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The discrete variational principle in Hamiltonian formalism and first integrals*

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The aim of this paper is to show that first integrals of discrete equation of motion for Hamiltonian systems can be determined explicitly by investigating the invariance properties of the discrete Lagrangian in phase space. The result obtained is a discrete analog of the theorem of Noether in the calculus of variations.

Keywords: discrete mechanics, Hamiltonian system, Noether's theorem, first integral
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1. Introduction

Discrete mechanics has become a field of intense research activity in recent years. The increasing interest in this subject is mainly due to its dual-character. On the one hand, discrete mechanics allows for the construction of integration schemes, the so-called mechanical integrators (i.e., an algorithm that concerns one or more of the fundamental properties of being symplectic, preserving energy, or preserving the momentum map), that turn out to be numerically competitive in many situations. On the other hand, many of the geometric properties of mechanical systems in the continuous case admit an appropriate counterpart in the discrete setting, which is a rich area to be explored. Both aspects of discrete mechanics interact mutually, since the geometric properties of the discrete model play a key role in the explanation of the good behaviour of the integrators derived from the model in a number of situations.

There are several numerical integration methods[1] that preserve some of the invariants in an autonomous mechanical system. In Ref.[2], Lee studies the possibility that time can be regarded as a bona fide dynamical variable giving a discrete time formulation of mechanics (see also Refs.[3,4]). In Ref.[5], Marsden and West derived the variational integrators for various mechanical systems based on the ideas of Veselov.[6−8] Guo [9−11] proposed the difference variational approach with variable step-length for discrete mechanics and field theory. These integration methods usually have better long-term simulation properties and computational efficiency than the conventional ones.

It is widely accepted that in the course of computation the discrete systems should be regarded as the discrete counterparts of the corresponding continuous systems. However, in order to discretize continuous systems, a working line is needed. In Ref.[12], Feng wrote "It is natural to look forward to those discrete systems which preserve as much as possible the intrinsic properties of the continuous system." In fact, this statement should be regarded as a criterion, the structure-preserving criterion, for constructing mostly quarried ones in all kinds of structure-preserving algorithms.

In view of these facts, the above-mentioned algorithms are mainly based upon preserving the symplectic, the energy map, or the momentum map. In Refs.[13,14], we have studied the properties of preservation of Noether symmetries for discrete mechanics in the Lagrangian formalism and expanded the idea of structure preservation. As in the standard mechanics, some of the problems are easier from a Lagrangian perspective and others are easier from a Hamiltonian perspective. In this paper, we make further study of

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this problem from the Hamiltonian perspective.

This paper is organized as follows. In Section 2, we review the discrete version of Lagrange's identity for difference operators and their adjoints. In Section 3, the discrete variational equation in Hamiltonian formalism is given. A discrete version of Noether's theorem for Hamiltonian systems is presented in Section 4. Finally, an example is given to illustrate the application of the results.

2. Preliminary remarks on difference operators

An essential role in obtaining a discrete variational formalism is played by the discrete version of Lagrange's identity for operators and their adjoints. The monograph by Miller[15] discusses adjoint difference operators in detail, so we will review in this section only the essential definitions and results which are required for our investigations on the one-dimensional problem.

We consider a pth-order linear difference operator O defined by

$$O = a_0(k)R^0 + a_1(k)R^1 + \cdots + a_p(k)R^p, \quad (1)$$

where R is the lag operator defined by

$$R^q r_k = r_{k-q}. \quad (2)$$

The coefficients $a_i(k), 0 \leq i \leq p$, are assumed to be defined on I_{p+m} where $m \in I$={integers}. It is also assumed that

$$a_0(k)a_p(k) \neq 0, \qquad k \in I_{p+m}, \quad (3)$$

in order that O be of order p. The adjoint operator O^* is defined in analogy with the theory of ordinary linear differential operators.

Definition 1 If O is given by Eq.(1), then the adjoint O^* of the operator O is

$$O^* = a_0^*(k)R^0 + a_1^*(k)R^1 + \cdots + a_p^*(k)R^p, \quad (4)$$

where $a_i^*(k) = a_{p-i}(k+p-i),\ 0 \leq i \leq p,\ k \in I_{p+m}$.

Clearly, O^* is also of pth-order since, from Eq.(3),

$$a_0^*(k)a_p^*(k) = a_p(k+p)a_0(k) \neq 0, \quad k \in I_{p+m}. \quad (5)$$

Lagrange's identity follows directly.

Theorem 1 Let O and O^* be defined by Eqs.(1) and (4), and let x_k and y_k be in the domain I_m. Then

$$y_k O\, x_k - x_k O^* y_{k+p} = \Delta B(x_k, y_k), \quad k \in I_{m+p}, \quad (6)$$

where

$$B(x_k, y_k) = -\sum_{i=1}^{p}\sum_{j=1}^{i} y_{k-j+i}x_{k-j}a_i(k-j+i), \quad (7)$$

and Δ is the difference operator, $\Delta r_k = r_{k+1} - r_k$.

We call Eq.(6) Lagrange's identity and Eq.(7) the Lagrange bilinear concomitant. Equation (6) will provide a mechanism analogous to the essential integration by parts in classical calculus of variations. That is, it will provide a method by which the variational derivatives can be isolated while at the same time certain boundary terms are generated. These variational derivative and boundary terms will lead to a discrete equation of motion and first integrals, respectively.

3. The fundamental variational equation in Hamiltonian formalism

We begin by recalling the ordinary variational principle in Hamiltonian formalism.[16,17] Suppose Q denotes the configuration space with coordinates q_s, and T^*Q the phase space with coordinates $[q_s(t), p_s(t)]$, $s = 1, 2, \cdots, n$. Consider a Hamiltonian $H : T^*Q \to R$. The corresponding action functional is defined by

$$J\left[q_s(t), p_s(t)\right] = \int_a^b \left[p_s\dot{q}_s - H(\bar{q}, \bar{p})\right]\mathrm{d}t, \quad (8)$$

where $[q_s(t), p_s(t)]$ is a C^2 curve in phase space T^*Q, and $\bar{q} = (q_1, q_2, \cdots, q_n)$, $\bar{p} = (p_1, p_2, \cdots, p_n)$.

The variational principle in the Hamiltonian formalism is to seek the curves $[q_s(t), p_s(t)]$ for which the action functional J is stationary under variations of $[q_s(t), p_s(t)]$ with fixed end points.

Let

$$q_s^*(t) = q_s(t) + \varepsilon\xi_s(t, \bar{q}, \bar{p}), \quad (9a)$$

$$p_s^*(t) = p_s(t) + \varepsilon\eta_s(t, \bar{q}, \bar{p}). \quad (9b)$$

For simplicity, we will use Einstein convention and omit the summation notation $\sum$ in the following. Now we calculate the variation of J at $[q_s(t), p_s(t)]$ as follows:

$$\begin{aligned}\delta J &= \int_{t_1}^{t_2} (\dot{q}_s \delta p_s + p_s \delta \dot{q}_s - \frac{\partial H}{\partial q_s}\delta q_s - \frac{\partial H}{\partial p_s}\delta p_s)\mathrm{d}t \\ &= \int_{t_1}^{t_2} \left[\dot{q}_s \delta p_s + \frac{\mathrm{d}}{\mathrm{d}t}(p_s \delta q_s) - \dot{p}_s \delta q_s - \frac{\partial H}{\partial q_s}\delta q_s - \frac{\partial H}{\partial p_s}\delta p_s\right] \mathrm{d}t \\ &= \int_{t_1}^{t_2} \left[(\dot{q}_s - \frac{\partial H}{\partial p_s})\delta p_s - (\dot{p}_s + \frac{\partial H}{\partial q_s})\delta q_s\right] \mathrm{d}t + p_s \delta q_s|_{t_1}^{t_2}, \end{aligned} \tag{10}$$

since $\delta q_s(t_1) = \delta q_s(t_2) = 0$ and the requirement of $\delta J = 0$ yield the Hamilton equation for $[q_s(t), p_s(t)]$:

$$\dot{q}_s = \frac{\partial H}{\partial p_s}, \tag{11a}$$

$$\dot{p}_s = -\frac{\partial H}{\partial q_s}. \tag{11b}$$

In a discrete case, the discrete Lagrangian $L_\mathrm{d}(\bar{q}_{k-1}, \bar{p}_{k-1}, \bar{q}_k, \bar{p}_k, k)$ can be obtained by substituting $q_{s,k} - q_{s,k-1}$ for $\dot{q}_s$, $q_{s,k-1}$ for q_s and $p_{s,k-1}$ for p_s respectively in a given Lagrangian $L(t, q_s, p_s, \dot{q}_s)$. The problem in the discrete variational calculus is to select from all finite sequence pairs $(q_{s,M}, p_{s,M})$, $(q_{s,M+1}, p_{s,M+1}), \cdots, (q_{s,N}, p_{s,N})$ the one which extremizes the sum

$$J(q_{s,k}, p_{s,k}) = \sum_{k=M}^{N} L_\mathrm{d}(\bar{q}_{k-1}, \bar{p}_{k-1}, \bar{q}_k, \bar{p}_k, k). \tag{12}$$

Certain boundary condition may be required, e.g.

$$\begin{cases} q_{s,M-1} = a_{s,b}, \\ p_{s,M-1} = b_{s,b}, \end{cases} \quad \text{and} \quad \begin{cases} q_{s,N} = a_{s,e}, \\ p_{s,N} = b_{s,e}, \end{cases} \tag{13}$$

in a fixed endpoint problem.

Proceeding in the way similar to that in the continuous case, we embed the sequence in a one-parameter family of sequences and calculate the derivative of J, or which is just the same, of L_d along this family. More precisely, we define the variations $\delta q_{s,k}$ and $\delta p_{s,k}$ respectively by

$$\delta q_{s,k} = \varepsilon u_{s,k}, \quad k = M, M+1, \cdots, N-1, \tag{14a}$$

$$\delta p_{s,k} = \varepsilon v_{s,k}, \quad k = M, M+1, \cdots, N-1, \tag{14b}$$

where ε is a parameter, $u_{s,k}$ and $v_{s,k}$ are sequences of real numbers. The resulting variation of L_d thus defined is the linear part in ε of the increment

$$L_\mathrm{d}(\bar{q}^*_{k-1}, \bar{p}^*_{k-1}, \bar{q}^*_k, \bar{p}^*_k, k) - L_\mathrm{d}(\bar{q}_{k-1}, \bar{p}_{k-1}, \bar{q}_k, \bar{p}_k, k), \tag{15}$$

where

$$q^*_{s,k} = q_{s,k} + \delta q_{s,k}, \tag{16a}$$

$$p^*_{s,k} = p_{s,k} + \delta p_{s,k}. \tag{16b}$$

We denote this variation by $\delta L_\mathrm{d}(\delta q_{s,k}, \delta p_{s,k})$, then

$$\delta L_\mathrm{d}(\delta q_{s,k}, \delta p_{s,k}) = \frac{\partial L_\mathrm{d}(\bar{q}_{k-1}, \bar{p}_{k-1}, \bar{q}_k, \bar{p}_k, k)}{\partial \varepsilon}|_{\varepsilon=0}, \tag{17}$$

and it is not difficult to show, by the chain rule and the fact that the operators R and δ commute, that

$$\begin{aligned} &\delta L_\mathrm{d}(\delta q_{s,k}, \delta p_{s,k}) \\ =&D_3 L_{d,s}(\bar{q}_{k-1}, \bar{p}_{k-1}, \bar{q}_k, \bar{p}_k, k)\delta q_{s,k} \\ &+ D_1 L_{d,s}(\bar{q}_{k-1}, \bar{p}_{k-1}, \bar{q}_k, \bar{p}_k, k)R\delta q_{s,k} \\ &+ D_4 L_{d,s}(\bar{q}_{k-1}, \bar{p}_{k-1}, \bar{q}_k, \bar{p}_k, k)\delta p_{s,k} \\ &+ D_2 L_{d,s}(\bar{q}_{k-1}, \bar{p}_{k-1}, \bar{q}_k, \bar{p}_k, k)R\delta p_{s,k}, \end{aligned} \tag{18}$$

where $D_i L_{\mathrm{d},s}$ denotes the partial derivative of L_d with respect to the s-th component of i-th argument. A procedure analogous to the integration by parts in classical calculus of variations can be performed on Eq.(18) using the results mentioned in Section 2. We notice that $\delta L_\mathrm{d}(\delta q_{s,k}, \delta p_{s,k})$ in Eq.(18) can be written as

$$\delta L_\mathrm{d}(\delta q_{s,k}, \delta p_{s,k}) = O(\delta q_{s,k}, \delta p_{s,k}), \tag{19}$$

where O is the difference operator

$$\begin{aligned} O =&[D_3 L_\mathrm{d}(\bar{q}_{k-1}, \bar{p}_{k-1}, \bar{q}_k, \bar{p}_k, k) \\ &+ D_4 L_\mathrm{d}(\bar{q}_{k-1}, \bar{p}_{k-1}, \bar{q}_k, \bar{p}_k, k)]R^0 \\ &+ [D_1 L_\mathrm{d}(\bar{q}_{k-1}, \bar{p}_{k-1}, \bar{q}_k, \bar{p}_k, k) \\ &+ D_2 L_\mathrm{d}(\bar{q}_{k-1}, \bar{p}_{k-1}, \bar{q}_k, \bar{p}_k, k)]R^1. \end{aligned} \tag{20}$$

According to definition 1, the adjoint of O is given by

$$\begin{aligned} O^* =&[D_1 L_\mathrm{d}(\bar{q}_k, \bar{p}_k, \bar{q}_{k+1}, \bar{p}_{k+1}, k+1) \\ &+ D_2 L_\mathrm{d}(\bar{q}_k, \bar{p}_k, \bar{q}_{k+1}, \bar{p}_{k+1}, k+1)]R^0 \\ &+ [D_3 L_\mathrm{d}(\bar{q}_{k-1}, \bar{p}_{k-1}, \bar{q}_k, \bar{p}_k, k) \\ &+ D_4 L_\mathrm{d}(\bar{q}_{k-1}, \bar{p}_{k-1}, \bar{q}_k, \bar{p}_k, k)]R^1, \end{aligned} \tag{21}$$

therefore, by Lagrange's identity (6) with $y_{s,k}=1$ and $x_{s,k}=(\delta q_{s,k},\delta p_{s,k})$, Eq.(18) can be written as

$$\begin{aligned}&O(\delta q_{s,k},\delta p_{s,k})\\=&(\delta q_{s,k},\delta p_{s,k})O^*(1)+\Delta B\left[(\delta q_{s,k},\delta p_{s,k}),1\right],\end{aligned}\tag{22}$$

where

$$\begin{aligned}&B\left[(\delta q_{s,k},\delta p_{s,k}),1\right]\\=&-\delta q_{s,k-1}D_1L_{d,s}(\bar q_{k-1},\bar p_{k-1},\bar q_k,\bar p_k,k)\\&-\delta p_{s,k-1}D_2L_{d,s}(\bar q_{k-1},\bar p_{k-1},\bar q_k,\bar p_k,k).\end{aligned}\tag{23}$$

Thus, from Eqs.(19), (21), (22), and (23) we conclude that

$$\begin{aligned}&\delta L_{\rm d}(\delta q_{s,k},\delta p_{s,k})\\=&[D_3L_{d,s}(\bar q_{k-1},\bar p_{k-1},\bar q_k,\bar p_k,k)\\&+D_1L_{d,s}(\bar q_k,\bar p_k,\bar q_{k+1},\bar p_{k+1},k+1)]\delta q_{s,k}\\&+\Delta[-\delta q_{s,k-1}D_1L_{d,s}(\bar q_{k-1},\bar p_{k-1},\bar q_k,\bar p_k,k)]\\&+[D_4L_{d,s}(\bar q_{k-1},\bar p_{k-1},\bar q_k,\bar p_k,k)\\&+D_2L_{d,s}(\bar q_k,\bar p_k,\bar q_{k+1},\bar p_{k+1},k+1)]\delta p_{s,k}\\&+\Delta[-\delta p_{s,k-1}D_2L_{{\rm d},s}(\bar q_{k-1},\bar p_{k-1},\bar q_k,\bar p_k,k)],\end{aligned}\tag{24}$$

which is the fundamental variational equation for $L_{\rm d}$. The expressions

$$\begin{aligned}\phi_k=&D_3L_{{\rm d},s}(\bar q_{k-1},\bar p_{k-1},\bar q_k,\bar p_k,k)\\&+D_1L_{{\rm d},s}(\bar q_k,\bar p_k,\bar q_{k+1},\bar p_{k+1},k+1),\end{aligned}\tag{25a}$$

$$\begin{aligned}\psi_k=&D_4L_{{\rm d},s}(\bar q_{k-1},\bar p_{k-1},\bar q_k,\bar p_k,k)\\&+D_2L_{{\rm d},s}(\bar q_k,\bar p_k,\bar q_{k+1},\bar p_{k+1},k+1),\end{aligned}\tag{25b}$$

$k=M,M+1,\cdots,N-1$, are called the discrete derivative.

In order to obtain the discrete Hamilton equation, which represents a necessary condition for J by

$$\delta J(\delta q_{s,k},\delta p_{s,k})=\sum_{k=M-1}^{N}\delta L_{\rm d}(\delta q_{s,k},\delta p_{s,k}),\tag{26}$$

using Eqs.(24) and (25), we obtain

$$\begin{aligned}&\delta J(\delta q_{s,k},\delta p_{s,k})\\=&\sum_{k=M}^{N-1}(\phi_{s,k}\delta q_{s,k}+\psi_{s,k}\delta p_{s,k})\\&+\delta q_{s,M-1}D_1L_{{\rm d},s}(\bar q_{M-1},\bar p_{M-1},\bar q_M,\bar p_M,M)\\&+\delta p_{s,M-1}D_2L_{{\rm d},s}(\bar q_{M-1},\bar p_{M-1},\bar q_M,\bar p_M,M)\\&+\delta q_{s,N}D_1L_{{\rm d},s}(\bar q_{N-1},\bar p_{N-1},\bar q_N,\bar p_N,N)\\&+\delta p_{s,N}D_1L_{{\rm d},s}(\bar q_{N-1},\bar p_{N-1},\bar q_N,\bar p_N,N).\end{aligned}\tag{27}$$

By using the condition (13), Eq.(27) becomes

$$\delta J(\delta q_{s,k},\delta p_{s,k})=\sum_{k=M}^{N-1}(\phi_{s,k}\delta q_{s,k}+\psi_{s,k}\delta p_{s,k}).\tag{28}$$

Let δJ vanish for all $\delta q_{s,k}$ and $\delta p_{s,k}$, then it follows that

$$\begin{aligned}&D_3L_{{\rm d},s}(\bar q_{k-1},\bar p_{k-1},\bar q_k,\bar p_k,k)\\&+D_1L_{{\rm d},s}(\bar q_k,\bar p_k,\bar q_{k+1},\bar p_{k+1},k+1)=0,\\&(k=M,\cdots,N-1),\end{aligned}\tag{29a}$$

$$\begin{aligned}&D_4L_{{\rm d},s}(\bar q_{k-1},\bar p_{k-1},\bar q_k,\bar p_k,k)\\&+D_2L_{{\rm d},s}(\bar q_k,\bar p_k,\bar q_{k+1},\bar p_{k+1},k+1)=0.\\&(k=M,\cdots,N-1).\end{aligned}\tag{29b}$$

These equations represent the Hamilton canonical equation for the discrete problem defined by Eq.(12).

4. First integrals

As in the continuous case, a systematic procedure for the establishment of first integrals of the discrete Hamilton canonical equation can be developed from a direct study of the invariance properties of the discrete Lagrangian $L_{\rm d}(\bar q_{k-1},\bar p_{k-1},\bar q_k,\bar p_k,k)$ in phase space.

We introduce the following infinitesimal transformation:

$$q^*_{s,k}=q_{s,k}+\varepsilon u_{s,k},\tag{30a}$$

$$p^*_{s,k}=p_{s,k}+\varepsilon v_{s,k},\tag{30b}$$

where ε is a parameter, $u_{s,k}=u_s(\bar q_k,\bar p_k,k)$ and $v_{s,k}=v_s(\bar q_k,\bar p_k,k)$ are two sequences depending upon k, $\bar q_k$ and $\bar p_k$, $k=M,\cdots,N-1$.

Definition 2 If there exists a sequence $g(\bar q_k,\bar p_k,k)$, $k=M,\cdots,N-1$ such that

$$\delta L_{\rm d}\left[\varepsilon u_s(\bar q_k,\bar p_k,k),\varepsilon v_s(\bar q_k,\bar p_k,k)\right]=\varepsilon\Delta g(\bar q_k,\bar p_k,k),\tag{31}$$

for each k, where $\delta L_{\rm d}$ is given by Eq.(24), then the discrete Lagrangian $L_{\rm d}(\bar q_{k-1},\bar p_{k-1},\bar q_k,\bar p_k,k)$ in phase space is difference invariant with respect to the infinitesimal transformation (9).

The following theorem, which is analogous to the classical Noether theorem, is valid. Actually, the following theorem is more similar to a statement about conservation laws, which in the continuous case follows as a corollary to the Noether theorem.

Theorem 2 If the discrete Lagrangian $L_{\rm d}(\bar q_{k-1},\bar p_{k-1},\bar q_k,\bar p_k,k)$ in phase space is difference invariant with respect to the infinitesimal transformation (30), and if Eq.(29) holds, then

$$\begin{aligned}&u_s(\bar q_{k-1},\bar p_{k-1},k-1)D_1L_{{\rm d},s}(\bar q_{k-1},\bar p_{k-1},\bar q_k,\bar p_k,k)\\&+v_s(\bar q_{k-1},\bar p_{k-1},k-1)D_2L_{{\rm d},s}(\bar q_{k-1},\bar p_{k-1},\bar q_k,\bar p_k,k)\\&+g(\bar q_k,\bar p,k)=\text{const}.\end{aligned}\tag{32}$$

Proof From Eqs.(31) and (24), one has

$$\begin{aligned}&\phi_{s,k}\delta q_{s,k}+\psi_{s,k}\delta p_{s,k}+\Delta[-\varepsilon u_s(\bar{q}_{k-1},\bar{p}_{k-1},k-1)\\&\times D_1L_{\mathrm{d},s}(\bar{q}_{k-1},\bar{p}_{k-1},\bar{q}_k,\bar{p}_k,k)]\\&+\Delta[-\varepsilon v_s(\bar{q}_{k-1},\bar{p}_{k-1},k-1)\\&\times D_2L_{\mathrm{d},s}(\bar{q}_{k-1},\bar{p}_{k-1},\bar{q}_k,\bar{p}_k,k)]\\=&\varepsilon\Delta g(\bar{q}_k,\bar{p}_k,k).\end{aligned}$$

Simplifying and using the hypothesis $\phi_{s,k}=0$ and $\psi_{s,k}=0$, one obtains

$$\begin{aligned}&\Delta[u_s(\bar{q}_{k-1},\bar{p}_{k-1},k-1)\\&\times D_1L_{\mathrm{d},s}(\bar{q}_{k-1},\bar{p}_{k-1},\bar{q}_k,\bar{p}_k,k)]\\&+\Delta[v_s(\bar{q}_{k-1},\bar{p}_{k-1},k-1)\\&D_2L_{\mathrm{d},s}(\bar{q}_{k-1},\bar{p}_{k-1},\bar{q}_k,\bar{p}_k,k)]\\&+\Delta g(\bar{q}_k,\bar{p}_k,k)=0,\end{aligned}$$

whence Eq.(32) holds. This completes the proof.

5. Example

To illustrate various aspects of the theory developed in preceding sections, we here give an example.

Example Considering a mechanical system of two degrees of freedom with discrete Lagrangian

$$\begin{aligned}L_{\mathrm{d}}=&p_{1,k-1}(q_{1,k}-q_{1,k-1})+p_{2,k-1}(q_{2,k}-q_{2,k-1})\\&-\frac{1}{2}(p_{1,k-1}^2+p_{2,k-1}^2)-q_{2,k-1},\end{aligned}\tag{33}$$

then the action sum is

$$\begin{aligned}J=\sum_{k=1}^{N}\Big\{&p_{1,k-1}(q_{1,k}-q_{1,k-1})+p_{2,k-1}(q_{2,k}-q_{2,k-1})\\&-\frac{1}{2}(p_{1,k-1}^2+p_{2,k-1}^2)-q_{2,k-1}\Big\};\end{aligned}\tag{34}$$

and, from Eq.(29), the discrete Hamilton canonical equations are the following difference equations:

$$p_{1,k}-p_{1,k-1}=0,\tag{35a}$$
$$q_{1,k+1}-q_{1,k}=p_{1,k},\tag{35b}$$
$$p_{2,k}-p_{2,k-1}=-1,\tag{35c}$$
$$q_{1,k+1}-q_{1,k}=p_{1,k}.\tag{35d}$$

Direct verification shows that

$$\begin{aligned}L_{\mathrm{d}}=&p_{1,k-1}(q_{1,k}-q_{1,k-1})+p_{2,k-1}(q_{2,k}-q_{2,k-1})\\&-\frac{1}{2}(p_{1,k-1}^2+p_{2,k-1}^2)-q_{2,k-1},\end{aligned}$$

is difference invariant (with $g=0$) with respect to the following infinitesimal transformations:

$$q_{1,k}^*=q_{1,k}+\varepsilon,\tag{36a}$$
$$q_{2,k}^*=q_{2,k},\tag{36b}$$
$$p_{1,k}^*=p_{1,k},\tag{36c}$$
$$p_{2,k}^*=q_{2,k}.\tag{36d}$$

Hence, from Theorem 2, one has

$$\begin{aligned}&u_s(\bar{q}_{k-1},\bar{p}_{k-1},k-1)\\&\times D_1L_{\mathrm{d},s}(\bar{q}_{k-1},\bar{p}_{k-1},\bar{q}_k,\bar{p}_k,k)=\mathrm{const},\end{aligned}$$

or

$$p_{1,k-1}=\mathrm{const}.\tag{37}$$

If we choose L_{d} in Eq.(33) as follows:

$$\begin{aligned}L_{\mathrm{d}}=&p_{1,k-1/2}(q_{1,k}-q_{1,k-1})+p_{2,k-1/2}(q_{2,k}-q_{2,k-1})\\&-\frac{1}{2}(p_{1,k-1/2}^2+p_{2,k-1/2}^2)-q_{2,k-1/2},\end{aligned}\tag{38}$$

where

$$q_{i,k-1/2}=\frac{q_{i,k-1}+q_{i,k}}{2},$$
$$q_{i,k+1/2}=\frac{q_{i,k}+q_{i,k+1}}{2},\quad i=1,2,$$

$$p_{i,k-1/2}=\frac{p_{i,k-1}+p_{i,k}}{2},$$
$$p_{i,k-1/2}=\frac{p_{2,k}+p_{2,k+1}}{2},\quad i=1,2,$$

and using Eq.(29), we can obtain the corresponding discrete Hamilton canonical equations

$$p_{1,k+1/2}-p_{1,k-1/2}=0,\tag{39a}$$
$$q_{1,k+1}-q_{1,k-1}=2(p_{1,k+1/2}+p_{1,k-1/2}),\tag{39b}$$
$$p_{2,k+1/2}-p_{2,k-1/2}=-1,\tag{39c}$$
$$q_{2,k+1}-q_{2,k-1}=2(p_{2,k-1/2}+p_{2,k+1/2}).\tag{39d}$$

It is easy to verify that

$$\begin{aligned}L_{\mathrm{d}}=&p_{1,k-1/2}(q_{1,k}-q_{1,k-1})+p_{2,k-1/2}(q_{2,k}-q_{2,k-1})\\&-\frac{1}{2}(p_{1,k-1/2}^2+p_{2,k-1/2}^2)-q_{2,k-1/2}\end{aligned}$$

is difference invariant (with $g=0$) with respect to the infinitesimal transformation (36). By using Theorem 2, one has

$$p_{1,k+1/2}=\mathrm{const}.\tag{40}$$

Obviously, there is no relation between the discrete first integral and the discrete form of the Lagrangian.

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