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Invariance and first integrals of continuous and discrete Hamiltonian equations

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Abstract The relation between symmetries and first integrals for both continuous canonical Hamiltonian equations and discrete Hamiltonian equations is considered. The observation that canonical Hamiltonian equations can be obtained by a variational principle from an action functional makes it possible to consider invariance properties of a functional in the same way as done in the Lagrangian formalism. The well-known Noether identity is rewritten in terms of the Hamiltonian function and symmetry operators. This approach, which is based on symmetries of the Hamiltonian action, provides a simple and clear way to construct first integrals of Hamiltonian equations without integration. A discrete analog of this identity is developed. It leads to a relation between symmetries and first integrals for discrete Hamiltonian equations that can be used to conserve structural properties of Hamiltonian equations in numerical implementation. The results are illustrated by a number of examples for both continuous and discrete Hamiltonian equations.

Keywords First integral · Discrete Hamiltonian equations · Symmetry

1 Introduction

It has been known since E. Noether's fundamental work that conservation laws of differential equations are connected with their symmetry properties [1]. For convenience we present here some well-known results (see also, for example, [2, Sect. 4.2], [3, Sect. 12-7], [4, Sect. 20]), for both Lagrangian and Hamiltonian approaches to conservation laws (first integrals).

Let us consider the functional

$$\mathbb{L}(u) = \int_{\Omega} L(x, u, u_1)\mathrm{d}x, \tag{1.1}$$

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where $x = (x^1, x^2, \dots, x^m)$ are independent variables, $u = (u^1, u^2, \dots, u^n)$ are dependent variables, $u_1 = (u_i^k)$ are all first-order derivatives $u_i^k = \frac{\partial u^k}{\partial x^i}$, Ω is a domain in $\mathbb{R}^m$ and $L(x, u, u_1)$ is a *first-order* Lagrangian. The functional (1.1) reaches its extremal values when $u(x)$ satisfies the Euler–Lagrange equations

$$\frac{\delta L}{\delta u^k} = \frac{\partial L}{\partial u^k} - D_i\left(\frac{\partial L}{\partial u_i^k}\right) = 0, \quad k = 1, \dots, n, \tag{1.2}$$

where

$$D_i = \frac{\partial}{\partial x^i} + u_i^k \frac{\partial}{\partial u^k} + u_{ji}^k \frac{\partial}{\partial u_j^k} + \cdots, \quad i = 1, \dots, m$$

are total differentiation operators with respect to the independent variables x^i. Here and below we assume summation over repeated indexes. Note that the equations of (1.2) are second-order PDEs.

We consider a Lie point transformation group G generated by the infinitesimal operator

$$X = \xi^i(x, u)\frac{\partial}{\partial x^i} + \eta^k(x, u)\frac{\partial}{\partial u^k} + \cdots, \tag{1.3}$$

where dots mean an appropriate prolongation of the operator on partial derivatives [5, Sect. 4], [6, Sect. 2.3], [7, Sect. 4], [8, Sect. 2.3]. The group G is called a variational symmetry of the functional $\mathbb{L}(u)$ if and only if the Lagrangian satisfies [1]

$$X(L) + LD_i(\xi^i) = 0, \tag{1.4}$$

where X is the first prolongation, i.e., the prolongation of the vector field X on the first derivatives u_i^k. We will actually need a weaker invariance condition than given by Eq. 1.4. The vector field X is a divergence symmetry of the functional $\mathbb{L}(u)$ if there exist functions $V^i(x, u, u_1), i = 1, \dots, m$ such that [9] (see also [6, Sect. 4.4], [7, Sect. 22], [8, Sect. 5.2])

$$X(L) + LD_i(\xi^i) = D_i(V^i). \tag{1.5}$$

An important result for us is the following: if X is a variational symmetry of the functional $\mathbb{L}(u)$, it is also a symmetry of the corresponding Euler–Lagrange equation. The symmetry group of (1.2) can of course be larger than the group generated by variational and divergence symmetries of the Lagrangian.

Noether's theorem [1] states that for a Lagrangian satisfying condition (1.4) there exists a conservation law of the Euler–Lagrange equations (1.2):

$$D_i\left(\xi^i L + (\eta^k - \xi^j u_j^k)\frac{\partial L}{\partial u_i^k}\right) = 0. \tag{1.6}$$

This result can be generalized: if X is a divergence symmetry of the functional $\mathbb{L}(u)$, i.e., Eq. 1.5 is satisfied, then there exists a conservation law

$$D_i\left(\xi^i L + (\eta^k - \xi^j u_j^k)\frac{\partial L}{\partial u_i^k} - V^i\right) = 0 \tag{1.7}$$

of the corresponding Euler–Lagrange equations.

The strong version of Noether's theorem [7, Sect. 22] states that there exists a conservation law of the Euler–Lagrange equations (1.2) in the form (1.6) if and only if condition (1.4) is satisfied on the solutions of (1.2).

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

$$\dot{q}^i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q^i}, \quad i = 1, \dots, n. \tag{1.8}$$

These equations can be obtained by the variational principle from the action functional

$$\delta \int_{t_1}^{t_2} (p_i \dot{q}^i - H(t, \mathbf{q}, \mathbf{p}))\mathrm{d}t = 0 \tag{1.9}$$

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, [10, Chap. 4], [11, Sect. 1.1]).

Let us note that the canonical Hamiltonian equations (1.8) can be obtained by action of the variational operators

$$\frac{\delta}{\delta p_i} = \frac{\partial}{\partial p_i} - D\frac{\partial}{\partial \dot{p}_i}, \quad i = 1, \ldots, n, \tag{1.10}$$

$$\frac{\delta}{\delta q^i} = \frac{\partial}{\partial q^i} - D\frac{\partial}{\partial \dot{q}^i}, \quad i = 1, \ldots, n, \tag{1.11}$$

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

$$D = \frac{\partial}{\partial t} + \dot{q}^i\frac{\partial}{\partial q^i} + \dot{p}_i\frac{\partial}{\partial p_i} + \cdots, \tag{1.12}$$

on the function

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

The Legendre transformation relates Hamiltonian and Lagrange functions

$$L(t, \mathbf{q}, \dot{\mathbf{q}}) = p_i\dot{q}^i - H(t, \mathbf{q}, \mathbf{p}), \tag{1.13}$$

where $\mathbf{p} = \partial L/\partial\dot{\mathbf{q}}$, $\dot{\mathbf{q}} = \partial H/\partial\mathbf{p}$. It makes possible to establish the equivalence of the Euler–Lagrange and Hamiltonian equations [4, Sect. 15]. Indeed, from the Euler–Lagrange equations for one independent variable ($m = 1$)

$$\frac{\delta L}{\delta q^i} = \frac{\partial L}{\partial q^i} - D\left(\frac{\partial L}{\partial \dot{q}^i}\right) = 0, \quad i = 1, \ldots, n \tag{1.14}$$

we can obtain the canonical Hamiltonian equations (1.8) using the Legendre transformation. It should be noticed that the Legendre transformation is not a point transformation. 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

$$X = \xi(t, \mathbf{q}, \mathbf{p})\frac{\partial}{\partial t} + \eta^i(t, \mathbf{q}, \mathbf{p})\frac{\partial}{\partial q^i} + \zeta_i(t, \mathbf{q}, \mathbf{p})\frac{\partial}{\partial p_i}. \tag{1.15}$$

The standard approach to conservation properties of the Hamiltonian equations is to consider so-called *Hamiltonian symmetries* [6, Sect. 6.3]. In the case of canonical Hamiltonian equations these are the evolutionary ($\xi = 0$) symmetries (1.15)

$$\bar{X} = \eta^i(t, \mathbf{q}, \mathbf{p})\frac{\partial}{\partial q^i} + \zeta_i(t, \mathbf{q}, \mathbf{p})\frac{\partial}{\partial p_i} \tag{1.16}$$

with

$$\eta^i = \frac{\partial I}{\partial p_i}, \quad \zeta^i = -\frac{\partial I}{\partial q^i}, \quad i = 1, \ldots, n \tag{1.17}$$

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

$$\bar{X}_I = \frac{\partial I}{\partial p_i}\frac{\partial}{\partial q^i} - \frac{\partial I}{\partial q^i}\frac{\partial}{\partial p_i}. \tag{1.18}$$

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 (1.18) the independent variable t is invariant and plays the role of a parameter.

Noether's theorem (Theorem 6.33 in [6]) relates Hamiltonian symmetries of the Hamiltonian equations with their first integrals. Restricting ourselves to the case of the canonical Hamiltonian equations, we may formulate this as follows:

Proposition 1.1 *An evolutionary vector field $\bar{X}$ of the form (1.16) generates a Hamiltonian symmetry group of the canonical Hamiltonian system (1.8) if and only if there exists a first integral $I(t,\mathbf{q},\mathbf{p})$ so that $\bar{X} = \bar{X}_I$ is the corresponding Hamiltonian vector field. Another function $\tilde{I}(t,\mathbf{q},\mathbf{p})$ determines the same Hamiltonian symmetry if and only if $\tilde{I} = I + F(t)$ for some time-dependent function $F(t)$.*

Thus, we obtain that the Hamiltonian symmetry determines a first integral of the canonical Hamiltonian equations up to some time-dependent function, which can be found with the help of these equations. This approach has two disadvantages. First, some transformations lose their geometrical sense if considered in the evolutionary form (1.18). Second, there is a necessity of integration to find first integrals with the help of (1.17). In this approach it is also unclear 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 (1.15) that are not restricted to the phase space and can also transform t. In contrast to Hamiltonian symmetries in the form (1.18) 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 identity for the Lagrangian approach. 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 only algebraic manipulations with symmetries of the action functional. The approach will be illustrated by a number of examples, including equations of the three-dimensional Kepler motion.

The paper is organized as follows: In Sect. 2 we introduce the definition of an invariant Hamiltonian and establish the necessary and sufficient condition for H to be invariant. Section 3 contains the main propositions of the present paper: Lemma 3.1 introduces a new identity, which is used in Theorem 3.2 to formulate the necessary and sufficient condition for the existence of first integrals of Hamiltonian equations (Hamiltonian version of Noether's theorem in the strong formulation). In Sect. 4, Lemma 4.1 introduces two further identities, which are used in Theorem 4.4 to formulate necessary and sufficient conditions for the canonical Hamiltonian equations to be invariant. Section 5 contains example ODEs which are considered as both Euler–Lagrange equations and canonical Hamiltonian equations. In particular, we consider the equations of Kepler motion. In Sect. 6 we present discrete Hamiltonian equations. Their symmetries and first integrals are shown to be related in the same way as those for the continuous canonical Hamiltonian equations. The final Sect. 7 contains concluding remarks.

2 Invariance of elementary Hamiltonian action

As an analog of the Lagrangian elementary action [6, Sect. 4.2], [7, Sect. 22], we consider the Hamiltonian elementary action

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

which can be invariant or not with respect to a group generated by an operator of the form (1.15).

Definition 2.1 We call a Hamiltonian function invariant with respect to a symmetry operator (1.15) 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 (1.15) 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 $\mathrm{d}q^i$, $i = 1, \dots, n$:

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

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

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

Remark 2.3 From the relation

$$L(t, \mathbf{q}, \dot{\mathbf{q}})\mathrm{d}t = p_i \mathrm{d}q^i - H(t, \mathbf{q}, \mathbf{p})\mathrm{d}t \tag{2.4}$$

it follows that if a Lagrangian is invariant with respect to a group of Lie point transformations, then the Hamiltonian is also invariant with respect to the same group (of point transformations). The converse statement is false. For example, symmetries providing components of the Runge–Lenz vector as first integrals of Kepler motion are point symmetries in the Hamiltonian framework (point 5.3). However, they are generalized symmetries in the Lagrangian framework [6, Chap. 5].

The proof follows from the action of operator (1.15) on relation (2.4).

Remark 2.4 The operator of total differentiation (1.12) applied to the Hamiltonian H and considered on the solutions of the Hamiltonian equations (1.8) coincides with partial differentiation with respect to time:

$$D(H)|_{\dot{\mathbf{q}}=H_{\mathbf{p}},\dot{\mathbf{p}}=-H_{\mathbf{q}}} = \left[\frac{\partial H}{\partial t} + \dot{q}^i \frac{\partial H}{\partial q^i} + \dot{p}_i \frac{\partial H}{\partial p_i}\right]_{\dot{\mathbf{q}}=H_{\mathbf{p}},\dot{\mathbf{p}}=-H_{\mathbf{q}}} = \frac{\partial H}{\partial t}. \tag{2.5}$$

3 The Hamiltonian identity and Noether-type theorem

Now we can relate conservation properties of the canonical Hamiltonian equations to the invariance of the Hamiltonian function.

Lemma 3.1 *The identity*

$$\zeta_i \dot{q}^i + p_i D(\eta^i) - X(H) - HD(\xi) \equiv \xi\left(D(H) - \frac{\partial H}{\partial t}\right) - \eta^i\left(\dot{p}_i + \frac{\partial H}{\partial q_i}\right) + \zeta_i\left(\dot{q}^i - \frac{\partial H}{\partial p_i}\right) + D[p_i\eta^i - \xi H] \tag{3.1}$$

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 3.2 *The canonical Hamiltonian equations (1.8) possess a first integral of the form*

$$I = p_i\eta^i - \xi H \tag{3.2}$$

if and only if the Hamiltonian function is invariant with respect to the operator (1.15) on the solutions of (1.8).

Proof The result follows from the identity (3.1). □

Theorem 3.2 corresponds to the strong version of the Noether theorem (i.e., necessary and sufficient condition) for invariant Lagrangians and Euler–Lagrange equations [7, Sect. 22].

Remark 3.3 Theorem 3.2 can be generalized to the case of the divergence invariance of the Hamiltonian action

$$\zeta_i \dot{q}^i + p_i D(\eta^i) - X(H) - HD(\xi) = D(V), \tag{3.3}$$

where $V = V(t, \mathbf{q}, \mathbf{p})$. If this condition holds on the solutions of the canonical Hamiltonian equations (1.8), then there is a first integral

$$I = p_i\eta^i - \xi H - V. \tag{3.4}$$

4 Invariance of canonical Hamiltonian equations

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 4.1 and Theorem 4.2 establish the sufficient conditions for canonical Hamiltonian equations to be invariant.

Lemma 4.1 *The following identities are true for any smooth function $H = H(t, \boldsymbol{q}, \boldsymbol{p})$:*

$$\frac{\delta}{\delta p_j}(\zeta_i \dot{q}^i + p_i D(\eta^i) - X(H) - HD(\xi)) \equiv D(\eta^j) - \dot{q}^j D(\xi) - X\left(\frac{\partial H}{\partial p_j}\right)$$
$$+\frac{\partial \xi}{\partial p_j}\left(D(H) - \frac{\partial H}{\partial t}\right) - \frac{\partial \eta^i}{\partial p_j}\left(\dot{p}_i + \frac{\partial H}{\partial q^i}\right) + \left(\frac{\partial \zeta_i}{\partial p_j} + \delta_{ij} D(\xi)\right)\left(\dot{q}^i - \frac{\partial H}{\partial p_i}\right), \quad j = 1, \ldots, n, \tag{4.1}$$

$$\frac{\delta}{\delta q^j}(\zeta_i \dot{q}^i + p_i D(\eta^i) - X(H) - HD(\xi)) \equiv -D(\zeta_j) + \dot{p}_j D(\xi) - X\left(\frac{\partial H}{\partial q_j}\right)$$
$$+\frac{\partial \xi}{\partial q^j}\left(D(H) - \frac{\partial H}{\partial t}\right) - \left(\frac{\partial \eta^i}{\partial q^j} + \delta_{ij} D(\xi)\right)\left(\dot{p}_i + \frac{\partial H}{\partial q^i}\right) + \frac{\partial \zeta_i}{\partial q^j}\left(\dot{q}^i - \frac{\partial H}{\partial p_i}\right), \quad j = 1, \ldots, n, \tag{4.2}$$

where the notation δ_{ij} stands for the Kronecker symbol.

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

Theorem 4.2 *If a Hamiltonian is invariant with respect to the symmetry (1.15), then the canonical Hamiltonian equations (1.8) are also invariant.*

Proof For invariance of the canonical Hamiltonian equations (1.8) we need the equations

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

to hold on the solutions of the Hamiltonian equations [6, Chap. 2]. These conditions follow from the identities (4.1) and (4.2). □

Remark 4.3 The statement of Theorem 4.2 remains valid if we consider divergence symmetries of the Hamiltonian, i.e., condition (3.3), because the term $D(V)$ belongs to the kernel of the variational operators (1.10), (1.11).

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 4.4 establishes the *necessary and sufficient* conditions for canonical Hamiltonian equations to be invariant.

Theorem 4.4 *The canonical Hamiltonian equations (1.8) are invariant with respect to the symmetry (1.15) if and only if the following conditions are true (on the solutions of the canonical Hamiltonian equations):*

$$\left.\frac{\delta}{\delta p_j}(\zeta_i \dot{q}^i + p_i D(\eta^i) - X(H) - HD(\xi))\right|_{\dot{\boldsymbol{q}}=H_{\boldsymbol{p}},\ \dot{\boldsymbol{p}}=-H_{\boldsymbol{q}}} = 0, \quad j = 1, \ldots, n, \tag{4.3}$$

$$\left.\frac{\delta}{\delta q^j}(\zeta_i \dot{q}^i + p_i D(\eta^i) - X(H) - HD(\xi))\right|_{\dot{\boldsymbol{q}}=H_{\boldsymbol{p}},\ \dot{\boldsymbol{p}}=-H_{\boldsymbol{q}}} = 0, \quad j = 1, \ldots, n. \tag{4.4}$$

Proof The statement follows from the identities (4.1) and (4.2). □

It should be noted that conditions (4.3) and (4.4) are true for all symmetries of canonical Hamiltonian equations. But not all of those symmetries yield the "variational integral" of these conditions, i.e.,

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

which gives first integrals in accordance with Theorem 3.2. *That is why not all symmetries of the canonical Hamiltonian equations provide first integrals*. In the next section we illustrate the theorems, given above, on a number of examples.

5 Applications

In this section we provide examples of how to find first integrals with the help of symmetries.

5.1 A scalar ODE

As a first example we consider the second-order ODE

$$\ddot{u} = \frac{1}{u^3}, \tag{5.1}$$

which admits Lie algebra L_3 with basis operators

$$X_1 = \frac{\partial}{\partial t}, \quad X_2 = 2t\frac{\partial}{\partial t} + u\frac{\partial}{\partial u}, \quad X_3 = t^2\frac{\partial}{\partial t} + tu\frac{\partial}{\partial u}. \tag{5.2}$$

5.1.1 Lagrangian approach

The Lagrangian function

$$L(t, u, \dot{u}) = \frac{1}{2}\left(\dot{u}^2 - \frac{1}{u^2}\right), \tag{5.3}$$

which provides Eq. 5.1 as its Euler–Lagrange equation, is invariant with respect to X_1 and X_2. Therefore, by means of Noether's theorem there exist first integrals

$$J_1 = -\frac{1}{2}\left(\dot{u}^2 + \frac{1}{u^2}\right), \quad J_2 = u\dot{u} - t\left(\dot{u}^2 + \frac{1}{u^2}\right). \tag{5.4}$$

The action of the third operator X_3 yields the divergence invariance condition

$$XL + LD(\xi) = u\dot{u} = D\left(\frac{u^2}{2}\right). \tag{5.5}$$

Due to the divergence invariance of the Lagrangian we can find the following first integral

$$J_3 = -\frac{1}{2}\left(\frac{t^2}{u^2} + (u - t\dot{u})^2\right). \tag{5.6}$$

Alternatively, one can find the last integral from another Lagrangian function

$$\tilde{L}(t, u, \dot{u}) = \left(\frac{u}{t} - \dot{u}\right)^2 - \frac{1}{u^2}, \tag{5.7}$$

which is exactly invariant with respect to X_3.

It should be mentioned that independence of first integrals obtained with the help of the Noether theorem is guaranteed only in the case when there is one Lagrangian which is invariant with respect to all symmetries. This condition is violated in the considered example. Therefore, the integrals obtained are not independent. The integrals (5.4),(5.6) are connected by the relation

$$4J_1J_3 - J_2^2 = 1. \tag{5.8}$$

Thus, any two integrals among (5.4), (5.6) are independent. Putting $J_1 = A/2$, $J_2 = B$ and excluding $\dot{u}$, we find the general solution of (5.1) as

$$Au^2 + (At - B)^2 + 1 = 0. \tag{5.9}$$

5.1.2 Hamiltonian framework

Let us transfer the preceding example into the Hamiltonian framework. We change variables:

$$q = u, \quad p = \frac{\partial L}{\partial \dot{u}} = \dot{u}.$$

The corresponding Hamiltonian is

$$H(t, q, p) = \dot{u}\frac{\partial L}{\partial \dot{u}} - L = \frac{1}{2}\left(p^2 + \frac{1}{q^2}\right). \tag{5.10}$$

The Hamiltonian equations

$$\dot{q} = p, \quad \dot{p} = \frac{1}{q^3} \tag{5.11}$$

admit symmetries

$$X_1 = \frac{\partial}{\partial t}, \quad X_2 = 2t\frac{\partial}{\partial t} + q\frac{\partial}{\partial q} - p\frac{\partial}{\partial p}, \quad X_3 = t^2\frac{\partial}{\partial t} + tq\frac{\partial}{\partial q} + (q - tp)\frac{\partial}{\partial p}. \tag{5.12}$$

We check the 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 3.2, we calculate the corresponding first integrals

$$I_1 = -H = -\frac{1}{2}\left(p^2 + \frac{1}{q^2}\right), \quad I_2 = pq - t\left(p^2 + \frac{1}{q^2}\right). \tag{5.13}$$

For the third symmetry operator the Hamiltonian is divergence invariant with $V_3 = q^2/2$. In accordance with Remark 3.3, this yields the following conserved quantity

$$I_3 = -\frac{1}{2}\left(\frac{t^2}{q^2} + (q - tp)^2\right). \tag{5.14}$$

Note that no integration is needed to provide solutions of (5.11). As we noted before, in the Lagrangian case only two first integrals are functionally independent. Putting $I_1 = A/2$ and $I_2 = B$, we find the solution of (5.11) as

$$Aq^2 + (At - B)^2 + 1 = 0, \quad p = \frac{B - At}{q}. \tag{5.15}$$

5.2 Repulsive one-dimensional motion.

As another example of an ODE we consider one-dimensional motion in a Coulomb field (the case of a repulsive force):

$$\ddot{u} = \frac{1}{u^2}, \tag{5.16}$$

which admits Lie algebra L_2 with basis operators

$$X_1 = \frac{\partial}{\partial t}, \quad X_2 = 3t\frac{\partial}{\partial t} + 2u\frac{\partial}{\partial u}. \tag{5.17}$$

5.2.1 Lagrangian approach

The Lagrangian function

$$L(t, u, \dot{u}) = \frac{\dot{u}^2}{2} - \frac{1}{u} \tag{5.18}$$

is invariant only with respect to X_1. Therefore, Noether's theorem yields the only first integral

$$J_1 = \frac{\dot{u}^2}{2} + \frac{1}{u}. \tag{5.19}$$

In this case the Euler–Lagrange equation admits two symmetries while the Lagrangian is invariant with respect to one symmetry operator only.

5.2.2 Hamiltonian framework

We change variables

$$q = u, \quad p = \frac{\partial L}{\partial \dot{u}} = \dot{u}$$

and find the Hamiltonian function

$$H(t, q, p) = \dot{u}\frac{\partial L}{\partial \dot{u}} - L = \frac{p^2}{2} + \frac{1}{q}. \tag{5.20}$$

The Hamiltonian equations have the form

$$\dot{q} = p, \quad \dot{p} = \frac{1}{q^2}. \tag{5.21}$$

We rewrite symmetries in the canonical variables as the following algebra L_2:

$$X_1 = \frac{\partial}{\partial t}, \quad X_2 = 3t\frac{\partial}{\partial t} + 2q\frac{\partial}{\partial q} - p\frac{\partial}{\partial p}. \tag{5.22}$$

The invariance of the Hamiltonian condition (2.2) is satisfied for operator X_1 only. Applying Theorem 3.2, we calculate the corresponding first integral

$$I_1 = -H = -\left(\frac{p^2}{2} + \frac{1}{q}\right). \tag{5.23}$$

Application of operator X_2 to the Hamiltonian action gives

$$\zeta\dot{q} + pD(\eta) - X(H) - HD(\xi) = p\dot{q} - \left(\frac{p^2}{2} + \frac{1}{q}\right) \neq 0. \tag{5.24}$$

Meanwhile, in accordance with Theorem 4.4 we have

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

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

We will show below that there exists a second integral of non-local character.

It was shown in [12] that Eq. 5.16 can be linearized by a contact transformation. For (5.21) this transformation is the following

$$p(t) = P(s), \quad Q^2(s) = \frac{2}{q(t)}, \quad \mathrm{d}t = -\frac{4}{Q^3}\mathrm{d}s. \tag{5.25}$$

The new Hamiltonian

$$H(s, Q, P) = \frac{1}{2}(P^2 + Q^2) \tag{5.26}$$

corresponds to the linear equations

$$\frac{\mathrm{d}Q}{\mathrm{d}s} = P, \quad \frac{\mathrm{d}P}{\mathrm{d}s} = -Q, \tag{5.27}$$

which describe the one-dimensional harmonic oscillator. These equations have two independent first integrals

$$I_1 = \frac{1}{2}(P^2 + Q^2), \quad I_2 = \arctan\left(\frac{P}{Q}\right) + s, \tag{5.28}$$

which allow us write down the general solution of (5.27) as

$$Q = A\sin s + B\cos s, \quad P = A\cos s - B\sin s, \tag{5.29}$$

where A and B are arbitrary constants. Applying the transformation (5.25) to integral I_2 we find the non-local integral for (5.21):

$$I_2^* = \arctan\left(\frac{p\sqrt{q}}{\sqrt{2}}\right) - \frac{1}{\sqrt{2}}\int_{t_0}^{t}\frac{\mathrm{d}t}{q^{3/2}}. \tag{5.30}$$

5.3 Kepler motion

The Kepler problem is a special case of the two-body problem, in which the two bodies interact by a central force that varies in strength as the inverse square of the distance between them [2, Chap. 9], [3, Chap. 3], [4, Chap. 2]. The three-dimensional Kepler motion of a body in a Newtonian gravitational field is given by the equations

$$\dot{\mathbf{q}} = \mathbf{p}, \quad \dot{\mathbf{p}} = -\frac{K^2}{r^3}\mathbf{q}, \quad r = |\mathbf{q}|, \quad \mathbf{q}, \mathbf{p} \in \mathbb{R}^3, \tag{5.31}$$

where K is a constant, with the initial data

$$\mathbf{q}(0) = \mathbf{q}_0, \quad \mathbf{p}(0) = \mathbf{p}_0.$$

These equations are Hamiltonian. They are defined by the Hamiltonian function

$$H(\mathbf{q}, \mathbf{p}) = \frac{1}{2}|\mathbf{p}|^2 - \frac{K^2}{r}. \tag{5.32}$$

Among the symmetries admitted by (5.31) there are

$$X_0 = \frac{\partial}{\partial t}, \quad X_1 = 3t\frac{\partial}{\partial t} + 2q^i\frac{\partial}{\partial q^i} - p_i\frac{\partial}{\partial p_i},$$

$$X_{ij} = -q^j\frac{\partial}{\partial q^i} + q^i\frac{\partial}{\partial q^j} - p_j\frac{\partial}{\partial p_i} + p_i\frac{\partial}{\partial p_j}, \quad i \neq j,$$

$$Y_l = (2q^l p_k - q^k p_l - (\mathbf{q}, \mathbf{p})\delta_{lk})\frac{\partial}{\partial q^k} + \left(p_l p_k - (\mathbf{p}, \mathbf{p})\delta_{lk} - \frac{K^2}{r^3}(q^l q^k - (\mathbf{q}, \mathbf{q})\delta_{lk})\right)\frac{\partial}{\partial p_k}, \quad l = 1, 2, 3,$$

where $(\mathbf{f}, \mathbf{g}) = \mathbf{f}^T\mathbf{g}$ is a scalar product of vectors.

The Hamiltonian function (5.32) is invariant for the symmetries X_0 and X_{ij}. Theorem 3.2 makes it possible to find the first integral for symmetry X_0

$$I_1 = -H,$$

which represents the conservation of the energy in Kepler motion. For symmetries X_{ij} we obtain the first integrals

$$I_{ij} = q^i p_j - q^j p_i, \quad i \neq j,$$

which are components of the angular momentum

$$\mathbf{L}(\mathbf{q}, \mathbf{p}) = \mathbf{q} \times \mathbf{p}. \tag{5.33}$$

Conservation of angular momentum shows that the orbit of motion of a body lies in a fixed plane perpendicular to the constant vector $\mathbf{L}$. It also follows that in this plane the position vector $\mathbf{q}$ sweeps out equal areas in equal time intervals, so that the sectorial velocity is constant [4, Sect. 7]. Therefore, Kepler's second law can be considered as a geometric reformulation of the conservation of angular momentum.

The scaling symmetry X_1 is not a Noether symmetry (neither variational, nor divergence symmetry) and does not lead to a conserved quantity.

For each of the symmetries Y_l the Hamiltonian is divergence-invariant with functions

$$V_l = q^l\left((\mathbf{p}, \mathbf{p}) + \frac{K^2}{r}\right) - p_l(\mathbf{q}, \mathbf{p}), \quad l = 1, 2, 3.$$

Hence, the operators Y_l yield the first integrals

$$I_l = q^l\left((\mathbf{p}, \mathbf{p}) - \frac{K^2}{r}\right) - p_l(\mathbf{q}, \mathbf{p}), \quad l = 1, 2, 3,$$

which are components of the Runge–Lenz vector

$$\mathbf{A}(\mathbf{q}, \mathbf{p}) = \mathbf{p} \times \mathbf{L} - \frac{K^2}{r}\mathbf{q} = \mathbf{q}\left(H(\mathbf{q}, \mathbf{p}) + \frac{1}{2}|\mathbf{p}|^2\right) - \mathbf{p}(\mathbf{q}, \mathbf{p}). \tag{5.34}$$

Physically, vector **A** lies along the major axis of the conic section determined by the orbit of the body. Its magnitude determines the eccentricity [13, p. 147].

Let us note that not all first integrals are independent. There are two relations between them given by the equations

$$|\mathbf{A}|^2 - 2H|\mathbf{L}|^2 = K^4 \quad \text{and} \quad (\mathbf{A}, \mathbf{L}) = 0.$$

The two-dimensional Kepler motion can be considered in a similar way. Let us remark that symmetries and first integrals of two-dimensional Kepler motion can be obtained by restricting the symmetries and first integrals of three-dimensional Kepler motion to the space (t, q^1, q^2, p_1, p_2). As the conserved quantities of two-dimensional Kepler motion one obtains the energy

$$H(\mathbf{q}, \mathbf{p}) = \frac{1}{2}|\mathbf{p}|^2 - \frac{K^2}{r}, \quad r = |\mathbf{q}|, \quad \mathbf{q} = (q^1, q^2), \quad \mathbf{p} = (p_1, p_2),$$

one component of the angular momentum

$$L_3 = q^1 p_2 - q^2 p_1$$

and two components of the Runge–Lenz vector

$$A_1 = q^1 \left(H(\mathbf{q}, \mathbf{p}) + \frac{1}{2}|\mathbf{p}|^2 \right) - p_1(\mathbf{q}, \mathbf{p}), \quad A_2 = q^2 \left(H(\mathbf{q}, \mathbf{p}) + \frac{1}{2}|\mathbf{p}|^2 \right) - p_2(\mathbf{q}, \mathbf{p}).$$

There is one relation between these conserved quantities, namely

$$A_1^2 + A_2^2 - 2HL_3^2 = K^4.$$

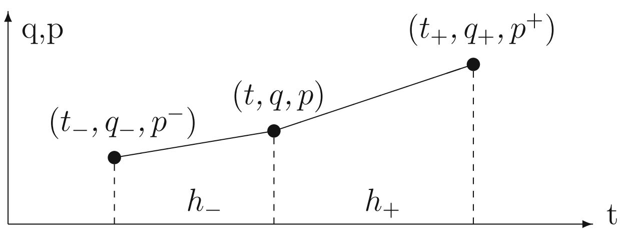
Further restriction to one-dimensional Kepler motion leaves only one first integral, which is the Hamiltonian function.

6 First integrals of discrete Hamiltonian equations

It is known that the preservation of first integrals (conservation laws) in numerical work is of great importance (see, for example, [14,15]). Therefore, it makes sense to establish a discrete analog of the results presented for the continuous Hamiltonian equations. An analogous discrete framework would allow one to construct numerical schemes with first integrals for various applied problems.

6.1 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 discrete equations we will need three points of a lattice. Prolongation of Lie group operator (1.15) for neighboring points $(t_-, \mathbf{q}_-, \mathbf{p}^-)$ and $(t_+, \mathbf{q}_+, \mathbf{p}^+)$ is the following:

$$X = \xi \frac{\partial}{\partial t} + \eta^i \frac{\partial}{\partial q^i} + \zeta_i \frac{\partial}{\partial p_i} + \xi_- \frac{\partial}{\partial t_-} + \eta^i_- \frac{\partial}{\partial q^i_-} + \zeta_i^- \frac{\partial}{\partial p_i^-}$$
$$+\xi_+ \frac{\partial}{\partial t_+} + \eta^i_+ \frac{\partial}{\partial q^i_+} + \zeta_i^+ \frac{\partial}{\partial p_i^+} + (\xi_+ - \xi) \frac{\partial}{\partial h_+} + (\xi - \xi_-) \frac{\partial}{\partial h_-}, \tag{6.1}$$

where

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

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

$$\mathbb{H}_h = \sum_{\Omega} (p_i^+ (q^i_+ - q^i) - \mathcal{H}(t, t_+, \mathbf{q}, \mathbf{p}^+) h_+). \tag{6.2}$$

Indeed, a variation of this functional along a curve $q^i = \phi_i(t)$, $p_i = \psi_i(t)$, $i = 1, \dots, n$ at some point $(t, \mathbf{q}, \mathbf{p})$ will effect only two terms of the sum (6.2):

$$\mathbb{H}_h = \dots + p_i(q^i - q^i_-) - \mathcal{H}(t_-, t, \mathbf{q}_-, \mathbf{p}) h_- + p_i^+(q^i_+ - q^i) - \mathcal{H}(t, t_+, \mathbf{q}, \mathbf{p}^+) h_+ + \cdots \tag{6.3}$$

Therefore, we get the following expression for the variation

$$\delta \mathbb{H}_h = \frac{\delta \mathcal{H}}{\delta p_i} \delta p_i + \frac{\delta \mathcal{H}}{\delta q^i} \delta q^i + \frac{\delta \mathcal{H}}{\delta t} \delta t, \tag{6.4}$$

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

$$\frac{\delta \mathcal{H}}{\delta p_i} = q^i - q^i_- - h_- \frac{\partial \mathcal{H}^-}{\partial p_i}, \quad \frac{\delta \mathcal{H}}{\delta q^i} = -\left(p_i^+ - p_i + h_+ \frac{\partial \mathcal{H}}{\partial q^i} \right), \quad i = 1, \dots, n,$$
$$\frac{\delta \mathcal{H}}{\delta t} = -\left(h_+ \frac{\partial \mathcal{H}}{\partial t} - \mathcal{H} + h_- \frac{\partial \mathcal{H}^-}{\partial t} + \mathcal{H}^- \right), \tag{6.5}$$

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 (6.2) we obtain the following system of $2n+1$ equations

$$\frac{\delta \mathcal{H}}{\delta p_i} = 0, \quad \frac{\delta \mathcal{H}}{\delta q^i} = 0, \quad i = 1, \dots, n, \quad \frac{\delta \mathcal{H}}{\delta t} = 0.$$

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

$$\underset{+h}{D}(q^i) = \frac{\partial \mathcal{H}}{\partial p_i^+}, \quad \underset{+h}{D}(p_i) = -\frac{\partial \mathcal{H}}{\partial q^i}, \quad i = 1, \dots, n, \quad h_+ \frac{\partial \mathcal{H}}{\partial t} - \mathcal{H} + h_- \frac{\partial \mathcal{H}^-}{\partial t} + \mathcal{H}^- = 0, \tag{6.6}$$

which we will call *discrete Hamiltonian equations*. For convenience we use the following total shift (left and right) operators and corresponding discrete differentiation operators:

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

Let us note that the first $2n$ equations (6.6) are first-order discrete equations, which correspond to the canonical Hamiltonian equations (1.8) in the continuous limit. The last equation is of second order. Its continuous counterpart (see Remark 2.4) 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.

It is interesting to note that the equations of (6.6) can be obtained from discrete variational equations in the Lagrangian framework [16,17], [18, Chap. 3], [19] with the help of a discrete Legendre transformation [20].

Remark 6.1 Equivalent formulation can be considered for the finite-difference functional

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

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

6.2 Invariance of the Hamiltonian action

Let us consider the functional (6.2) on some lattice, given by equation

$$\Omega(t, h_+, h_-, \mathbf{q}, \mathbf{p}) = 0. \tag{6.7}$$

Definition 6.2 We call a discrete Hamiltonian function $\mathcal{H}$ considered on the mesh (6.7) *invariant* with respect to a group generated by the operator (6.1), if the action (6.2) considered on the mesh (6.7) is an invariant manifold of a group.

Theorem 6.3 *A Hamiltonian function considered together with the mesh* (6.7) *is invariant with respect to a group generated by the operator* (6.1) *if and only if the following conditions hold*

$$\left.\zeta_i^+ \underset{+h}{D}(q^i) + p_i^+ \underset{+h}{D}(\eta^i) - X(\mathcal{H}) - \mathcal{H} \underset{+h}{D}(\xi)\right|_{\Omega=0} = 0, \quad X\Omega(t, h_+, h_-, \boldsymbol{q}, \boldsymbol{p})|_{\Omega=0} = 0. \tag{6.8}$$

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 a mesh, which is obtained by the action of the symmetry operator on the mesh equation (6.7). □

6.3 Discrete Hamiltonian identity and discrete Noether-type theorem

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

Lemma 6.4 *The following identity is true for any smooth function* $\mathcal{H} = \mathcal{H}(t, t_+, \mathbf{q}, \mathbf{p}^+)$*:*

$$\begin{aligned}\zeta_i^+ \underset{+h}{D}(q^i) + p_i^+ \underset{+h}{D}(\eta^i) - X(\mathcal{H}) - \mathcal{H} \underset{+h}{D}(\xi) &\equiv \xi \left(\underset{+h}{D}(\mathcal{H}^-) - \frac{\partial \mathcal{H}}{\partial t} - \frac{h_-}{h_+}\frac{\partial \mathcal{H}^-}{\partial t}\right) \\ -\eta^i \left(\underset{+h}{D}(p_i) + \frac{\partial \mathcal{H}}{\partial q^i}\right) + \zeta_i^+ \left(\underset{+h}{D}(q^i) - \frac{\partial \mathcal{H}}{\partial p_i^+}\right) &+ \underset{+h}{D}\left[\eta^i p_i - \xi\left(\mathcal{H}^- + h_- \frac{\partial \mathcal{H}^-}{\partial t}\right)\right]\end{aligned} \tag{6.9}$$

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 6.5 *The discrete Hamiltonian equations* (6.6)*, invariant with respect to the symmetry operator* (6.1)*, possess a first integral*

$$\mathcal{I} = \eta^i p_i - \xi\left(\mathcal{H}^- + h_- \frac{\partial \mathcal{H}^-}{\partial t}\right) \tag{6.10}$$

if and only if the Hamiltonian function is invariant with respect to the same symmetry on the solutions of (6.6).

Proof This result is a consequence of the identity (6.9). The invariance of the discrete Hamiltonian equations is needed to guarantee the invariance of the mesh, which is defined by these equations. □

Remark 6.6 Theorem 6.5 can be generalized to the case of divergence invariance of the Hamiltonian action, i.e.,

$$\zeta_i^+ \underset{+h}{D}(q^i) + p_i^+ \underset{+h}{D}(\eta^i) - X(\mathcal{H}) - \mathcal{H} \underset{+h}{D}(\xi) = \underset{+h}{D}(V), \tag{6.11}$$

where $V = V(t, \mathbf{q}, \mathbf{p})$. If this condition holds on the solutions of the discrete Hamiltonian equations (6.6), then there is a first integral

$$\mathcal{I} = \eta^i p_i - \xi \left(\mathcal{H}^- + h_- \frac{\partial \mathcal{H}^-}{\partial t} \right) - V. \tag{6.12}$$

Remark 6.7 For discrete 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 discrete Hamiltonian equations (6.6) are related to symplectic-momentum-energy preserving variational integrations introduced for the discrete Lagrangian framework in [21]. Note that $\mathcal{H}$ is not the discrete energy; it has the meaning of a generating function for discrete Hamiltonian flow.

6.4 Applications

6.4.1 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

$$\dot{q} = p, \quad \dot{p} = -q. \tag{6.13}$$

This system of Hamiltonian equations is generated by the Hamiltonian function

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

As a discretization of (6.13) we consider the application of the midpoint rule

$$\frac{q_+ - q}{h_+} = \frac{p + p_+}{2}, \quad \frac{p_+ - p}{h_+} = -\frac{q + q_+}{2} \tag{6.14}$$

on a uniform mesh $h_+ = h_- = h$. The presented discretization can be rewritten as the following system of equations

$$\underset{+h}{D}(q) = \frac{4}{4 - h_+^2}\left(p_+ + \frac{h_+}{2} q \right), \quad \underset{+h}{D}(p) = -\frac{4}{4 - h_+^2}\left(q + \frac{h_+}{2} p_+ \right), \quad h_+ = h_-. \tag{6.15}$$

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

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

Indeed, the first and second equations of (6.6) are exactly the same as those of (6.15). The last equation of (6.6) takes the form

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

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

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

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

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

The system of difference equations (6.15) admits, in particular, the following symmetries

$$X_1 = \sin(\omega t)\frac{\partial}{\partial q} + \cos(\omega t)\frac{\partial}{\partial p}, \quad X_2 = \cos(\omega t)\frac{\partial}{\partial q} - \sin(\omega t)\frac{\partial}{\partial p},$$

$$X_3 = \frac{\partial}{\partial t}, \quad X_4 = q\frac{\partial}{\partial q} + p\frac{\partial}{\partial p}, \quad X_5 = p\frac{\partial}{\partial q} - q\frac{\partial}{\partial p},$$

where

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

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 (6.15) with functions $V_1 = q\cos(\omega t)$ and $V_2 = -q\sin(\omega t)$, respectively. Therefore, we obtain two corresponding first integrals

$$\mathcal{I}_1 = p\sin(\omega t) - q\cos(\omega t), \quad \mathcal{I}_2 = p\cos(\omega t) + q\sin(\omega t). \tag{6.16}$$

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

$$\mathcal{I}_3 = -\frac{4}{4-h_-^2}\left(\frac{4+h_-^2}{4-h_-^2}\frac{q_-^2 + p^2}{2} + \frac{4h_-}{4-h_-^2}q_- p\right). \tag{6.17}$$

Using the first and second equations of (6.15), we can simplify it as

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

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

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

The three first integrals $\mathcal{I}_1, \mathcal{I}_2, \tilde{\mathcal{I}}_3$ are sufficient for integration of the system (6.14). We obtain the solution

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

on the lattice

$$t_i = t_0 + ih, \quad i = 0, \pm 1, \pm 2, \dots, \quad h = \tilde{\mathcal{I}}_3.$$

6.4.2 Modified discrete harmonic oscillator (exact scheme)

The discrete harmonic oscillator of the preceding example follows the same trajectory as the continuous harmonic oscillator, but with a different velocity. This numerical error can be corrected by time reparametrization. In this case we will get the exact discretization of the harmonic oscillator, i.e., a discretization which gives the exact solution of the underlying ODEs.

In this case the harmonic oscillator (6.13) is discretized as

$$\frac{q_+ - q}{h_+} = \Omega \frac{p + p_+}{2}, \quad \frac{p_+ - p}{h_+} = -\Omega \frac{q + q_+}{2}, \quad h_+ = h_- = h, \tag{6.18}$$

where

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

represents a time reparametrization. Similarly to the preceding example it can be shown that this discrete model of the harmonic oscillator is generated by the discrete Hamiltonian

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

The system of difference equations (6.18) admits the following symmetries

$$X_1 = \sin t \frac{\partial}{\partial q} + \cos t \frac{\partial}{\partial p}, \quad X_2 = \cos t \frac{\partial}{\partial q} - \sin t \frac{\partial}{\partial p},$$
$$X_3 = \frac{\partial}{\partial t}, \quad X_4 = q \frac{\partial}{\partial q} + p \frac{\partial}{\partial p}, \quad X_5 = p \frac{\partial}{\partial q} - q \frac{\partial}{\partial p}.$$

For symmetries X_1 and X_2, which satisfy the divergence invariance condition (6.11) on the solutions of equations (6.18) with functions $V_1 = q \cos t$ and $V_2 = -q \sin t$, we obtain two first integrals

$$\mathcal{I}_1 = p \sin t - q \cos t, \quad \mathcal{I}_2 = p \cos t + q \sin t. \tag{6.19}$$

The operator X_3 satisfies the invariance condition (6.8) and provides us with the first integral $\mathcal{I}_3$, which (similarly to the preceding example) can be taken in an equivalent form:

$$\tilde{\mathcal{I}}_3 = h_-. \tag{6.20}$$

The scheme (6.18) gives the exact solution of the harmonic oscillator, which can be found with the help of first integrals $\mathcal{I}_1$ and $\mathcal{I}_2$ as

$$q = \mathcal{I}_2 \sin t - \mathcal{I}_1 \cos t, \quad p = \mathcal{I}_1 \sin t + \mathcal{I}_2 \cos t.$$

This discrete solution is given on the lattice

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

The exact schemes for two- and four-dimensional harmonic oscillators were used in [22] to construct exact schemes for two- and three-dimensional Kepler motion, respectively.

6.4.3 A nonlinear motion

We consider a difference analog of (5.11), and choose

$$\mathcal{H}(t, t_+, q, p_+) = \frac{1}{2}\left(p_+^2 + \frac{1}{q^2}\right). \tag{6.21}$$

Then, in accordance with (6.6) we obtain the discrete Hamiltonian equations:

$$\underset{+h}{D}(q) = p_+, \quad \underset{+h}{D}(p) = \frac{1}{q^3}, \quad p_+^2 + \frac{1}{q^2} = p^2 + \frac{1}{q_-^2} \tag{6.22}$$

It is easy to check the invariance conditions for $\mathcal{H}$ with respect to the symmetry operators X_1 and X_2, given in (5.12). Application of Theorem 6.5 for these symmetries yields the first integrals

$$\mathcal{I}_1 = -\frac{1}{2}\left(p^2 + \frac{1}{q_-^2}\right), \quad \mathcal{I}_2 = qp - t\left(p^2 + \frac{1}{q_-^2}\right). \tag{6.23}$$

Therefore, the solution of the discrete system (6.22) satisfies the relation

$$\mathcal{I}_2 = qp + 2t\mathcal{I}_1$$

in all points of the lattice.

7 Conclusion

The goal of the present paper has been to present a method to find first integrals of canonical Hamiltonian equations and to establish a way of preserving Hamiltonian structure in finite-difference schemes. To achieve this we have used invariance of the 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 formulated 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 variational consequences of the Hamiltonian identity make it possible to establish necessary and sufficient conditions for the canonical Hamiltonian equations to be invariant. These conditions make it clear why not every symmetry of the Hamiltonian equations provides a first integral.

The Hamiltonian version of Noether's theorem, as formulated in the paper, gives a constructive way of finding first integrals of the canonical Hamiltonian equations once their symmetries are known. This simple method does not require integration, as was illustrated by a number of examples. In particular, we considered the equations of Kepler motion in various dimensions. The presented approach gives a possibility to consider canonical Hamiltonian equations and find their first integrals without exploiting the relationship with the Lagrangian formulation (see, for example, [23]).

The approach developed for the continuous case was applied to discrete Hamiltonian equations, which can be obtained by a variational principle from finite-difference functionals. Similarly to the continuous case we related invariance of discrete Hamiltonian functions to first integrals of the discrete Hamiltonian equations. In particular, energy-conserving numerical schemes can be obtained as discrete Hamiltonian equations generated by Hamiltonian functions invariant with respect to time translations.

The results presented here can be used to find first integrals of continuous and discrete canonical Hamiltonian equations. They also provide guidelines on how to construct conservative finite-difference schemes in the Hamiltonian framework that are important in numerical implementations.

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