Variational symmetries in the Hamiltonian formalism

G. F. Torres del Castillo

Instituto de Ciencias, Benemérita Universidad Autónoma de Puebla,
72570 Puebla, Pue., México

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We consider the effect on the Hamilton equations of an arbitrary coordinate transformation in the extended configuration space, $q'_i = q'_i(q_j, t)$, $t' = t'(q_j, t)$ (which may not be canonical) and we show that when the Hamiltonian is invariant under a one-parameter family of these transformations, there is an associated nontrivial constant of motion.

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1. Introduction

A common point of interest in classical mechanics, quantum mechanics, classical field theory and quantum field theory is the study of symmetry, which can be defined directly in terms of the equations of motion (*e.g.*, Newton's second law, Schrödinger's equation, etc.) or through Lagrangians or Hamiltonians. One advantage of finding symmetries of a Lagrangian or a Hamiltonian for a given system is that one can associate conserved quantities with one-parameter families of symmetries if the notion of symmetry is appropriately defined. (By contrast, the symmetries of the equations of motion alone do not lead to constants of motion, see, *e.g.*, Ref. [1].)

In the case of a system with a finite number of degrees of freedom described by a Lagrangian, $L(q_i, \dot{q}_i, t)$, it is useful to define a variational symmetry (also called a divergence symmetry) as a coordinate transformation in the extended configuration space,

$$q'_i = q'_i(q_1, \ldots, q_n, t), \quad t' = t'(q_1, \ldots, q_n, t), \qquad (1)$$

such that

$$L\left(q'_i, \frac{\mathrm{d}q'_i}{\mathrm{d}t'}, t'\right) \frac{\mathrm{d}t'}{\mathrm{d}t} = L\left(q_i, \frac{\mathrm{d}q_i}{\mathrm{d}t}, t\right) + \frac{\mathrm{d}}{\mathrm{d}t}F(q_i, t), \qquad (2)$$

where F is some function defined on the extended configuration space. The usefulness of this definition comes from the fact that the "infinitesimal" generators of the one-parameter groups of variational symmetries of a Lagrangian can be found by means of a systematic procedure (though somewhat lengthy in most cases) and with each generator we get a nontrivial constant of motion (see, *e.g.*, Refs [2, 3]). However, not all constants of motion can be obtained in this way (perhaps the best known example is the Laplace–Runge–Lenz vector found in the Kepler problem).

On the other hand, within the Hamiltonian formalism, *any* constant of motion is associated with a one-parameter group of canonical transformations that leave invariant the Hamiltonian of the system under consideration. However, finding these groups is as complicated as finding the constants of motion directly.

By contrast with the variational symmetries defined in the Lagrangian formalism, where the time can be replaced by some function, t', of the original coordinates and the time [see Eqs. (1)], in the canonical transformations, the phase space coordinates, q_i, p_i, can be substituted by new coordinates $Q_i = Q_i(q_j, p_j, t)$, $P_i = P_i(q_j, p_j, t)$, but the time remains unaltered.

The aim of this paper is to show in an elementary way that given a Hamiltonian, $H(q_i, p_i, t)$, and a coordinate transformation (1) in the extended configuration space, we can find a new Hamiltonian, $H'(q'_i, p'_i, t')$, and new canonical momenta, p'_i, such that the Hamilton equations with the primed variables are equivalent to the Hamilton equations with the unprimed variables. In Sec. 2 we give the formulas relating the new Hamiltonian and canonical momenta with the initial ones. In Sec. 3 we show that if a Hamiltonian is invariant under a one-parameter family of coordinate transformations in the extended configuration space then there is a nontrivial constant of motion associated with the symmetry.

2. Transformation of the Hamiltonian under coordinate transformations in the extended configuration space

As is well known, the Hamilton equations can be derived from Hamilton's principle: the actual path followed by a system with Hamiltonian $H(q_i, p_i, t)$ is such that the line integral

$$\int_C \big(p_i \mathrm{d}q_i - H \mathrm{d}t\big), \qquad (3)$$

has an extreme (or a stationary value) compared with other curves with the same endpoints in the extended configuration space. The value of the integral (3) does not change if we perform the coordinate transformation (1) and, at the same time, H and p_i are replaced by H' and p'_i in such a way that

$$p_i \mathrm{d}q_i - H \mathrm{d}t = p'_i \mathrm{d}q'_i - H' \mathrm{d}t'.$$

Furthermore, if $F(q_i, t)$ is an arbitrary function, the addition of $\mathrm{d}F$ to the integrand of (3) only adds the difference of the values of F at the endpoints of the curve C to the value of the integral, but this difference has the same value for all the curves with the same endpoints as C. Hence, the addition of $\mathrm{d}F$ in the integrand of (3) does not modify the Hamilton equations. Thus, the Hamilton equations are unchanged if H' and p'_i are such that

$$p_i \mathrm{d}q_i - H\mathrm{d}t = p'_i \mathrm{d}q'_i - H'\mathrm{d}t' + \mathrm{d}F. \tag{4}$$

Since q'_i and t' (as well as F) are functions of (q_j, t) only, the right-hand side of (4) is equivalent to

$$p'_i \left(\frac{\partial q'_i}{\partial q_j}\mathrm{d}q_j + \frac{\partial q'_i}{\partial t}\mathrm{d}t \right) - H' \left(\frac{\partial t'}{\partial q_j}\mathrm{d}q_j + \frac{\partial t'}{\partial t}\mathrm{d}t \right) + \frac{\partial F}{\partial q_j}\mathrm{d}q_j + \frac{\partial F}{\partial t}\mathrm{d}t.$$

Comparing this last expression with the left-hand side of (4) it follows that

$$H = \frac{\partial t'}{\partial t}H' - \frac{\partial q'_i}{\partial t}p'_i - \frac{\partial F}{\partial t} \tag{5}$$

and

$$p_j = \frac{\partial q'_i}{\partial q_j}p'_i - \frac{\partial t'}{\partial q_j}H' + \frac{\partial F}{\partial q_j}. \tag{6}$$

It may be noticed that, by contrast with the canonical transformations, the transformation of the canonical momenta [Eq. (6)] depends on the Hamiltonian. In the Lagrangian formalism, a transformation of the form (1) defines in a unique way the relation between the primed and unprimed generalized velocities, regardless of the Lagrangian under consideration. The function F is arbitrary and it can be chosen in a convenient way, usually to adjust H' to some particular form (see below).

By interchanging the primed and the unprimed quantities in Eqs. (5)–(6) we have the equivalent expressions

$$H' = \frac{\partial t}{\partial t'}H - \frac{\partial q_i}{\partial t'}p_i + \frac{\partial F}{\partial t'} \tag{7}$$

and

$$p'_j = \frac{\partial q_i}{\partial q'_j}p_i - \frac{\partial t}{\partial q'_j}H - \frac{\partial F}{\partial q'_j}. \tag{8}$$

A simple application of these formulas is given by the Hamiltonian

$$H' = \frac{p'^2}{2m}, \tag{9}$$

which is the standard one for a free particle. The solution of the corresponding equations of motion is given by

$$q' = A + Bt',$$

where A, B are constants. On the other hand, the solution of the equations of motion of a damped harmonic oscillator is given by

$$q = A\mathrm{e}^{-\gamma t}\cos\sqrt{\omega^2-\gamma^2}\,t + B\mathrm{e}^{-\gamma t}\sin\sqrt{\omega^2-\gamma^2}\,t,$$

where ω, γ are constants (we shall assume that $\gamma < \omega$) and A, B are constants determined by the initial conditions. The two solutions can be connected by the transformation

$$q' = \mathrm{e}^{\gamma t} q \sec\sqrt{\omega^2-\gamma^2}\,t, \quad t' = \frac{\tan\sqrt{\omega^2-\gamma^2}\,t}{\sqrt{\omega^2-\gamma^2}} \tag{10}$$

(*cf.* Ref. [4]). Then, Eq. (6) gives

$$p' = \mathrm{e}^{-\gamma t}\left(p - \frac{\partial F}{\partial q}\right)\cos\sqrt{\omega^2-\gamma^2}\,t$$

and from Eq. (5) we obtain

$$H = \frac{\mathrm{e}^{-2\gamma t}}{2m}\left(p - \frac{\partial F}{\partial q}\right)^2 - \left(p - \frac{\partial F}{\partial q}\right) q \left(\gamma + \sqrt{\omega^2-\gamma^2}\tan\sqrt{\omega^2-\gamma^2}\,t\right) - \frac{\partial F}{\partial t}. \tag{11}$$

As pointed out above, the function $F(q, t)$ is arbitrary, but if F is appropriately chosen we can get some convenient or recognizable expression for H.

Since most Hamiltonians do not contain linear terms in the momenta, we can look for a function F such that the linear terms in p are eliminated from (11). This condition amounts to

$$\frac{\partial F}{\partial q} = -mq\mathrm{e}^{2\gamma t}\left(\gamma + \sqrt{\omega^2-\gamma^2}\tan\sqrt{\omega^2-\gamma^2}\,t\right).$$

This equation determines the function F up to an additive function of t only. Taking

$$F = -\frac{m}{2}q^2\mathrm{e}^{2\gamma t}\left(\gamma + \sqrt{\omega^2-\gamma^2}\tan\sqrt{\omega^2-\gamma^2}\,t\right) \tag{12}$$

one finds that (11) reduces to

$$H = \mathrm{e}^{-2\gamma t}\frac{p^2}{2m} + \mathrm{e}^{2\gamma t}\frac{m}{2}\omega^2 q^2. \tag{13}$$

According to the previous discussion this last Hamiltonian must correspond to a damped harmonic oscillator, as one can verify making use of the Hamilton equations. It may be noticed that when the damping is absent ($\gamma = 0$), this is the standard Hamiltonian for a harmonic oscillator.

3. Invariance of the Hamiltonian under coordinate transformations in the extended configuration space

The transformation (1) preserves the form of the equations of motion defined by the Hamiltonian $H(q_i, p_i, t)$ if

$$H'(q_i, p_i, t) = H(q'_i, p'_i, t') \tag{14}$$

that is [see Eq. (5)] ,

$$H(q_i, p_i, t) = \frac{\partial t'}{\partial t}H(q'_i, p'_i, t') - \frac{\partial q'_i}{\partial t}p'_i - \frac{\partial F}{\partial t}, \tag{15}$$

for some function $F(q_i, t)$. Due to their connection with the symmetries defined by (2), the transformations satisfying (14) or (15) will also be called variational symmetries.

As pointed out at the Introduction, the one-parameter families of transformations satisfying (15) are especially important because they lead to nontrivial constants of motion. Indeed, if

$$q'_i = q'_i(q_j, t, s), \qquad t' = t'(q_i, t, s), \tag{16}$$

is a family of transformations depending on the parameter s, such that $q'_i(q_j, t, 0) = q_i$ and $t'(q_i, t, 0) = t$ (that is, when $s = 0$ the transformation is the identity), with the definitions

$$\eta_i(q_j, t) \equiv \left.\frac{\partial q'_i(q_j, t, s)}{\partial s}\right|_{s=0}, \qquad \xi(q_i, t) \equiv \left.\frac{\partial t'(q_i, t, s)}{\partial s}\right|_{s=0}, \tag{17}$$

taking the partial derivative of both sides of (6) with respect to s, at $s = 0$, we obtain

$$0 = \left.\frac{\partial p'_j}{\partial s}\right|_{s=0} + p_i\frac{\partial \eta_i}{\partial q_j} - H\frac{\partial \xi}{\partial q_j} + \frac{\partial G}{\partial q_j},$$

with $G(q_i, t) \equiv \partial F/\partial s|_{s=0}$. Then, taking the partial derivative of both sides of (15) with respect to s, at $s = 0$, we get

$$0 = \frac{\partial \xi}{\partial t}H + \frac{\partial H}{\partial q_i}\eta_i + \frac{\partial H}{\partial p_i}\left(-p_j\frac{\partial \eta_j}{\partial q_i} + H\frac{\partial \xi}{\partial q_i} - \frac{\partial G}{\partial q_i}\right) + \frac{\partial H}{\partial t}\xi - \frac{\partial \eta_i}{\partial t}p_i - \frac{\partial G}{\partial t}. \tag{18}$$

For a given Hamiltonian this last equation determines the $n + 1$ functions η_i, ξ of the $n + 1$ variables q_i, t, which generate a local one-parameter group of symmetries of H (see the example below). If the Hamilton equations are satisfied then Eq. (18) reduces to

$$\frac{\mathrm{d}}{\mathrm{d}t}\big(\xi H - \eta_i p_i - G\big) = 0, \tag{19}$$

which means that $\xi H - \eta_i p_i - G$ is a (nontrivial) constant of motion.

A simple but illustrative example is given by the Hamiltonian (13). In order to find the one-parameter groups of symmetries of (13) we substitute this expression into Eq. (18), which gives

$$\begin{aligned} 0 \;\; = \;\; & \frac{\partial \xi}{\partial t}\left(\mathrm{e}^{-2\gamma t}\frac{p^2}{2m} + \mathrm{e}^{2\gamma t}\frac{m}{2}\omega^2 q^2\right) + \mathrm{e}^{2\gamma t}m\omega^2 q\eta + \mathrm{e}^{-2\gamma t}\frac{p}{m}\left[-p\frac{\partial \eta}{\partial q} + \left(\mathrm{e}^{-2\gamma t}\frac{p^2}{2m} + \mathrm{e}^{2\gamma t}\frac{m}{2}\omega^2 q^2\right)\frac{\partial \xi}{\partial q} - \frac{\partial G}{\partial q}\right] \\ & + \left(-\mathrm{e}^{-2\gamma t}\frac{\gamma p^2}{m} + \mathrm{e}^{2\gamma t}m\gamma\omega^2 q^2\right)\xi - \frac{\partial \eta}{\partial t}p - \frac{\partial G}{\partial t}. \end{aligned}$$

Fortunately, the right-hand side of the last equation is a (third degree) polynomial in p, which must vanish for all values of q, p and t (which at this level are independent); hence, equating to zero the coefficients of p^3, p^2, p^1 and p^0 we get

$$\mathrm{e}^{-4\gamma t}\frac{1}{2m^2}\frac{\partial \xi}{\partial q} = 0, \tag{20}$$

$$\mathrm{e}^{-2\gamma t}\left(\frac{1}{2m}\frac{\partial \xi}{\partial t} - \frac{1}{m}\frac{\partial \eta}{\partial q} - \frac{\gamma}{m}\xi\right) = 0, \tag{21}$$

$$\frac{1}{2}\omega^2 q^2 \frac{\partial \xi}{\partial q} - \frac{1}{m}\mathrm{e}^{-2\gamma t}\frac{\partial G}{\partial q} - \frac{\partial \eta}{\partial t} = 0, \tag{22}$$

$$\mathrm{e}^{2\gamma t}\left(\frac{m}{2}\omega^2 q^2 \frac{\partial \xi}{\partial t} + m\omega^2 q\eta + m\gamma\omega^2 q^2 \xi\right) - \frac{\partial G}{\partial t} = 0. \tag{23}$$

Equations (20) and (21) imply that

$$\xi = A(t), \quad \eta = \left(\frac{1}{2}\frac{\mathrm{d}A}{\mathrm{d}t} - \gamma A\right) q + B(t), \tag{24}$$

where $A(t)$ and $B(t)$ are functions of t only. Then, Eqs. (22)–(23) yield

$$\frac{\partial G}{\partial q} = -m\mathrm{e}^{2\gamma t}\left(\frac{1}{2}\frac{\mathrm{d}^2 A}{\mathrm{d}t^2} q - \gamma\frac{\mathrm{d}A}{\mathrm{d}t} q + \frac{\mathrm{d}B}{\mathrm{d}t}\right) \tag{25}$$

and

$$\frac{\partial G}{\partial t} = m\mathrm{e}^{2\gamma t}\omega^2\left(\frac{\mathrm{d}A}{\mathrm{d}t} q^2 + Bq\right). \tag{26}$$

The equality of the mixed second partial derivatives of G gives the condition

$$2\gamma^2\frac{\mathrm{d}A}{\mathrm{d}t} q - 2\gamma\frac{\mathrm{d}B}{\mathrm{d}t} - \frac{1}{2}\frac{\mathrm{d}^3 A}{\mathrm{d}t^3} q - \frac{\mathrm{d}^2 B}{\mathrm{d}t^2} = 2\omega^2\frac{\mathrm{d}A}{\mathrm{d}t} q + \omega^2 B,$$

which must hold for all values of q. Hence,

$$\frac{\mathrm{d}^3 A}{\mathrm{d}t^3} + 4(\omega^2 - \gamma^2)\frac{\mathrm{d}A}{\mathrm{d}t} = 0, \qquad \frac{\mathrm{d}^2 B}{\mathrm{d}t^2} + 2\gamma\frac{\mathrm{d}B}{\mathrm{d}t} + \omega^2 B = 0. \tag{27}$$

The general solution of the first of Eqs. (27) contains three arbitrary constants while the general solution of the second one contains two additional arbitrary constants; therefore, the Hamiltonian (13) possesses five one-parameter groups of variational symmetries. Perhaps the simplest of these groups corresponds to $A = c_1$, $B = 0$, where c_1 is a constant. Then, $\xi = c_1$ and $\eta = -c_1\gamma q$. From Eqs. (25)–(26) we see that G can be taken equal to zero and the constant of motion associated with this symmetry is [see Eq. (19)]

$$\xi H - \eta_i p_i - G = c_1 H + c_1\gamma qp = c_1\left(\mathrm{e}^{-2\gamma t}\frac{p^2}{2m} + \mathrm{e}^{2\gamma t}\frac{m}{2}\omega^2 q^2 + \gamma qp\right).$$

It may be noticed that when $\gamma = 0$ the expression inside the parenthesis is the energy of an undamped harmonic oscillator. (The one-parameter group of transformations generated by $\xi = c_1$, $\eta = -c_1\gamma q$ is given by $t' = t + c_1 s$, $q' = q\mathrm{e}^{-\gamma c_1 s}$ [see Eqs. (17)]).

4. Concluding remarks

The results of Sec. 2 show once again that the form of the Hamilton equations can be preserved by coordinate transformations that are not canonical transformations (another example are the canonoid transformations, see, *e.g.*, Ref. [3], Sec. 5.5).

Even though the one-parameter families of variational symmetries of a Lagrangian or a Hamiltonian may not lead to all the conserved quantities of the corresponding system, the fact that they are determined by the functions ξ and η_i, which depend on q_i and t only, simplifies their finding, as illustrated in the example given above.

As shown in Ref. [4], each solution of the Schrödinger equation for a harmonic oscillator can be expressed as the product of a solution of the Schrödinger equation for a free particle by certain fixed factor, making use of the coordinate transformation (1) with $\gamma = 0$. It turns out that a similar result is applicable in the example given in Sec. 2: each solution of the Schrödinger equation corresponding to the Hamiltonian (13), $\Psi(q,t)$, can be expressed as the product of a solution of the Schrödinger equation for a free particle, $\Psi'(q',t')$, by a fixed factor, making use of the coordinate transformation (1). Specifically,

$$\Psi(q,t) = (\mathrm{e}^{\gamma t} \sec \sqrt{\omega^2 - \gamma^2} t)^{1/2} \, \mathrm{e}^{\mathrm{i}F/\hbar} \, \Psi'(q',t')$$

with F defined by (12), provided that the coordinates (q,t) are related to (q',t') through (1). Moreover, Ψ is normalized if and only if Ψ' is normalized (thanks to the factor $(\mathrm{e}^{\gamma t} \sec \sqrt{\omega^2 - \gamma^2} t)^{1/2}$).

In the transformations considered here the time can be transformed in an arbitrary manner jointly with the coordinates, and in this sense we obtain a treatment similar to that of the generally covariant systems studied in field theory (see, *e.g.*, Ref. [5]).

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