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First integrals of difference Hamiltonian equations

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Abstract
In the present paper, the well-known Noether's identity, which represents the connection between symmetries and first integrals of Euler–Lagrange equations, is rewritten in terms of the Hamiltonian function. This approach, based on the Hamiltonian identity, provides a simple and clear way to find first integrals of canonical Hamiltonian equations without integration. A discrete analog of the Hamiltonian identity is developed. It leads to a connection between symmetries and first integrals of difference Hamiltonian equations that can be used to conserve the structural properties of Hamiltonian equations under discretizaton. The results are illustrated by a number of examples for both continuous and difference Hamiltonian equations.

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1. Introduction

In the present paper, we are interested in canonical Hamiltonian equations

$$\dot{q}^i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q^i}, \qquad i = 1, \ldots, n, \tag{1.1}$$

which can be obtained by the variational principle from the action functional

$$\delta \int_{t_1}^{t_2} (p_i \dot{q}^i - H(t, \mathbf{q}, \mathbf{p}))\, \mathrm{d}t = 0 \tag{1.2}$$

in the phase space $(\mathbf{q}, \mathbf{p})$, where $\mathbf{q} = (q^1, q^2, \ldots, q^n)$, $\mathbf{p} = (p_1, p_2, \ldots, p_n)$ (see, for example, [1, 2]).

Let us note that the canonical Hamiltonian equations (1.1) can be obtained by the action of the variational operators

$$\frac{\delta}{\delta p_i} = \frac{\partial}{\partial p_i} - D\frac{\partial}{\partial \dot{p}_i}, \qquad \frac{\delta}{\delta q^i} = \frac{\partial}{\partial q^i} - D\frac{\partial}{\partial \dot{q}^i}, \qquad i = 1, \ldots, n, \tag{1.3}$$

where D is the operator of total differentiation with respect to time

$$D = \frac{\partial}{\partial t} + \dot{q}^i \frac{\partial}{\partial q^i} + \dot{p}_i \frac{\partial}{\partial p_i} + \cdots, \tag{1.4}$$

on the function

$$p_i \dot{q}^i - H(t, \mathbf{q}, \mathbf{p}).$$

The Legendre transformation relates Hamiltonian and Lagrange functions:

$$L(t, \mathbf{q}, \dot{\mathbf{q}}) = p_i \dot{q}^i - H(t, \mathbf{q}, \mathbf{p}), \tag{1.5}$$

where $\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}}$, $\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}$. It makes it possible to establish the equivalence of the Euler–Lagrange and Hamiltonian equations [3]. It should be noted that the Legendre transformation is not a point one. Hence, there is no conservation of Lie group properties of the corresponding Euler–Lagrange equations and Hamiltonian equations within the class of point transformations.

Lie point symmetries in the space $(t, \mathbf{q}, \mathbf{p})$ are generated by operators of the form [4–6]

$$X = \xi(t, \mathbf{q}, \mathbf{p}) \frac{\partial}{\partial t} + \eta^i(t, \mathbf{q}, \mathbf{p}) \frac{\partial}{\partial q^i} + \zeta_i(t, \mathbf{q}, \mathbf{p}) \frac{\partial}{\partial p_i}. \tag{1.6}$$

The standard approach to symmetry properties of the Hamiltonian equations is to consider so-called *Hamiltonian symmetries* [5]. In the case of canonical Hamiltonian equations these are the evolutionary ($\xi = 0$) symmetries (1.6):

$$\bar{X} = \eta^i(t, \mathbf{q}, \mathbf{p}) \frac{\partial}{\partial q^i} + \zeta_i(t, \mathbf{q}, \mathbf{p}) \frac{\partial}{\partial p_i} \tag{1.7}$$

with

$$\eta^i = \frac{\partial I}{\partial p_i}, \qquad \zeta^i = -\frac{\partial I}{\partial q^i}, \qquad i = 1, \ldots, n, \tag{1.8}$$

for some function $I(t, \mathbf{q}, \mathbf{p})$, namely, symmetries of the form

$$\bar{X}_I = \frac{\partial I}{\partial p_i} \frac{\partial}{\partial q^i} - \frac{\partial I}{\partial q^i} \frac{\partial}{\partial p_i}. \tag{1.9}$$

These symmetries are restricted to the phase space $(\mathbf{q}, \mathbf{p})$ and are generated by the function $I = I(t, \mathbf{q}, \mathbf{p})$. For symmetry (1.9) the independent variable t is invariant and plays a role of a parameter.

Noether's theorem (theorem 6.33 in [5]) relates the Hamiltonian symmetries of the Hamiltonian equations with their first integrals. This approach has some disadvantages. First, some transformations lose their geometrical sense if considered in the evolutionary form (1.9). Second, there is a necessity of integration to find first integrals with the help of (1.8). Third, a specific disadvantage is a big difficulty to preserve evolutionary symmetries (1.7) in discrete models [7]. In this approach, it is also not clear why some point symmetries of Hamiltonian equations yield integrals, while others do not.

In the present paper, we will consider symmetries of the general form (1.6), which are not restricted to the phase space and can also transform t. In contrast to the Hamiltonian symmetries in the form (1.9) the underlying symmetries have a clear geometric sense in finite space and do not require integration to find first integrals. We will provide a Hamiltonian version of Noether's theorem (in the strong formulation) based on a newly established Hamiltonian identity, which is an analog of the well-known Noether's identity in the Lagrangian framework. The Hamiltonian identity links directly an invariant Hamiltonian function with first integrals of the canonical Hamiltonian equations. This approach provides a simple and clear way to construct first integrals by means of merely algebraic manipulations with symmetries of the action functional. The approach will be illustrated on a number of examples.

The paper is organized as follows. In section 2, we introduce the definition of an invariant Hamiltonian and establish the necessary and sufficient condition for H to be invariant. The main proposition of this section is lemma 2.3 which introduces a new identity, used in theorem 2.4 to formulate the necessary and sufficient condition for existence of first integrals of Hamiltonian equations (Hamiltonian version of Noether's theorem in the strong formulation). Lemma 2.7 introduces two more identities, which are used in theorem 2.9 to formulate necessary and sufficient conditions for the canonical Hamiltonian equations to be invariant. This section also contains examples of canonical Hamiltonian equations with first integrals. Section 3 is devoted to difference Hamiltonian equations. Their symmetries and first integrals are shown to be related in the same way as those of the continuous canonical Hamiltonian equations. Final section 4 contains concluding remarks.

2. Invariance of Hamiltonian action and first integrals

As an analog of the Lagrangian elementary action [5, 6] we consider the Hamiltonian elementary action

$$p_i\,\mathrm{d}q^i - H\,\mathrm{d}t, \tag{2.1}$$

which can be invariant with respect to a group generated by an operator of the form (1.6).

Definition 2.1. *We call a Hamiltonian function invariant with respect to a symmetry operator (1.6) if the elementary action (2.1) is an invariant of the group generated by this operator.*

Theorem 2.2. *A Hamiltonian is invariant with respect to a group generated by the operator (1.6) if and only if the following condition holds:*

$$\zeta_i\dot{q}^i + p_i D(\eta^i) - X(H) - HD(\xi) = 0. \tag{2.2}$$

Proof. The invariance condition follows directly from the action of the operator X prolonged on the differentials $\mathrm{d}t$ and $\mathrm{d}q^i$, $i = 1, \ldots, n$:

$$X = \xi(t,\mathbf{q},\mathbf{p})\frac{\partial}{\partial t} + \eta^i(t,\mathbf{q},\mathbf{p})\frac{\partial}{\partial q^i} + \zeta_i(t,\mathbf{q},\mathbf{p})\frac{\partial}{\partial p_i} + D(\xi)\,\mathrm{d}t\frac{\partial}{\partial(\mathrm{d}t)} + D(\eta^i)\,\mathrm{d}t\frac{\partial}{\partial\,(\mathrm{d}q^i)}. \tag{2.3}$$

Application of (2.3) to the Hamiltonian elementary action (2.1) yields

$$X(p_i dq^i - H\,\mathrm{d}t) = (\zeta_i\dot{q}^i + p_i D(\eta^i) - X(H) - HD(\xi))\,\mathrm{d}t = 0. \qquad \square$$

Now we can relate the conservation properties of the canonical Hamiltonian equations to the invariance of the Hamiltonian function. Generally, Hamiltonization of Lagrangian systems can lead to Hamiltonian equations with constraints. The Hamiltonian form of the Noether identity for such systems can be found in [8, 9]. In the present paper, we restrict ourselves to Hamiltonian systems without constraints.

Lemma 2.3. *The identity*

$$\zeta_i\dot{q}^i + p_i D(\eta^i) - X(H) - HD(\xi) \equiv \xi\left(D(H) - \frac{\partial H}{\partial t}\right)$$
$$- \eta^i\left(\dot{p}_i + \frac{\partial H}{\partial q^i}\right) + \zeta_i\left(\dot{q}^i - \frac{\partial H}{\partial p_i}\right) + D[p_i\eta^i - \xi H] \tag{2.4}$$

is true for any smooth function $H = H(t,\mathbf{q},\mathbf{p})$.

Proof. The identity can be established by direct calculation. □

We call this identity the *Hamiltonian identity*. This identity makes it possible to develop the following result.

Theorem 2.4. *The canonical Hamiltonian equations (1.1) possess a first integral of the form*

$$I = p_i\eta^i - \xi H \tag{2.5}$$

if and only if the Hamiltonian function is invariant with respect to the operator (1.6) on the solutions of equations (1.1).

Proof. The result follows from identity (2.4). Note that we use the following: the operator of total differentiation (1.4) applied to Hamiltonian H and considered on the solutions of Hamiltonian equations (1.1) coincides with partial differentiation with respect to time:

$$D(H)|_{\dot{\mathbf{q}}=H_{\mathbf{p}},\ \dot{\mathbf{p}}=-H_{\mathbf{q}}} = \left[\frac{\partial H}{\partial t} + \dot{q}^i\frac{\partial H}{\partial q^i} + \dot{p}_i\frac{\partial H}{\partial p_i}\right]_{\dot{\mathbf{q}}=H_{\mathbf{p}},\ \dot{\mathbf{p}}=-H_{\mathbf{q}}} = \frac{\partial H}{\partial t}.$$
□

Theorem 2.4 corresponds to the strong version [6] (i.e. necessary and sufficient condition) of the Noether theorem [10] for invariant Lagrangians and Euler–Lagrange equations.

Remark 2.5. Theorem 2.4 can be generalized to the case of the divergence invariance of the Hamiltonian action (see [11] for this result in the Lagrangian framework)

$$\zeta_i\dot{q}^i + p_iD(\eta^i) - X(H) - HD(\xi) = D(V), \tag{2.6}$$

where $V = V(t, \mathbf{q}, \mathbf{p})$. If this condition holds on the solutions of the canonical Hamiltonian equations (1.1), then there is a first integral

$$I = p_i\eta^i - \xi H - V. \tag{2.7}$$

Remark 2.6. Let us note that according to definition 2.1 any Hamiltonian is invariant with respect to the family of operators

$$X_* = \zeta_i(t, \mathbf{q}, \mathbf{p})\frac{\partial}{\partial p_i} \tag{2.8}$$

on the solutions of the corresponding Hamiltonian equations. These operators do not provide non-trivial first integrals (they give $I = 0$). Therefore, it makes sense to consider symmetry operators up to the set of operators (2.8). It should be mentioned that in general operators X_* are not symmetries of the Hamiltonian equations (1.1).

In the Lagrangian framework, the variational principle provides us with the Euler–Lagrange equations. It is known that the invariance of the Euler–Lagrange equations follows from the invariance of the action integral. The following lemma 2.7 and theorem 2.8 establish the sufficient conditions for canonical Hamiltonian equations to be invariant.

Lemma 2.7. *The following identities are true for any smooth function $H = H(t, \mathbf{q}, \mathbf{p})$:*

$$\begin{aligned}\frac{\delta}{\delta p_j}(\zeta_i\dot{q}^i + p_iD(\eta^i) - X(H) - HD(\xi)) &\equiv D(\eta^j) - \dot{q}^jD(\xi) - X\left(\frac{\partial H}{\partial p_j}\right)\\ &+ \frac{\partial \xi}{\partial p_j}\left(D(H) - \frac{\partial H}{\partial t}\right) - \frac{\partial \eta^i}{\partial p_j}\left(\dot{p}_i + \frac{\partial H}{\partial q^i}\right)\\ &+ \left(\frac{\partial \zeta_i}{\partial p_j} + \delta_{ij}D(\xi)\right)\left(\dot{q}^i - \frac{\partial H}{\partial p_i}\right), \qquad j = 1, \ldots, n,\end{aligned} \tag{2.9}$$

$$\frac{\delta}{\delta q^j}(\zeta_i \dot{q}^i + p_i D(\eta^i) - X(H) - HD(\xi)) \equiv -D(\zeta_j) + \dot{p}_j D(\xi) - X\left(\frac{\partial H}{\partial q_j}\right) + \frac{\partial \xi}{\partial q^j}\left(D(H) - \frac{\partial H}{\partial t}\right) - \left(\frac{\partial \eta^i}{\partial q^j} + \delta_{ij} D(\xi)\right) \times \left(\dot{p}_i + \frac{\partial H}{\partial q^i}\right) + \frac{\partial \zeta_i}{\partial q^j}\left(\dot{q}^i - \frac{\partial H}{\partial p_i}\right), \qquad j = 1, \ldots, n, \tag{2.10}$$

where δ_{ij} is the Kronecker symbol.

Proof. The identities can be easily obtained by direct computation. □

Theorem 2.8. *If a Hamiltonian is invariant or divergence invariant with respect to the symmetry (1.6), then the canonical Hamiltonian equations (1.1) are also invariant.*

Proof. For invariance of the canonical Hamiltonian equations (1.1) we need the equations

$$D(\eta^j) - \dot{q}^j D(\xi) = X\left(\frac{\partial H}{\partial p_j}\right), \qquad D(\zeta_j) - \dot{p}_j D(\xi) = -X\left(\frac{\partial H}{\partial q^j}\right), \qquad j = 1, \ldots, n$$

to hold on the solutions of the Hamiltonian equations [5]. These conditions follow from the identities (2.9) and (2.10). In the case of divergence invariance the term $D(V)$ disappears because it belongs to the kernel of the variational operators (1.3). □

The invariance of the Hamiltonian is a *sufficient condition* for the canonical Hamiltonian equations to be invariant. The symmetry group of the canonical Hamiltonian equations can of course be larger than that of the Hamiltonian. The following theorem 2.9 establishes the *necessary and sufficient* conditions for canonical Hamiltonian equations to be invariant.

Theorem 2.9. *Canonical Hamiltonian equations (1.1) are invariant with respect to the symmetry (1.6) if and only if the following conditions are true (on the solutions of the canonical Hamiltonian equations):*

$$\left.\frac{\delta}{\delta p_j}(\zeta_i \dot{q}^i + p_i D(\eta^i) - X(H) - HD(\xi))\right|_{\dot{\mathbf{q}}=H_{\mathbf{p}},\ \dot{\mathbf{p}}=-H_{\mathbf{q}}} = 0, \qquad j = 1, \ldots, n, \tag{2.11}$$

$$\left.\frac{\delta}{\delta q^j}(\zeta_i \dot{q}^i + p_i D(\eta^i) - X(H) - HD(\xi))\right|_{\dot{\mathbf{q}}=H_{\mathbf{p}},\ \dot{\mathbf{p}}=-H_{\mathbf{q}}} = 0, \qquad j = 1, \ldots, n. \tag{2.12}$$

Proof. The statement follows from identities (2.9) and (2.10). □

It should be noted that conditions (2.11) and (2.12) are true for all symmetries of canonical Hamiltonian equations. But not all of those symmetries yield the 'variational integral' of these conditions, i.e.

$$(\zeta_i \dot{q}^i + p_i D(\eta^i) - X(H) - HD(\xi))|_{\dot{\mathbf{q}}=H_{\mathbf{p}},\ \dot{\mathbf{p}}=-H_{\mathbf{q}}} = 0, \tag{2.13}$$

which gives first integrals in accordance with theorem 2.4. That is why not all symmetries of the canonical Hamiltonian equations provide first integrals. Below we illustrate the theorems, given above, by examples.

2.1. Applications

In this point we present two examples of canonical Hamiltonian equations with first integrals.

2.1.1. Repulsive one-dimensional motion. Let us consider one-dimensional motion in the Coulomb field (the case of a repulsive force):

$$\dot{q} = p, \qquad \dot{p} = \frac{1}{q^2}. \tag{2.14}$$

These equations are generated by the Hamiltonian function

$$H(t, q, p) = \frac{p^2}{2} + \frac{1}{q}.$$

Equations (2.14) admit Lie algebra with basis operators

$$X_1 = \frac{\partial}{\partial t}, \qquad X_2 = 3t\frac{\partial}{\partial t} + 2q\frac{\partial}{\partial q} - p\frac{\partial}{\partial p}. \tag{2.15}$$

The invariance of Hamiltonian condition (2.2) is satisfied for the operator X_1 only. Applying theorem 2.4, we calculate the corresponding first integral

$$I_1 = -H = -\left(\frac{p^2}{2} + \frac{1}{q}\right). \tag{2.16}$$

Application of operator X_2 to the Hamiltonian action gives

$$\zeta\dot{q} + pD(\eta) - X(H) - HD(\xi) = p\dot{q} - \left(\frac{p^2}{2} + \frac{1}{q}\right) \neq 0.$$

Meanwhile, in accordance with theorem 2.9 we have

$$\frac{\delta}{\delta p}\left(\zeta\dot{q} + pD(\eta) - X(H) - HD(\xi)\right)\Big|_{\dot{q}=p,\ \dot{p}=\frac{1}{q^2}} = (\dot{q} - p)|_{\dot{q}=p,\ \dot{p}=\frac{1}{q^2}} = 0,$$

$$\frac{\delta}{\delta q}\left(\zeta\dot{q} + pD(\eta) - X(H) - HD(\xi)\right)\Big|_{\dot{q}=p,\ \dot{p}=\frac{1}{q^2}} = \left(-\dot{p} + \frac{1}{q^2}\right)\Big|_{\dot{q}=p,\ \dot{p}=\frac{1}{q^2}} = 0.$$

Thus, the operator X_2 is a symmetry of the Hamiltonian equations (2.14), which does not produce a first integral.

2.1.2. Nonlinear motion. As the next example we consider the equations

$$\dot{q} = p, \qquad \dot{p} = \frac{1}{q^3}, \tag{2.17}$$

corresponding to the Hamiltonian

$$H(t, q, p) = \frac{1}{2}\left(p^2 + \frac{1}{q^2}\right).$$

These equations admit symmetries

$$X_1 = \frac{\partial}{\partial t}, \qquad X_2 = 2t\frac{\partial}{\partial t} + q\frac{\partial}{\partial q} - p\frac{\partial}{\partial p}, \qquad X_3 = t^2\frac{\partial}{\partial t} + tq\frac{\partial}{\partial q} + (q - tp)\frac{\partial}{\partial p}. \tag{2.18}$$

We check invariance of H in accordance with theorem 2.2 and find that condition (2.2) is satisfied for the operators X_1 and X_2. Using theorem 2.4, we calculate the corresponding first integrals

$$I_1 = -H = -\frac{1}{2}\left(p^2 + \frac{1}{q^2}\right), \qquad I_2 = pq - t\left(p^2 + \frac{1}{q^2}\right). \tag{2.19}$$

For the third symmetry operator the Hamiltonian is divergence invariant with $V_3 = q^2/2$. In accordance with remark 2.5, it yields the conserved quantity

$$I_3 = -\frac{1}{2}\left(\frac{t^2}{q^2} + (q - tp)^2\right). \tag{2.20}$$

The first integrals (2.19), (2.20) are not independent. They are connected by the relation

$$4I_1 I_3 - I_2^2 = 1. \tag{2.21}$$

Putting $I_1 = A/2$ and $I_2 = B$, we find the solution of (2.17) as

$$Aq^2 + (At - B)^2 + 1 = 0, \qquad p = \frac{B - At}{q}. \tag{2.22}$$

Note that no integration is needed to provide solutions of (2.17).

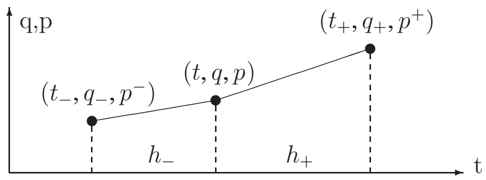
In [12] the Hamiltonian form of Noether's theorem, presented in this section, was applied to find first integrals of Kepler motion.

3. First integrals of difference Hamiltonian equations

The preservation of first integrals (conservation laws) in numerical work is of great importance (see, for example, [13, 14]). Therefore, it makes sense to establish a discrete analog of the results presented in the preceding section for the continuous Hamiltonian equations.

3.1. The discrete version of Hamiltonian action

We will consider finite-difference equations and discrete Hamiltonians at some point $(t, \mathbf{q}, \mathbf{p})$ of a lattice. Generally, the lattice is not regular. The notations are clear from the following picture.



To consider difference equations we will need three points of a lattice. Prolongation of the Lie group operator (1.6) for neighboring points $(t_-, \mathbf{q}_-, \mathbf{p}^-)$ and $(t_+, \mathbf{q}_+, \mathbf{p}^+)$ is as follows [7]:

$$X = \xi\frac{\partial}{\partial t} + \eta^i\frac{\partial}{\partial q^i} + \zeta_i\frac{\partial}{\partial p_i} + \xi_-\frac{\partial}{\partial t_-} + \eta^i_-\frac{\partial}{\partial q^i_-} + \zeta_i^-\frac{\partial}{\partial p_i^-}$$
$$+\xi_+\frac{\partial}{\partial t_+} + \eta^i_+\frac{\partial}{\partial q^i_+} + \zeta_i^+\frac{\partial}{\partial p_i^+} + (\xi_+ - \xi)\frac{\partial}{\partial h_+} + (\xi - \xi_-)\frac{\partial}{\partial h_-}, \tag{3.1}$$

where

$$\xi_- = \xi(t_-, \mathbf{q}_-, \mathbf{p}^-), \qquad \eta^i_- = \eta^i(t_-, \mathbf{q}_-, \mathbf{p}^-), \qquad \zeta_i^- = \zeta^i(t_-, \mathbf{q}_-, \mathbf{p}^-),$$
$$\xi_+ = \xi(t_+, \mathbf{q}_+, \mathbf{p}^+), \qquad \eta^i_+ = \eta^i(t_+, \mathbf{q}_+, \mathbf{p}^+), \qquad \zeta_i^+ = \zeta^i(t_+, \mathbf{q}_+, \mathbf{p}^+).$$

Hamiltonian equations can be obtained by the variational principle from the finite-difference functional

$$\mathbb{H}_h = \sum_{\Omega}\left(p_i^+(q^i_+ - q^i) - \mathcal{H}(t, t_+, \mathbf{q}, \mathbf{p}^+)h_+\right). \tag{3.2}$$

Indeed, a variation of this functional along a curve $q^i = \phi_i(t)$, $p_i = \psi_i(t)$, $i = 1, \ldots, n$, at some point $(t, \mathbf{q}, \mathbf{p})$ will affect only two terms of the sum (3.2):

$$\mathbb{H}_h = \cdots + p_i\left(q^i - q_-^i\right) - \mathcal{H}(t_-, t, \mathbf{q}_-, \mathbf{p})h_- + p_i^+\left(q_+^i - q^i\right) - \mathcal{H}(t, t_+, \mathbf{q}, \mathbf{p}^+)h_+ + \cdots . \tag{3.3}$$

Therefore, we get the following expression for the variation:

$$\delta\mathbb{H}_h = \frac{\delta\mathcal{H}}{\delta p_i}\delta p_i + \frac{\delta\mathcal{H}}{\delta q^i}\delta q^i + \frac{\delta\mathcal{H}}{\delta t}\delta t, \tag{3.4}$$

where $\delta q^i = \phi_i'\delta t$, $\delta p_i = \psi_i'\delta t$, $i = 1, \ldots, n$, and

$$\begin{aligned} &\frac{\delta\mathcal{H}}{\delta p_i} = q^i - q_-^i - h_-\frac{\partial\mathcal{H}^-}{\partial p_i}, \qquad \frac{\delta\mathcal{H}}{\delta q^i} = -\left(p_i^+ - p_i + h_+\frac{\partial\mathcal{H}}{\partial q^i}\right), \qquad i = 1, \ldots, n, \\ &\frac{\delta\mathcal{H}}{\delta t} = -\left(h_+\frac{\partial\mathcal{H}}{\partial t} - \mathcal{H} + h_-\frac{\partial\mathcal{H}^-}{\partial t} + \mathcal{H}^-\right), \end{aligned} \tag{3.5}$$

where $\mathcal{H} = \mathcal{H}(t, t_+, \mathbf{q}, \mathbf{p}^+)$ and $\mathcal{H}^- = \mathcal{H}(t_-, t, \mathbf{q}_-, \mathbf{p})$.

For the stationary value of the finite-difference functional (3.2) we obtain the system of $2n + 1$ equations

$$\frac{\delta\mathcal{H}}{\delta p_i} = 0, \qquad \frac{\delta\mathcal{H}}{\delta q^i} = 0, \qquad i = 1, \ldots, n, \qquad \frac{\delta\mathcal{H}}{\delta t} = 0. \tag{3.6}$$

Thus, we arrive at the system of $2n + 1$ equations

$$\begin{aligned} &\underset{h}{D}(q^i) = \frac{\partial\mathcal{H}}{\partial p_i^+}, \qquad \underset{h}{D}(p_i) = -\frac{\partial\mathcal{H}}{\partial q^i}, \qquad i = 1, \ldots, n, \\ &h_+\frac{\partial\mathcal{H}}{\partial t} - \mathcal{H} + h_-\frac{\partial\mathcal{H}^-}{\partial t} + \mathcal{H}^- = 0, \end{aligned} \tag{3.7}$$

which we will call *difference Hamiltonian equations*. For convenience we use the following total right-shift operator and the corresponding discrete differentiation operator:

$$\underset{h}{S}f(t) = f(t_+), \qquad \underset{h}{D} = \frac{\underset{h}{S} - 1}{h_+}.$$

Let us note that the first $2n$ equations (3.7) are first-order difference equations, which correspond to the canonical Hamiltonian equations (1.1) in the continuous limit. The last equation is of second order. Its continuous counterpart is automatically satisfied on the solutions of canonical Hamiltonian equations. In the discrete case it defines the lattice on which the canonical Hamiltonian equations are discretized. Being a second-order difference equation it needs one more initial value (first step of lattice) to state the initial-value problem.

Let us note that equations (3.7) can be obtained from discrete variational equations in the Lagrangian framework [7, 15–17] with the help of discrete Legendre transform [18].

Remark 3.1. Equivalent formulation can be considered for the finite-difference functional

$$\mathbb{H}_h = \sum_{\Omega}\left(p_i\left(q_+^i - q^i\right) - \mathcal{H}(t, t_+, \mathbf{q}_+, \mathbf{p})h_+\right) \tag{3.8}$$

and a discrete Hamiltonian function $\mathcal{H}(t, t_+, \mathbf{q}_+, \mathbf{p})$.

3.2. Symplecticity of difference Hamiltonian equations

The canonical Hamiltonian equations generate symplectic transformations in the phase space $(\mathbf{q}, \mathbf{p})$. For the solution $(\mathbf{q}(t), \mathbf{p}(t))$ of the system (1.1) with initial data $\mathbf{q}(t_0) = \mathbf{q}_0, \mathbf{p}(t_0) = \mathbf{p}^0$ this property can be expressed as a conservation of the two-form

$$\mathrm{d}p_i \wedge \mathrm{d}q^i = \mathrm{d}p_i^0 \wedge \mathrm{d}q_0^i. \tag{3.9}$$

This property is used to select symplectic numerical integrators [19, 20] as numerical schemes with the property

$$\mathrm{d}p_i^{n+1} \wedge \mathrm{d}q_{n+1}^i = \mathrm{d}p_i^n \wedge \mathrm{d}q_n^i, \qquad n = 0, 1, \ldots. \tag{3.10}$$

Definition (3.10) for conservation of symplecticity cannot be used for discretizations on solution-dependent meshes such as difference Hamiltonian equations (3.7). Generally, variations of the dependent variables involve variations of the lattice points. It is clearly seen from the variational equations for the system (3.7):

$$\mathrm{d}q_+^i - \mathrm{d}q^i = \frac{\partial^2(\mathcal{H}h_+)}{\partial p_i^+ \partial t}\,\mathrm{d}t + \frac{\partial^2(\mathcal{H}h_+)}{\partial p_i^+ \partial t_+}\,\mathrm{d}t_+ + \frac{\partial^2(\mathcal{H}h_+)}{\partial p_i^+ \partial q^j}\,\mathrm{d}q^j + \frac{\partial^2(\mathcal{H}h_+)}{\partial p_i^+ \partial p_j^+}\,\mathrm{d}p_j^+, \qquad i = 1, \ldots, n,$$

$$\mathrm{d}p_i^+ - \mathrm{d}p_i = -\frac{\partial^2(\mathcal{H}h_+)}{\partial q^i \partial t}\,\mathrm{d}t - \frac{\partial^2(\mathcal{H}h_+)}{\partial q^i \partial t_+}\,\mathrm{d}t_+ - \frac{\partial^2(\mathcal{H}h_+)}{\partial q^i \partial q^j}\,\mathrm{d}q^j - \frac{\partial^2(\mathcal{H}h_+)}{\partial q^i \partial p_j^+}\,\mathrm{d}p_j^+, \quad i = 1, \ldots, n,$$

$$\frac{\partial^2(\mathcal{H}h_+)}{\partial t^2}\,\mathrm{d}t + \frac{\partial^2(\mathcal{H}h_+)}{\partial t \partial t_+}\,\mathrm{d}t_+ + \frac{\partial^2(\mathcal{H}h_+)}{\partial t \partial q^j}\,\mathrm{d}q^j + \frac{\partial^2(\mathcal{H}h_+)}{\partial t \partial p_j^+}\,\mathrm{d}p_j^+$$
$$+ \frac{\partial^2(\mathcal{H}^- h_-)}{\partial t \partial t_-}\,\mathrm{d}t_- + \frac{\partial^2(\mathcal{H}^- h_-)}{\partial t^2}\,\mathrm{d}t + \frac{\partial^2(\mathcal{H}^- h_-)}{\partial t \partial q_-^j}\,\mathrm{d}q_-^j + \frac{\partial^2(\mathcal{H}^- h_-)}{\partial t \partial p_j}\,\mathrm{d}p_j = 0.$$

For $\mathrm{d}t_+, \mathrm{d}\mathbf{q}_+, \mathrm{d}\mathbf{p}^+$, i.e. the variations in the next point of the lattice, these equations are a system of $2n + 1$ linear algebraic equations. Thus, the variational equations considered in the phase space (without variations of the independent variable) form an overdetermined system of $2n + 1$ equations for $2n$ variables, which in the general case has only trivial solutions.

Therefore, we are forced to look for symplecticity in the extended phase space $(t, \mathbf{q}, \mathbf{p})$ (see also general considerations for the continuous case in [21]).

Theorem 3.2. *The difference Hamiltonian equations (3.7) possess the conservation of symplecticity*

$$\mathrm{d}p_i^+ \wedge \mathrm{d}q_+^i - \mathrm{d}\mathcal{E}_+ \wedge \mathrm{d}t_+ = \mathrm{d}p_i \wedge \mathrm{d}q^i - \mathrm{d}\mathcal{E} \wedge \mathrm{d}t, \tag{3.11}$$

where

$$\mathcal{E}_+ = \mathcal{H} + h_+ \frac{\partial \mathcal{H}}{\partial t_+}, \qquad \mathcal{E} = \mathcal{H}^- + h_- \frac{\partial \mathcal{H}^-}{\partial t} \tag{3.12}$$

are discrete energies for lattice points t_+ and t.

Proof. From the first $2n$ variational equations we obtain

$$\mathrm{d}p_i^+ \wedge \mathrm{d}q_+^i - \mathrm{d}p_i \wedge \mathrm{d}q^i = \frac{\partial^2(\mathcal{H}h_+)}{\partial p_i^+ \partial t}\,\mathrm{d}p_i^+ \wedge \mathrm{d}t + \frac{\partial^2(\mathcal{H}h_+)}{\partial p_i^+ \partial t_+}\,\mathrm{d}p_i^+ \wedge \mathrm{d}t_+$$
$$+ \frac{\partial^2(\mathcal{H}h_+)}{\partial q^i \partial t}\,\mathrm{d}q^i \wedge \mathrm{d}t + \frac{\partial^2(\mathcal{H}h_+)}{\partial q^i \partial t_+}\,\mathrm{d}q^i \wedge \mathrm{d}t_+. \tag{3.13}$$

With the help of the relations for variations

$$\mathrm{d}\mathcal{E}_+ = \frac{\partial^2(\mathcal{H}h_+)}{\partial t \partial t_+}\,\mathrm{d}t + \frac{\partial^2(\mathcal{H}h_+)}{\partial t_+^2}\,\mathrm{d}t_+ + \frac{\partial^2(\mathcal{H}h_+)}{\partial q^j \partial t_+}\,\mathrm{d}q^j + \frac{\partial^2(\mathcal{H}h_+)}{\partial p_j^+ \partial t_+}\,\mathrm{d}p_j^+$$

and

$$\begin{aligned} d\mathcal{E} &= \frac{\partial^2(\mathcal{H}^- h_-)}{\partial t_- \partial t}\, dt_- + \frac{\partial^2(\mathcal{H}^- h_-)}{\partial t^2}\, dt + \frac{\partial^2(\mathcal{H}^- h_-)}{\partial q_-^j \partial t}\, dq_-^j + \frac{\partial^2(\mathcal{H}^- h_-)}{\partial p_j \partial t}\, dp_j \\ &= -\frac{\partial^2(\mathcal{H} h_+)}{\partial t^2}\, dt - \frac{\partial^2(\mathcal{H} h_+)}{\partial t_+ \partial t}\, dt_+ - \frac{\partial^2(\mathcal{H} h_+)}{\partial q^j \partial t}\, dq^j - \frac{\partial^2(\mathcal{H} h_+)}{\partial p_j^+ \partial t}\, dp_j^+, \end{aligned}$$

where the last variational equation was used, we get

$$\begin{aligned} d\mathcal{E}_+ \wedge dt_+ - d\mathcal{E} \wedge dt &= \frac{\partial^2(\mathcal{H} h_+)}{\partial p_i^+ \partial t}\, dp_i^+ \wedge dt + \frac{\partial^2(\mathcal{H} h_+)}{\partial p_i^+ \partial t_+}\, dp_i^+ \wedge dt_+ \\ &\quad + \frac{\partial^2(\mathcal{H} h_+)}{\partial q^i \partial t}\, dq^i \wedge dt + \frac{\partial^2(\mathcal{H} h_+)}{\partial q^i \partial t_+}\, dq^i \wedge dt_+. \end{aligned} \tag{3.14}$$

Comparing right-hand sides of (3.13) and (3.14), we conclude the statement of the theorem. □

3.3. Invariance of the Hamiltonian action

Let us consider the functional (3.2) on some lattice, given by the equation

$$\Omega(t, h_+, h_-, \mathbf{q}, \mathbf{p}, \mathbf{q}_-, \mathbf{p}^-, \mathbf{q}_+, \mathbf{p}^+) = 0. \tag{3.15}$$

Definition 3.3. *We call a discrete Hamiltonian function $\mathcal{H}$ considered on the lattice (3.15) invariant with respect to a group generated by the operator (3.1), if the action (3.2) considered on the mesh (3.15) is an invariant manifold of the group.*

Theorem 3.4. *A Hamiltonian function considered together with the mesh (3.15) is invariant with respect to a group generated by the operator (3.1) if and only if the following conditions hold:*

$$\left. \zeta_i^+ \underset{h}{D}(q^i) + p_i^+ \underset{h}{D}(\eta^i) - X(\mathcal{H}) - \mathcal{H} \underset{h}{D}(\xi) \right|_{\Omega=0} = 0, \qquad X\Omega|_{\Omega=0} = 0. \tag{3.16}$$

Proof. The invariance condition follows directly from the action of X on the functional:

$$X\left(\sum_{\Omega} p_i^+(q_+^i - q^i) - \mathcal{H} h_+\right) = \sum_{\Omega} \left(\zeta_i^+ \underset{h}{D}(q^i) + p_i^+ \underset{h}{D}(\eta^i) - X(\mathcal{H}) - \mathcal{H} \underset{h}{D}(\xi)\right) h_+ = 0.$$

It should be provided with the invariance of the mesh, which is obtained by the action of the symmetry operator on the mesh equation (3.15). □

3.4. Discrete Hamiltonian identity and Noether-type theorem

As in the continuous case, the invariance of a discrete Hamiltonian on a specified mesh yields first integrals of the corresponding difference Hamiltonian equations.

Lemma 3.5. *The following identity is true for any smooth function $\mathcal{H} = \mathcal{H}(t, t_+, \mathbf{q}, \mathbf{p}^+)$:*

$$\begin{aligned} \zeta_i^+ \underset{h}{D}(q^i) + p_i^+ \underset{h}{D}(\eta^i) - X(\mathcal{H}) - \mathcal{H} \underset{h}{D}(\xi) &\equiv \xi \left(\underset{h}{D}(\mathcal{H}^-) - \frac{\partial \mathcal{H}}{\partial t} - \frac{h_-}{h_+} \frac{\partial \mathcal{H}^-}{\partial t} \right) \\ - \eta^i \left(\underset{h}{D}(p_i) + \frac{\partial \mathcal{H}}{\partial q^i} \right) + \zeta_i^+ &\left(\underset{h}{D}(q^i) - \frac{\partial \mathcal{H}}{\partial p_i^+} \right) + \underset{h}{D}\left[\eta^i p_i - \xi \left(\mathcal{H}^- + h_- \frac{\partial \mathcal{H}^-}{\partial t} \right) \right]. \end{aligned} \tag{3.17}$$

Proof. The identity can be established by direct calculation. □

We call this identity the *discrete Hamiltonian identity*. It allows us to state the following result.

Theorem 3.6. *The difference Hamiltonian equations (3.7), invariant with respect to symmetry operator (3.1), possess a first integral*

$$\mathcal{I} = \eta^i p_i - \xi \left(\mathcal{H}^- + h_- \frac{\partial \mathcal{H}^-}{\partial t} \right) \tag{3.18}$$

if and only if the Hamiltonian function is invariant with respect to the same symmetry on the solutions of equations (3.7).

Proof. This result is a consequence of identity (3.17). The invariance of the difference Hamiltonian equations is needed to guarantee the invariance of the mesh, which is defined by these equations. □

Remark 3.7. Theorem 3.6 can be generalized to the case of the divergence invariance of the Hamiltonian action, i.e.

$$\zeta_i^+ \underset{h}{D}(q^i) + p_i^+ \underset{h}{D}(\eta^i) - X(\mathcal{H}) - \mathcal{H} \underset{h}{D}(\xi) = \underset{h}{D}(V), \tag{3.19}$$

where $V = V(t, \mathbf{q}, \mathbf{p})$. If this condition holds on the solutions of the difference Hamiltonian equations (3.7), then there is a first integral

$$\mathcal{I} = \eta^i p_i - \xi \left(\mathcal{H}^- + h_- \frac{\partial \mathcal{H}^-}{\partial t} \right) - V. \tag{3.20}$$

Remark 3.8. For difference Hamiltonian equations with Hamiltonian functions invariant with respect to time translations, i.e. $\mathcal{H} = \mathcal{H}(h_+, \mathbf{q}, \mathbf{p}^+)$, where $h_+ = t_+ - t$, there is a conservation of energy:

$$\mathcal{E} = \mathcal{H}^- + h_- \frac{\partial \mathcal{H}^-}{\partial h_-} = \mathcal{H} + h_+ \frac{\partial \mathcal{H}}{\partial h_+}.$$

In this case the difference Hamiltonian equations (3.7) are related to symplectic-momentum-energy preserving variational integrations introduced for the discrete Lagrangian framework in [22]. Note that in contrast to the continuous case, where Hamiltonian $H(t, \mathbf{q}, \mathbf{p})$ represents the energy of the system, the discrete Hamiltonian $\mathcal{H}$ is different from the discrete energy; it has a meaning of a generating function for discrete Hamiltonian flow.

3.5. Applications

3.5.1. Discrete harmonic oscillator. The harmonic oscillator model is very important in physics. A mass at equilibrium under the influence of any conservative force behaves as a simple harmonic oscillator (in the limit of small motions). Harmonic oscillators are exploited in many man-made devices, such as clocks and radio circuits.

Let us consider the one-dimensional harmonic oscillator

$$\dot{q} = p, \qquad \dot{p} = -q. \tag{3.21}$$

This system of Hamiltonian equations is generated by the Hamiltonian function

$$H(t, q, p) = \tfrac{1}{2}(q^2 + p^2).$$

As a discretization of equations (3.21) we consider the application of the midpoint rule

$$\frac{q_+ - q}{h_+} = \Omega \frac{p + p_+}{2}, \qquad \frac{p_+ - p}{h_+} = -\Omega \frac{q + q_+}{2} \tag{3.22}$$

on a uniform mesh $h_+ = h_- = h$. The parameter Ω will be chosen later. The presented discretization can be rewritten as the following system of equations:

$$\underset{h}{D}(q) = \frac{4\Omega}{4 - \Omega^2 h_+^2}\left(p_+ + \frac{\Omega h_+}{2} q\right), \qquad \underset{h}{D}(p) = -\frac{4\Omega}{4 - \Omega^2 h_+^2}\left(q + \frac{\Omega h_+}{2} p_+\right). \tag{3.23}$$
$$h_+ = h_-.$$

It can be shown that this system is generated by the discrete Hamiltonian function

$$\mathcal{H}(t, t_+, q, p_+) = \frac{2\Omega}{4 - \Omega^2 h_+^2}\left(q^2 + p_+^2 + \Omega h_+ q p_+\right).$$

Indeed, the first and second equations of (3.7) are exactly the same as those of (3.23). The last equation of (3.7) takes the form

$$-\frac{2\Omega\left(4 + \Omega^2 h_+^2\right)}{\left(4 - \Omega^2 h_+^2\right)^2}\left(q^2 + p_+^2\right) - \frac{16\Omega^2 h_+}{\left(4 - \Omega^2 h_+^2\right)^2} q p_+ + \frac{2\Omega\left(4 + \Omega^2 h_-^2\right)}{\left(4 - \Omega^2 h_-^2\right)^2}\left(q_-^2 + p^2\right)$$
$$+\frac{16\Omega^2 h_-}{\left(4 - \Omega^2 h_-^2\right)^2} q_- p = 0.$$

Using the first and second equations, we can rewrite it as

$$\left(-\frac{2\Omega}{4 + \Omega^2 h_+^2} + \frac{2\Omega}{4 + \Omega^2 h_-^2}\right)\left(q^2 + p^2\right) = 0.$$

Therefore, for the case $q^2 + p^2 \neq 0$ this equation can be taken in an equivalent form

$$h_+ = h_- = h.$$

The system of difference equations (3.23) on a uniform mesh admits, in particular, the following symmetries:

$$X_1 = \sin(\omega t)\frac{\partial}{\partial q} + \cos(\omega t)\frac{\partial}{\partial p}, \qquad X_2 = \cos(\omega t)\frac{\partial}{\partial q} - \sin(\omega t)\frac{\partial}{\partial p},$$
$$X_3 = \frac{\partial}{\partial t}, \qquad X_4 = q\frac{\partial}{\partial q} + p\frac{\partial}{\partial p}, \qquad X_5 = p\frac{\partial}{\partial q} - q\frac{\partial}{\partial p}, \tag{3.24}$$

where

$$\omega = \frac{\arctan(\Omega h/2)}{h/2}.$$

For the symmetry operators X_1 and X_2 we have the divergence invariance conditions

$$\zeta_+ \underset{h}{D}(q) + p_+ \underset{h}{D}(\eta) - X(\mathcal{H}) - \mathcal{H}\underset{h}{D}(\xi) = \underset{h}{D}(V)$$

fulfilled on the solutions of equations (3.23) with functions $V_1 = q\cos(\omega t)$ and $V_2 = -q\sin(\omega t)$, respectively. Therefore, we obtain two corresponding first integrals

$$\mathcal{I}_1 = p\sin(\omega t) - q\cos(\omega t), \qquad \mathcal{I}_2 = p\cos(\omega t) + q\sin(\omega t). \tag{3.25}$$

The symmetry operator X_3 satisfies the invariance condition

$$\zeta_+ \underset{h}{D}(q) + p_+ \underset{h}{D}(\eta) - X(\mathcal{H}) - \mathcal{H}\underset{h}{D}(\xi) = 0.$$

Thus, we get the first integral

$$\mathcal{I}_3 = -\frac{4\Omega}{4-\Omega^2 h_-^2}\left(\frac{4+\Omega^2 h_-^2}{4-\Omega^2 h_-^2}\frac{q_-^2+p^2}{2} + \frac{4\Omega h_-}{4-\Omega^2 h_-^2} q_- p\right). \tag{3.26}$$

Using the first and second equations of (3.23), we can simplify it as

$$\mathcal{I}_3 = -\frac{4\Omega}{4+\Omega^2 h_-^2}\frac{q^2+p^2}{2}.$$

Since from the first integrals $\mathcal{I}_1$ and $\mathcal{I}_2$ we have the conservation law

$$\mathcal{I}_1^2 + \mathcal{I}_2^2 = q^2 + p^2 = \text{const},$$

it follows that we can take the third first integral equivalently as

$$\tilde{\mathcal{I}}_3 = h_-. \tag{3.27}$$

The three first integrals $\mathcal{I}_1, \mathcal{I}_2, \tilde{\mathcal{I}}_3$ are sufficient for integration of the system (3.22). We obtain the solution

$$q = \mathcal{I}_2 \sin(\omega t) - \mathcal{I}_1 \cos(\omega t), \qquad p = \mathcal{I}_1 \sin(\omega t) + \mathcal{I}_2 \cos(\omega t) \tag{3.28}$$

on the lattice

$$t_i = t_0 + ih, \qquad i = 0, \pm 1, \pm 2, \ldots, \qquad h = \tilde{\mathcal{I}}_3. \tag{3.29}$$

Let us consider different choices for the parameter Ω:

(i) $\Omega = 1$ or no additional parameter.
This is the natural choice for the discretization of equations (3.21). In this case the symmetry operators X_1 and X_2 contain the parameter

$$\omega = \frac{\arctan(h/2)}{h/2},$$

which represents the deformation of the corresponding symmetry operators admitted by the underlying differential equations (3.21). The discrete harmonic oscillator follows the same trajectory as the continuous harmonic oscillator, but with a different velocity.

(ii) Modified discrete harmonic oscillator (exact scheme).
The numerical error of the preceding point can be eliminated by time reparametrization. If we chose the parameter

$$\Omega = \frac{\tan(h/2)}{h/2},$$

we get $\omega = 1$. In this case the symmetry operators (3.24) are the same as the corresponding symmetries of the underlying differential equations. We obtain the exact discretization of the harmonic oscillator, i.e. a discretization which gives the exact solution of the underlying ODEs.

The exact schemes for two- and four-dimensional harmonic oscillators were used in [23] to construct exact schemes for two- and three-dimensional Kepler motion, respectively.

3.5.2. Nonlinear motion. Let us consider a discrete model for equations (2.17). We chose a discretization

$$\frac{q_+ - q}{h_+} = \frac{qp + q_+p_+}{q + q_+}, \qquad \frac{p_+ - p}{h_+} = \frac{1}{q^2q_+^2}\frac{q + q_+}{2}, \tag{3.30}$$

which is invariant with respect to Lie group operators (2.18). The discretization will be considered on the invariant lattice

$$\frac{h_+}{qq_+} = \frac{h_-}{qq_-}. \tag{3.31}$$

This discrete system can be found with the help of the method of finite-difference invariants [24].

Difference equations (3.30) can be rewritten as

$$\frac{q_+ - q}{h_+} = p_+ - \frac{h_+}{2q\tilde{q}^2}, \qquad \frac{p_+ - p}{h_+} = \frac{1}{q^2\tilde{q}^2}\frac{q + \tilde{q}}{2}, \tag{3.32}$$

where $\tilde{q} = \tilde{q}(h_+, q, p_+)$ is the solution of the cubic equation

$$\tilde{q}^3 - (q + h_+p_+)\tilde{q}^2 + \frac{h_+^2}{2q} = 0 \tag{3.33}$$

expressed in terms of the equation parameters h_+, q and p_+ (the expression for $\tilde{q}$ can be written down explicitly; we do not provide it here because of the size of the expression). These equations are generated by the Hamiltonian function

$$\mathcal{H}(t, t_+, q, p_+) = \frac{1}{2}\left(\left(p_+ - \frac{h_+}{2q\tilde{q}^2}\right)^2 + \frac{2\tilde{q} - q}{q\tilde{q}^2}\right), \qquad \tilde{q} = \tilde{q}(h_+, q, p_+).$$

The last difference Hamiltonian equation of (3.7) takes the form

$$-\frac{1}{2}\left(\left(p_+ - \frac{h_+}{2q\tilde{q}^2}\right)^2 + \frac{1}{q\tilde{q}}\right) + \frac{1}{2}\left(\left(p - \frac{h_-}{2\tilde{q}_-^2q_-}\right)^2 + \frac{1}{\tilde{q}_-q_-}\right) = 0, \tag{3.34}$$

where $\tilde{q}_- = \tilde{q}(h_-, q_-, p)$ solves the equation

$$\tilde{q}_-^3 - (q_- + h_-p)\tilde{q}_-^2 + \frac{h_-^2}{2q_-} = 0, \tag{3.35}$$

which is equation (3.33) shifted to the left. It can be shown that lattice equation (3.34), generated by the Hamiltonian, is equivalent to lattice equation (3.31) on the solutions of (3.32).

The Hamiltonian function is invariant with respect to the symmetry operators X_1 and X_2. For the symmetry X_3 we have divergence invariance with $V_3 = q^2/2$. Thus, these symmetries yield three first integrals

$$\begin{aligned} \mathcal{I}_1 &= -\frac{1}{2}\left(\left(p - \frac{h_-}{2q^2q_-}\right)^2 + \frac{1}{qq_-}\right), \\ \mathcal{I}_2 &= qp - t\left(\left(p - \frac{h_-}{2q^2q_-}\right)^2 + \frac{1}{qq_-}\right), \\ \mathcal{I}_3 &= tqp - \frac{t^2}{2}\left(\left(p - \frac{h_-}{2q^2q_-}\right)^2 + \frac{1}{qq_-}\right) - \frac{q^2}{2}. \end{aligned} \tag{3.36}$$

Note that on the solutions of (3.30) we have the relation

$$4\mathcal{I}_1\mathcal{I}_3 - \mathcal{I}_2^2 = 1 - \frac{1}{4}\left(\frac{h_-}{qq_-}\right)^2, \tag{3.37}$$

which explains the choice of the lattice (3.31). In contrast to the differential case (see relation (2.21)) the first integrals $\mathcal{I}_1$, $\mathcal{I}_2$ and $\mathcal{I}_3$ are independent.

In order to integrate the discrete system (3.30), (3.31) we use all three first integrals. Setting $\mathcal{I}_1 = A/2, \mathcal{I}_2 = B$ and

$$\frac{h_-}{q_- q} = \varepsilon,$$

we obtain the solution

$$Aq^2 + (At - B)^2 + 1 = \frac{\varepsilon^2}{4}, \qquad p = \frac{B - At}{q}. \tag{3.38}$$

The solution agrees with the solution of the underlying differential equation, given by (2.22), up to the order ε^2. Complete integration of the difference equations (3.30), (3.31) requires integration of the lattice equation. It can be found in [17].

3.5.3. Nonlinear ODEs. The equations

$$\dot{q} = \frac{4}{p^2}, \qquad \dot{p} = 1 \tag{3.39}$$

are generated by the Hamiltonian

$$H = -\frac{4}{p} - q.$$

We consider the discretization

$$\frac{q_+ - q}{h_+} = \frac{4}{(p_+ - h_+/2)(p + h_+/2)}, \qquad \frac{p_+ - p}{h_+} = 1 \tag{3.40}$$

on the lattice

$$\frac{h_+}{p_+ - h_+/2} = \frac{h_-}{p - h_-/2}. \tag{3.41}$$

This scheme is invariant with respect to Lie group operators

$$X_1 = \frac{\partial}{\partial t}, \qquad X_2 = \frac{\partial}{\partial q}, \qquad X_3 = t\frac{\partial}{\partial t} - q\frac{\partial}{\partial q} + p\frac{\partial}{\partial p}. \tag{3.42}$$

The difference equations (3.40) can be rewritten as

$$\frac{q_+ - q}{h_+} = \frac{4}{(p_+ - h_+/2)^2}, \qquad \frac{p_+ - p}{h_+} = 1. \tag{3.43}$$

These equations are generated by the discrete Hamiltonian function

$$\mathcal{H}(t, t_+, q, p_+) = -\frac{4}{p_+ - h_+/2} - q.$$

The last discrete Hamiltonian equation (3.7) is

$$-\frac{4p_+}{(p_+ - h_+/2)^2} + q - \frac{4p}{(p - h_-/2)^2} - q_- = 0. \tag{3.44}$$

On the solutions of (3.40) this equation leads to the lattice equation (3.41).

The Hamiltonian function is invariant with respect to the symmetry operators X_1 and X_3. For the symmetry X_2 we have divergence invariance with $V_2 = t$. Therefore, these symmetries provide us with three first integrals

$$\mathcal{I}_1 = \frac{4p_+}{(p - h_-/2)^2} + q_-, \qquad \mathcal{I}_2 = p - t, \qquad \mathcal{I}_3 = -qp + t\left(\frac{4p}{(p - h_-/2)^2} + q_-\right). \tag{3.45}$$

The first integrals satisfy the relation

$$4 - \mathcal{I}_1\mathcal{I}_2 - \mathcal{I}_3 = \left(\frac{h_-}{p - h_-/2}\right)^2 \tag{3.46}$$

on the solutions of the difference equations (3.40) that justifies the lattice (3.41). Setting

$$\mathcal{I}_1 = A, \qquad \mathcal{I}_2 = B, \qquad \frac{h_-}{p - h_-/2} = \varepsilon,$$

we find the solution of the discrete model as

$$q = A - \frac{4}{t + B}\left(1 - \frac{\varepsilon^2}{4}\right), \qquad p = t + B. \tag{3.47}$$

Integration of the lattice equation can be found in [17].

4. Conclusion

The goal of this paper is to present a method to find first integrals of canonical Hamiltonian equations and difference Hamiltonian equations as well as to establish a way to preserve the Hamiltonian structure in finite-difference schemes. We introduce invariance of a Hamiltonian action functional and its relation to first integrals of canonical Hamiltonian equations. The conservation properties of the canonical Hamiltonian equations are based on the newly written identity, called the Hamiltonian identity. This identity can be viewed as a 'translation' of the well-known Noether identity into the Hamiltonian framework. The identity makes it possible to establish a one-to-one correspondence between invariance of the Hamiltonian and first integrals of the canonical Hamiltonian equations (the strong version of Noether's theorem). The Hamiltonian version of Noether's theorem, formulated in this paper, gives a constructive way to find first integrals of the canonical Hamiltonian equations once their symmetries are known. This simple method does not require integration as it was illustrated by examples. The presented approach gives a possibility of considering canonical Hamiltonian equations and find their first integrals without exploiting the relationship to the Lagrangian formulation (see, for example, [25]).

The variational consequences of the Hamiltonian identity make it possible to establish the necessary and sufficient conditions for invariance of canonical Hamiltonian equations. These conditions make it clear why not each symmetry of the Hamiltonian equations provides a first integral.

The approach developed for the continuous case was applied to difference Hamiltonian equations, which can be obtained by a variational principle from finite-difference functionals. Similar to the continuous case we related invariance of discrete Hamiltonian functions to first integrals of the difference Hamiltonian equations. In particular, energy conserving numerical schemes can be obtained as difference Hamiltonian equations generated by Hamiltonian functions invariant with respect to time translation. The results presented in this paper provide guidelines how to construct conservative finite-difference schemes in the Hamiltonian framework that are important in numerical implementation.

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