size $h = 0.4$. The exponential increase in the positional errors for both Cheby4 and GauLe4 are due to the effect of roundoff error in combination with the exponentially increasing nature of the exact solution for position.

From equations (6.3) and (6.2), it can be easily verified that $q_{n+1} p_{n+1} = q_n p_n$. Thus both the Cheby4 and GauLe4 methods preserve the energy $H = qp$ exactly in infinite precision arithmetic. In practice, numerical roundoff error results in a small drift in the numerically observed energy error when the computations are performed in floating-point arithmetic. Figure 4 shows the energy errors of the Cheby4 and GauLe4 methods for a relatively long time interval.

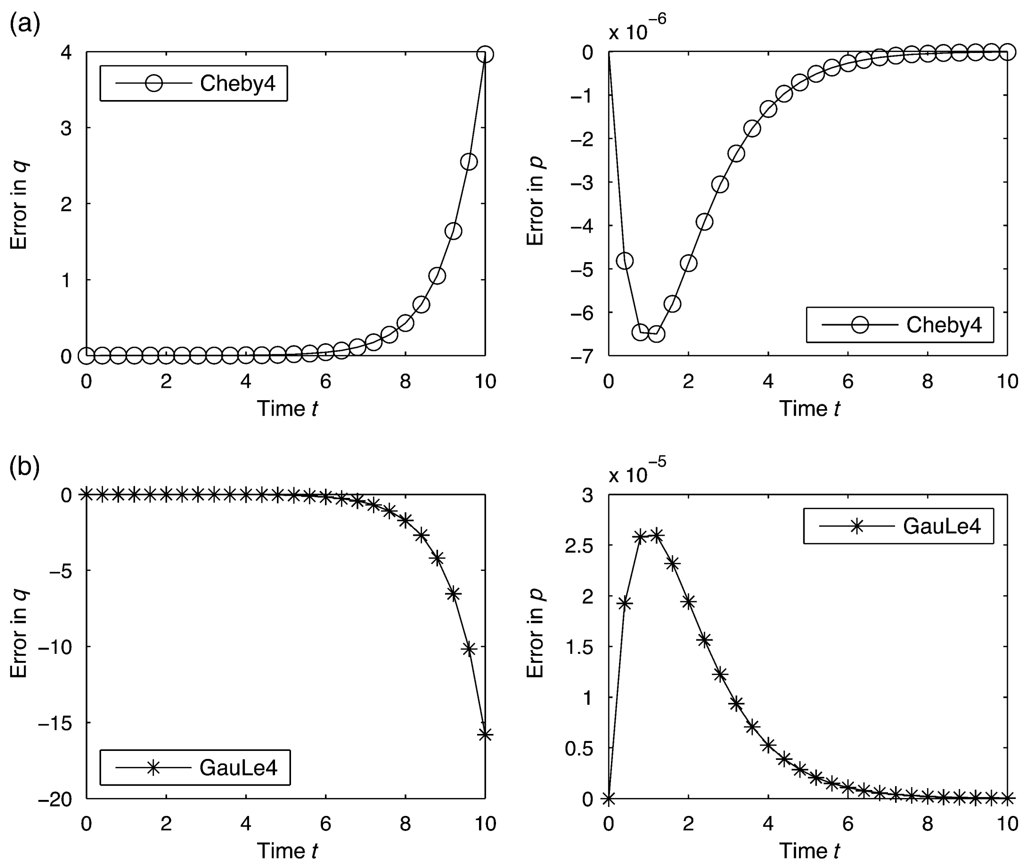

FIG. 3. Degenerate Hamiltonian example. Errors in the position (q) and momentum (p) for (a) the Cheby4 and (b) the GauLe4 methods with the step size $h = 0.4$.

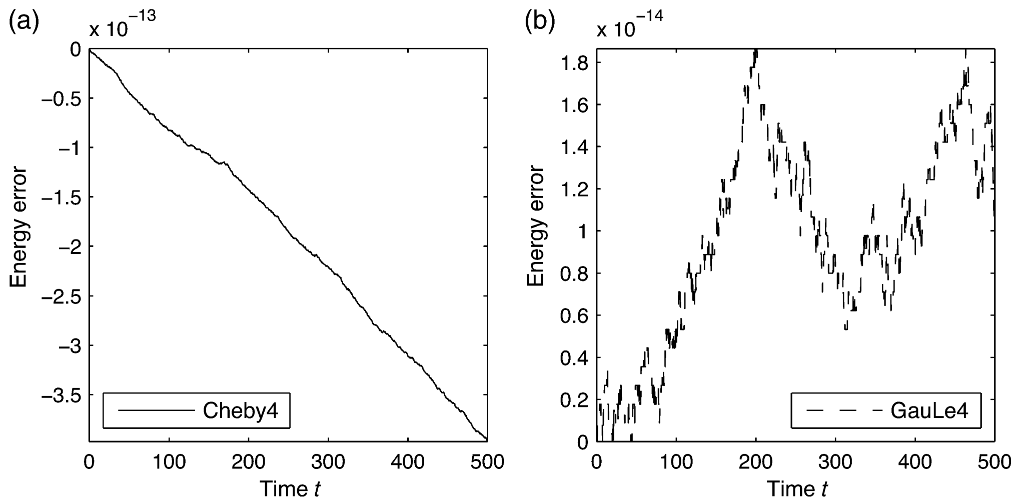

FIG. 4. Degenerate Hamiltonian example. Energy errors of (a) the Cheby4 and (b) the GauLe4 methods with the step size $h = 0.4$.

EXAMPLE 6.2. We consider the harmonic oscillator with Hamiltonian $H = \frac{p^2+\omega^2 q^2}{2}$. The associated Hamilton's equations are

$$\dot{q} = p, \quad \dot{p} = -\omega^2 q. \tag{6.4}$$

Given the initial conditions $q(0) = q_0$ and $p(0) = p_0$, the exact solution of this system is $q(t) = \cos(\omega t) q_0 + \frac{1}{\omega}\sin(\omega t) p_0$ and $p(t) = -\omega \sin(\omega t) q_0 + \cos(\omega t) p_0$.

For our numerical experiments we consider the harmonic oscillator with the initial conditions $(q_0, p_0) = (2, 1)$. The Cheby4 method applied to the harmonic oscillator yields the explicit scheme

$$\begin{aligned} q_{n+1} &= \frac{(-h^6 w^6 + 228 h^4 w^4 - 4320 h^2 w^2 + 9216) q_n}{h^6 w^6 - 12 h^4 w^4 + 288 h^2 w^2 + 9216} + \frac{(36 h^5 w^4 - 1248 h^3 w^2 + 9216 h) p_n}{h^6 w^6 - 12 h^4 w^4 + 288 h^2 w^2 + 9216}, \\ p_{n+1} &= \frac{(-12 h^5 w^6 + 1248 h^3 w^4 - 9216 h w^2) q_n}{h^6 w^6 - 12 h^4 w^4 + 288 h^2 w^2 + 9216} + \frac{(-h^6 w^6 + 228 h^4 w^4 - 4320 h^2 w^2 + 9216) p_n}{h^6 w^6 - 12 h^4 w^4 + 288 h^2 w^2 + 9216}, \end{aligned} \tag{6.5}$$

and the GauLe4 method for the harmonic oscillator is given by

$$\begin{aligned} q_{n+1} &= \frac{(h^4 w^4 - 60 h^2 w^2 + 144) q_n}{h^4 w^4 + 12 h^2 w^2 + 144} + \frac{(-12 h^3 w^2 + 144 h) p_n}{h^4 w^4 + 12 h^2 w^2 + 144}, \\ p_{n+1} &= \frac{(12 h^3 w^4 - 144 h w^2) q_n}{h^4 w^4 + 12 h^2 w^2 + 144} + \frac{(h^4 w^4 - 60 h^2 w^2 + 144) p_n}{h^4 w^4 + 12 h^2 w^2 + 144}. \end{aligned} \tag{6.6}$$

As before, we present a numerical verification of the order of accuracy of these two methods in Fig. 5 by noting that the global error lines in position (q) and momentum (p) are parallel to the dashed reference line with slope 4, which implies that these two methods are fourth-order accurate.

The error in the position (q) and momentum (p) are given in Fig. 6 for the initial conditions $(q_0, p_0) = (2, 1)$ and step size $h = 0.5$. Note that the errors in the position and momentum for the

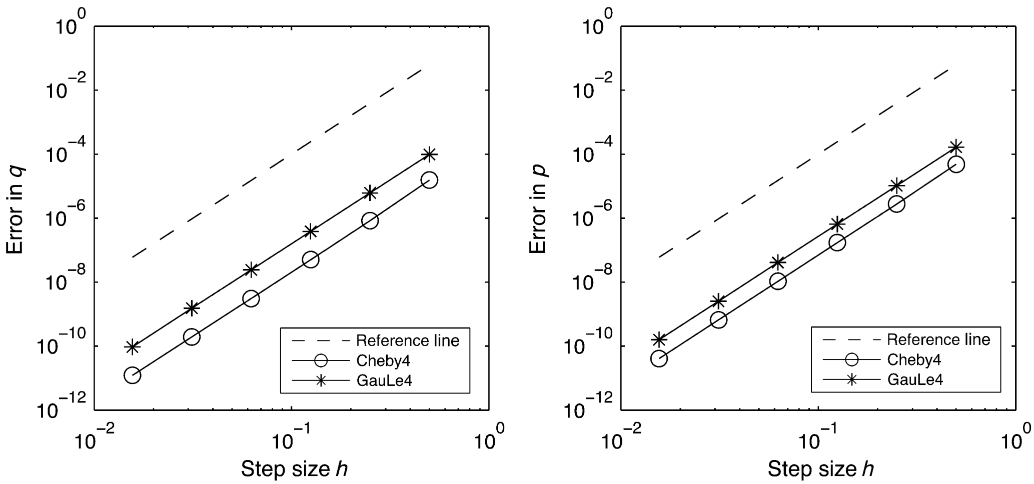

FIG. 5. Harmonic oscillator ($\omega = 1$). Global errors for the position (q) and momentum (p) at six step sizes h for the GauLe4 and Cheby4 methods on a log–log scale.

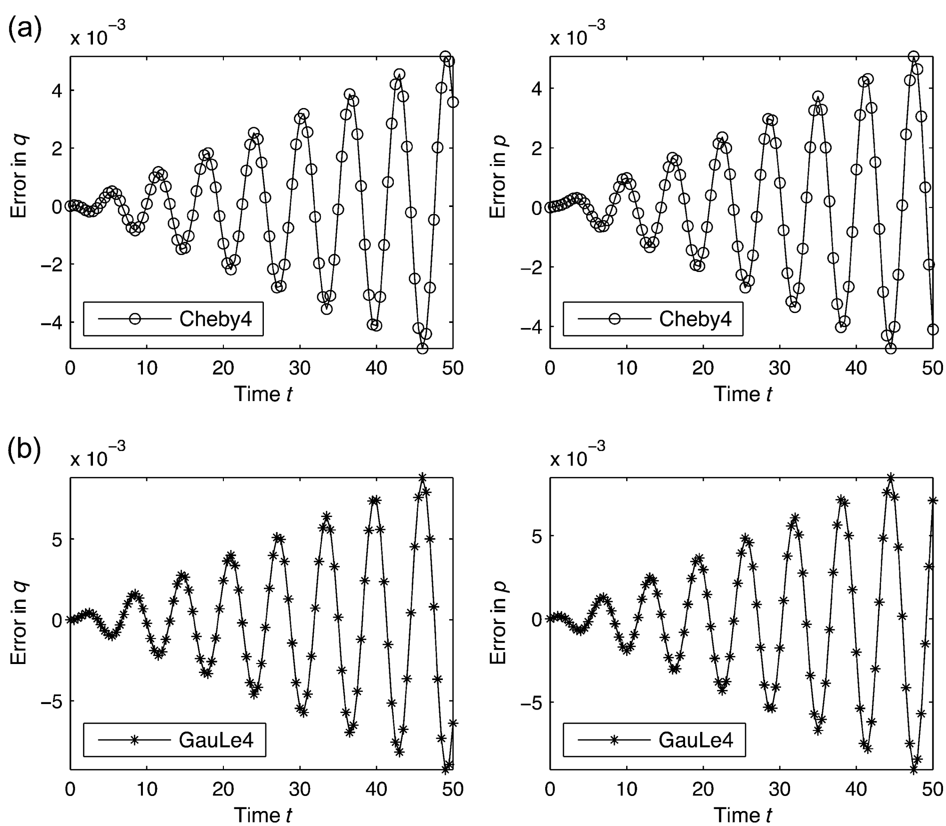

FIG. 6. Harmonic oscillator ($\omega = 1$). Errors in the position (q) and momentum (p) for (a) the Cheby4 and (b) the GauLe4 methods with the step size $h = 0.5$.

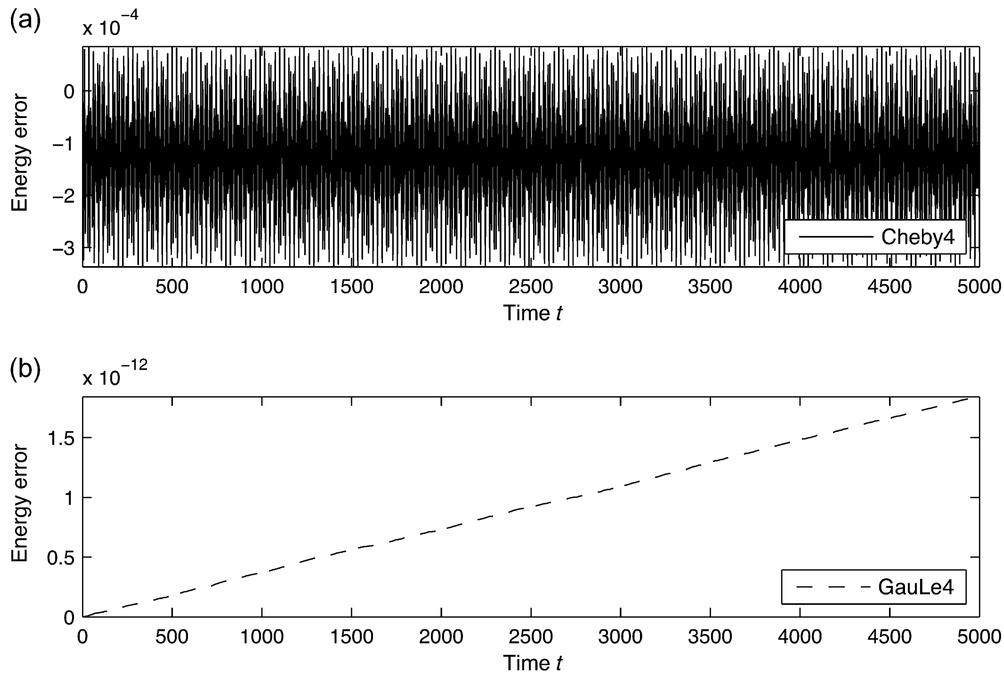

FIG. 7. Harmonic oscillator ($\omega = 1$). Energy errors of (a) the Cheby4 and (b) GauLe4 methods with the step size $h = 0.5$.

Cheby4 method are slightly smaller than for the GauLe4 method, even though, as we will see, the Cheby4 method has poorer energy properties than GauLe4.

It is well known that the energy $H = \frac{1}{2}(p^2 + \omega^2 q^2)$ is an invariant of (6.4). By direct computation, it can be proved that the GauLe4 method (6.6) exactly preserves the energy, that is , $\frac{1}{2}(p_{n+1}^2 + \omega^2 q_{n+1}^2) = \frac{1}{2}(p_n^2 + \omega^2 q_n^2)$. However, the Cheby4 method (6.5) does not possess this property. In Fig. 7 we give the energy error evolution over a long time interval [0, 5000], where the error is plotted for every tenth point. As shown in Fig. 7, the GauLe4 method exhibits an energy error evolution that is dominated by roundoff error, while the Cheby4 method exhibits a bounded energy oscillation that is typical of symplectic methods.

The energy behaviour of the two methods for the two numerical examples is consistent with the fact that symplectic Runge–Kutta methods preserve all quadratic invariants, whereas SPRK methods only preserve quadratic invariants of the form $q^{\mathrm{T}}Cp$, where C is a constant matrix (Hairer *et al.*, 2006). Thus the GauLe4 method, which is a symplectic Runge–Kutta method, preserves the energy up to roundoff error for both numerical examples, whereas the Cheby4 method, which is an SPRK method, only preserves energy to roundoff error for the case of the degenerate Hamiltonian $H(q, p) = qp$.

7. Conclusions and future directions

In this paper we provided a variational characterization of the Type II generating function that generates the exact flow of Hamilton's equations and showed how this is a Type II analogue of Jacobi's solution of the Hamilton–Jacobi equation. This corresponds to the exact discrete Hamiltonian for discrete

Hamiltonian mechanics, and Galerkin approximations of this lead to computable discrete Hamiltonians. In addition, we introduced a discrete Type II Hamilton–Jacobi equation, which can be viewed as a composition theorem for discrete Hamiltonians.

We introduced generalized Galerkin variational integrators from both the Hamiltonian and the Lagrangian approaches, and when the Hamiltonian is hyperregular these two approaches are equivalent. Furthermore, we demonstrated how these methods can be implemented as SPRK methods and derived several examples using this framework. Finally, we characterized the invariance properties of a discrete Hamiltonian that ensure that the discrete Hamiltonian flow preserves the momentum map.

We are interested in the following topics for future work.

- *Lie–Poisson reduction and connections to the Hamilton–Pontryagin principle.* Since we provided a method for constructing discrete Hamiltonians that yields a numerical method that is momentum preserving, it is natural to consider discrete analogues of Lie–Poisson reduction. In particular, the constrained variational formulation of continuous Lie–Poisson reduction (Cendra *et al.*, 2003) appears to be related to the Hamilton–Pontryagin variational principle (Yoshimura & Marsden, 2006). It would be interesting to develop discrete Lie–Poisson reduction (Marsden *et al.*, 1999) from the Hamiltonian perspective, in the context of the discrete Hamilton–Pontryagin principle (Leok & Ohsawa, 2008; Stern, 2010).

- *Extensions to multisymplectic Hamiltonian PDEs.* Multisymplectic integrators have been developed in the setting of Lagrangian variational integrators (Lew *et al.*, 2003) and Hamiltonian multisymplectic integrators (Bridges & Reich, 2001). In the paper by Marsden *et al.* (1998) the Lagrangian formulation of multisymplectic field theory is related to Hamiltonian multisymplectic field theory (Bridges, 1997). It would be interesting to construct Hamiltonian variational integrators for multisymplectic PDEs by generalizing the variational characterization of discrete Hamiltonian mechanics and the generalized Galerkin construction for computable discrete Hamiltonians to the setting of Hamiltonian multisymplectic field theories.

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