The action of canonical transformations on functions defined on the configuration space

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The effect of an arbitrary canonical transformation on functions defined on the configuration space is defined in such a way that a solution to the time-independent Hamilton–Jacobi equation is mapped into another solution if the Hamiltonian is invariant under the canonical transformation.

Keywords: Canonical transformations; Hamilton-Jacobi equation.

Se define el efecto de una transformación canónica arbitraria sobre funciones definidas en el espacio de configuración en tal forma que una solución de la ecuación de Hamilton–Jacobi independiente del tiempo es enviada en otra solución si la hamiltoniana es invariante bajo la transformación canónica.

Descriptores: Transformaciones canónicas; ecuación de Hamilton-Jacobi.

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1. Introduction

In the Hamiltonian formalism of classical mechanics, the solution to the equations of motion can be obtained with the aid of the Hamilton–Jacobi (HJ) equation; a complete solution to the HJ equation is the generating function of a canonical transformation that relates the original phase space coordinates to a new set of canonical coordinates that are constant in time (see, *e.g.*, Refs. 1 to 3). The HJ equation is the classical limit of the Schrödinger equation and, therefore, the solutions to the HJ equation provide the lowest-order part of the semiclassical approximation for the solutions to the Schrödinger equation (see, *e.g.*, Ref. 4).

The HJ equation and the Schrödinger equation involve only the time and one half of the phase space coordinates (usually a set of coordinates of the configuration space). In the framework of quantum mechanics, the problem of finding the effect of an arbitrary change of coordinates has been recognized, and has only been solved in the case of point transformations or of linear canonical transformations (see, *e.g.*, Refs. 5, 6, and the references cited therein).

The aim of this paper is to give a natural definition for the action of a canonical transformation on Hamilton's characteristic function (which satisfies the time-independent HJ equation), or on any function defined on the configuration space. We show that, in the case of a time-independent Hamiltonian, this definition has the property that a solution to the HJ equation is mapped into another solution of the same equation if the canonical transformation leaves the Hamiltonian invariant.

In Sec. 2 we derive the action of an arbitrary time-independent canonical transformation on functions defined in the configuration space, giving some explicit examples. In Sec. 3, we show that the action of a one-parameter group of canonical transformations on a function defined in the configuration space is determined by a partial differential equation involving the generating function of the group and that, from each constant of motion and each solution to the HJ equation, a one-parameter family of solutions to the HJ equation can be obtained; that is, each continuous group of canonical transformations that leave the Hamiltonian invariant allows one to add one parameter to a given solution of the HJ equation. Throughout this paper only Hamiltonians that do not depend explicitly on time are considered.

2. The effect of an arbitrary canonical transformation

We begin by reviewing some elementary facts about canonical transformations that will be employed in what follows.

Let

$$q'^i = q'^i(q^j, p_j), \quad p'_i = p'_i(q^j, p_j) \tag{1}$$

be a (time-independent) canonical transformation. Then, there exists (at least locally) a function, $\Lambda(q^j, p_j)$, defined up to an additive constant, such that

$$p'_i \mathrm{d}q'^i = p_i \mathrm{d}q^i + \mathrm{d}\Lambda, \tag{2}$$

with summation over repeated indices (see, *e.g.*, Refs. 1-3). When one starts from an arbitrary change of coordinates in the configuration space of the form $q'^i = q'^i(q^j)$ (or point transformation), the elementary definition $p_i{=}\partial L/\partial \dot{q}^i$, where L is the Lagrangian, implies that this change of coordinates is accompanied by the transformation of the canonical momenta

$$p'_i = \frac{\partial L}{\partial \dot{q}'^i} = \frac{\partial L}{\partial \dot{q}^j}\frac{\partial \dot{q}^j}{\partial \dot{q}'^i} = p_j \frac{\partial q^j}{\partial q'^i} \tag{3}$$

and therefore, in this particular case,

$$p'_i \mathrm{d}q'^i = p_i \mathrm{d}q^i, \tag{4}$$

that is, we can take $\Lambda = 0$.

Under the canonical transformation (1), a given Hamiltonian, $H(q^i, p_i)$, becomes a new Hamiltonian function H' given by

$$H'(q'^i(q^j, p_j), p'_i(q^j, p_j)) = H(q^i, p_i). \tag{5}$$

(The Hamiltonian H is *invariant* under the canonical transformation (1) if $H' = H$.) For example, the coordinate transformation relating $(q^1, q^2, p_1, p_2) = (z, w, p_z, p_w)$ with $(q'^1, q'^2, p'_1, p'_2) = (x, y, p_x, p_y)$, given by [7]

$$x = z - \frac{p_z p_w}{m^2 g}, \quad y = w - \frac{{p_z}^2}{2m^2 g},$$
$$p_x = p_z, \qquad p_y = p_w, \tag{6}$$

where m and g are arbitrary nonzero constants, is canonical. In fact, a straightforward computation gives

$$p_x \mathrm{d}x + p_y \mathrm{d}y = p_z \mathrm{d}z + p_w \mathrm{d}w + \mathrm{d}\left(-\frac{{p_z}^2 p_w}{m^2 g}\right)$$

[*cf.* Eq. (2)]. Under the transformation (6), the Hamiltonian function

$$H = \frac{{p_w}^2}{2m} + mgw \tag{7}$$

is transformed into

$$\frac{p_y^2}{2m} + mg\left(y + \frac{p_x^2}{2m^2 g}\right) = \frac{p_x^2 + p_y^2}{2m} + mgy \equiv H'(q'^i, p'_i) \tag{8}$$

(which corresponds to a particle of mass m in a uniform gravitational field with acceleration due to gravity g).

Going back to our preceding discussion, we note that Eq. (2) implies that

$$p'_i{=}p_j \frac{\partial q^j}{\partial q'^i} + \frac{\partial \Lambda}{\partial q^j}\frac{\partial q^j}{\partial q'^i} + \frac{\partial \Lambda}{\partial p_j}\frac{\partial p_j}{\partial q'^i} \tag{9}$$

(which duly reduces to Eq. (3) when $\Lambda = 0$). Hence, Eq. (5) is equivalent to

$$H'\left(q'^i, p_j \frac{\partial q^j}{\partial q'^i} + \frac{\partial \Lambda}{\partial q^j}\frac{\partial q^j}{\partial q'^i} + \frac{\partial \Lambda}{\partial p_j}\frac{\partial p_j}{\partial q'^i}\right) = H(q^i, p_i), \tag{10}$$

where it is understood that the q'^i, and the partial derivatives $\partial q^j/\partial q'^i$, $\partial p_j/\partial q'^i$ on the left-hand side, are expressed in terms of q^i, p_i.

2.1. The Hamilton–Jacobi equation

With any Hamiltonian, $H(q^i, p_i)$, we can associate the (time-independent) Hamilton–Jacobi (HJ) equation

$$H\left(q^i, \frac{\partial W}{\partial q^i}\right) = E, \tag{11}$$

where E is a constant, which is a, possibly nonlinear, first-order partial differential equation (provided that $\partial H/\partial p_i \neq 0$) for the *characteristic function* $W(q^i)$. As is well known, a complete solution to the HJ equation allows one to obtain the solution to the equations of motion [1-3]. By replacing p_i by $\partial W/\partial q^i$ in Eq. (10), where W is a solution to the HJ equation (11), we obtain

$$H'\left(q'^i, \frac{\partial W}{\partial q^j}\frac{\partial q^j}{\partial q'^i} + \frac{\partial \Lambda}{\partial q^j}\frac{\partial q^j}{\partial q'^i} + \frac{\partial \Lambda}{\partial p_j}\frac{\partial p_j}{\partial q'^i}\right) = E, \tag{12}$$

where it is understood that the partial derivatives are evaluated at points such that $p_i = \partial W/\partial q^i$.

We now look for a way of relating the solutions to the HJ equation (11) with those of the HJ equation corresponding to the Hamiltonian H', obtained from H by means of a canonical transformation [see Eq. (5)].

Keeping in mind that the characteristic function must depend on the coordinates only, and not on the momenta, we shall assume that the equations

$$p_i = \frac{\partial W}{\partial q^i}, \qquad q'^i = q'^i(q^j, p_j), \tag{13}$$

allow us to express the q^j in terms of the q'^i only [eliminating the p_i from Eqs. (13)]; we define

$$W'(q'^i) \equiv W(q^j(q'^i)) + \Lambda\left(q^j(q'^i), p_j(q^k(q'^i))\right), \tag{14}$$

assuming that the right-hand side is expressed as a function of the q'^i only, with the aid of Eqs. (13) (see the examples below). On the other hand, from Eq. (14), using the elementary expression for the differential of a function, we obtain

$$\mathrm{d}W' = \left(\frac{\partial W}{\partial q^j} + \frac{\partial \Lambda}{\partial q^j}\right)\left(\frac{\partial q^j}{\partial q'^i}\mathrm{d}q'^i + \frac{\partial q^j}{\partial p'_i}\mathrm{d}p'_i\right) + \frac{\partial \Lambda}{\partial p_j}\left(\frac{\partial p_j}{\partial q'^i}\mathrm{d}q'^i + \frac{\partial p_j}{\partial p'_i}\mathrm{d}p'_i\right),$$

which must reduce to

$$\mathrm{d}W' = \left(\frac{\partial W}{\partial q^j} + \frac{\partial \Lambda}{\partial q^j}\right)\frac{\partial q^j}{\partial q'^i}\mathrm{d}q'^i + \frac{\partial \Lambda}{\partial p_j}\frac{\partial p_j}{\partial q'^i}\mathrm{d}q'^i,$$

on the submanifold defined by Eqs. (13) and, therefore, on this submanifold,

$$\frac{\partial W'}{\partial q'^i} = \left(\frac{\partial W}{\partial q^j} + \frac{\partial \Lambda}{\partial q^j}\right)\frac{\partial q^j}{\partial q'^i} + \frac{\partial \Lambda}{\partial p_j}\frac{\partial p_j}{\partial q'^i},$$

thus showing that Eq. (12) amounts to

$$H'\left(q'^i, \frac{\partial W'}{\partial q'^i}\right) = E,$$

in other words, $W'(q'^i)$ *is a solution to the HJ equation for the Hamiltonian* H' [with the same value of the constant E appearing in Eq. (11)].

As pointed out above, in the special case where one starts from an arbitrary transformation in the configuration space (*e.g.*, a translation or a rotation), $q'^i = q'^i(q^j)$, we can assume that the momenta transform according to Eq. (3), with the function Λ equal to zero. Then Eq. (14) reduces to

$$W'(q'^i) = W(q^j(q'^i)), \tag{15}$$

i.e., W' is obtained from W by simply expressing the coordinates q^i in terms of the q'^i.

2.1.1. *Example. Particle in a uniform gravitational field*

In the example considered above [Eqs. (6)-(8)], the HJ equation associated with the Hamiltonian (7),

$$\frac{1}{2m}\left(\frac{\partial W}{\partial w}\right)^2 + mgw = E,$$

has the solution

$$W = \pm \int^{w} \sqrt{2m(E - mgs)}\,\mathrm{d}s + F(z),$$

where F is an arbitrary function. Choosing $F(z){=}\alpha z$, where α is a constant, we find that the equations $p_i{=}\partial W/\partial q^i$ amount to

$$p_z = \alpha, \qquad p_w = \sqrt{2m(E - mgw)}.$$

(The fact that z is an ignorable coordinate in the Hamiltonian (7) implies that p_z is a constant of motion and, therefore, $F(z)$ must depend linearly on z.) Then, making use of Eqs. (6), we find that

$$z = x + \frac{\alpha\sqrt{2m(E - mgw)}}{m^2 g}, \qquad w = y + \frac{\alpha^2}{2m^2 g}$$

and recalling that in this case $\Lambda = -{p_z}^2 p_w/(m^2 g)$, from Eq. (14) we obtain

$$\begin{aligned} W' = \pm &\int^{y+\alpha^2/(2m^2 g)} \sqrt{2m(E{-}mgs)}\mathrm{d}s \\ &+\alpha\left(x+\frac{\alpha\sqrt{2m(E{-}mgw)}}{m^2 g}\right)-\frac{\alpha^2\sqrt{2m(E{-}mgw)}}{m^2 g} \\ =\pm &\int^{y+\alpha^2/(2m^2 g)} \sqrt{2m(E{-}mgs)}\mathrm{d}s+\alpha x, \end{aligned}$$

which is indeed a (complete) solution to the HJ equation corresponding to the Hamiltonian (8), as one can readily verify.

2.1.2. *Example. Particle in a uniform magnetic field*

Another example is provided by the (linear) canonical transformation from $(q^1, q^2, p_1, p_2){=}(u, v, p_u, p_v)$ to $(q'^1, q'^2, p'_1, p'_2) = (x, y, p_x, p_y)$, given by [8]

$$\begin{aligned} x &= u + v, \qquad y = \frac{c}{eB}(p_u - p_v), \\ p_x &= \frac{1}{2}(p_u + p_v), \qquad p_y = \frac{eB}{2c}(v - u), \end{aligned} \tag{16}$$

where e, B, and c are constants. We have

$$p_x \mathrm{d}x + p_y \mathrm{d}y = p_u \mathrm{d}u + p_v \mathrm{d}v + \mathrm{d}\left[\tfrac{1}{2}(v - u)(p_u - p_v)\right],$$

which allows us to identify the function Λ. The Hamiltonian

$$H = \frac{{p_u}^2}{2m} + \frac{m\omega^2}{2}u^2, \tag{17}$$

which is the usual one for a one-dimensional harmonic oscillator, is then expressed as

$$H{=}\frac{1}{2m}\left(p_x{+}\frac{eB}{2c}y\right)^2 + \frac{m\omega^2}{2}\frac{c^2}{e^2B^2}\left(p_y{-}\frac{eB}{2c}x\right)^2, \tag{18}$$

which corresponds to a particle of mass m and electric charge e moving on the xy-plane under the influence of a magnetic field B, perpendicular to this plane, if $\omega = eB/mc$.

One can readily verify that the solutions to the HJ equation corresponding to the Hamiltonian (17) are of the form

$$W = \pm \int^{u} \sqrt{2mE - m^2\omega^2 s^2}\,\mathrm{d}s + G(v),$$

where G is an arbitrary function. Taking $G(v) = \alpha v$, where α is a constant, and making use of Eqs. (13), (14), and (16), we obtain

$$\begin{aligned} W' = \pm &\int^{\sqrt{2mE-(eBy/c+\alpha)^2}/(m\omega)} \sqrt{2mE{-}m^2\omega^2 s^2}\,\mathrm{d}s \\ &+\alpha x{+}\frac{eB}{2c}xy{-}\frac{1}{m\omega}\left(\frac{eBy}{c}{+}\alpha\right)\sqrt{2mE{-}\left(\frac{eBy}{c}{+}\alpha\right)}. \end{aligned}$$

This last expression can be simplified with the aid of the change of variable $z = (\sqrt{2mE - m^2\omega^2 s^2} - \alpha)/(m\omega)$, integrating by parts

$$W' = \mp \int^{y} \sqrt{2mE - \left(\frac{eBz}{c} + \alpha\right)}\,\mathrm{d}z + \alpha x + \frac{eB}{2c}xy.$$

It may be noticed that this function is not separable.

2.1.3. Example. The exchange transformation

As is well known, the transformation

$$q'^i = p_i, \qquad p'_i = -q^i, \tag{19}$$

is canonical. In fact, one readily verifies that

$$p'_i \mathrm{d}q'^i = p_i \mathrm{d}q^i + \mathrm{d}(-p_i q^i)$$

[*cf.* Eq. (2)]. An *arbitrary* Hamiltonian, $H(q^i, p_i)$, is transformed into

$$H'(q'^i, p'_i) = H(-p'_i, q'^i)$$

[see Eq. (5)] and from a given solution, W, of the HJ equation (11) one obtains a solution to the HJ equation

$$H\left(-\frac{\partial W'}{\partial p_i}, p_i\right) = E \tag{20}$$

given by [see Eq. (14)]

$$W'(p_i) = W(q^i) - q^i \frac{\partial W}{\partial q^i}, \tag{21}$$

where it is understood that the q^i appearing on the right-hand side are eliminated in favor of the p_i by means of [see Eq. (13)]

$$p_i = \frac{\partial W}{\partial q^i}.$$

Thus, in this case, W' is obtained from W by making use of the Legendre transformation. (This result is the analog of the well-known fact that, in quantum mechanics, the relation between the wave function in momentum space and the wave function in the configuration space is given by the Fourier transform.)

3. One-parameter groups of canonical transformations

As is well known, the differentiable functions defined on the phase space generate one-parameter groups of canonical transformations. In particular, the canonical transformations generated by a constant of motion map a solution to the equations of motion into other solutions, with the same value of the Hamiltonian.

The one-parameter group of canonical transformations defined by a differentiable function $f(q^i, p_i)$ is given by the solution of the system of ordinary differential equations

$$\frac{\mathrm{d}q^i}{\mathrm{d}s} = \frac{\partial f}{\partial p_i}, \qquad \frac{\mathrm{d}p_i}{\mathrm{d}s} = -\frac{\partial f}{\partial q^i}. \tag{22}$$

Hence, to first order in the parameter s,

$$q^i(s) \simeq q^i(0) + s\frac{\partial f}{\partial p_i}, \qquad p_i(s) \simeq p_i(0) - s\frac{\partial f}{\partial q^i},$$

and therefore

$$p_i(s)\mathrm{d}q^i(s) \simeq \left(p_i(0) - s\frac{\partial f}{\partial q^i}\right)\left(\mathrm{d}q^i(0) + s\,\mathrm{d}\frac{\partial f}{\partial p_i}\right)$$
$$\simeq p_i(0)\mathrm{d}q^i(0) + s\,\mathrm{d}\left(p_i\frac{\partial f}{\partial p_i} - f\right)$$

i.e., $\Lambda \simeq s\big(p_i \partial f/\partial p_i - f\big)$ and from Eq. (14) we have

$$W'\left(q^i(0) + s\frac{\partial f}{\partial p_i}\right) \simeq W(q^i(0))$$
$$+ s\frac{\partial W}{\partial q^i}\frac{\partial f}{\partial p_i} - sf\left(q^j(0), \frac{\partial W}{\partial q^j}\right).$$

On the other hand, to first order in s,

$$W'\left(q^i(0) + s\frac{\partial f}{\partial p_i}\right) \simeq W'(q^i(0)) + s\frac{\partial W'}{\partial q^i}\frac{\partial f}{\partial p_i}$$
$$\simeq W'(q^i(0)) + s\frac{\partial W}{\partial q^i}\frac{\partial f}{\partial p_i}$$

hence, taking into account that the initial conditions $q^i(0)$ are arbitrary,

$$W'(q^i) \simeq W(q^i) - sf\left(q^j, \frac{\partial W}{\partial q^j}\right).$$

Thus, denoting by $W(q^i, s)$ the function $W'(q^i)$ obtained by the transformation $q'^i = q^i(s)$, $p'_i = p_i(s)$, where $q^i(s)$, $p_i(s)$ is the solution to Eqs. (22), from the last equation we obtain the partial differential equation

$$\frac{\partial W}{\partial s} = -f\left(q^i, \frac{\partial W}{\partial q^i}\right), \tag{23}$$

which defines the action of the one-parameter group of canonical transformations generated by f on a function W, defined on the configuration space.

Thus, from each constant of motion and a particular solution to the HJ equation, we obtain a one-parameter family of solutions to the HJ equation with a fixed value of E (although, in some cases, these transformations only add a constant to W; see the example below).

3.1. Example. Free particle in the plane

A very simple example is given by the HJ equation for a free particle in the xy plane. Taking $H = ({p_x}^2 + {p_y}^2)/2m$, the HJ equation reads

$$\frac{1}{2m}\left[\left(\frac{\partial W}{\partial x}\right)^2 + \left(\frac{\partial W}{\partial y}\right)^2\right] = E \tag{24}$$

and a particular solution is given by

$$W_0 = \sqrt{2mE}\,x. \tag{25}$$

Since H is invariant under rigid rotations, according to the discussion above [see Eq. (15)], the images of (25) under the rotations about the origin,

$$W = \sqrt{2mE}\,(x\cos s + y\sin s) \tag{26}$$

form a one-parameter family of solutions of (24) which is, in fact, a *complete* solution to Eq. (24). (One can readily verify that the function (26) satisfies Eq. (23) with the constant of motion $f = xp_y - yp_x$.)

On the other hand, $f = p_x$ is also a constant of motion, and the corresponding solution to Eq. (23), with W_0 given by Eq. (25), is just $W = \sqrt{2mE}\,(x - s)$, that is, $W_0 + \text{const.}$

It should be clear that Eq. (23) defines a one-parameter family of functions defined on the configuration space, starting from any function $W_0(q^i)$ (not necessarily the characteristic function), with an arbitrary function $f(q^i, p_i)$ (not necessarily a constant of motion). For instance, choosing $f = p_k$, Eq. (23) yields $W(q^i, s) = W_0(q^1, \ldots, q^k - s, \ldots, q^n)$, in accordance with the fact that p_k generates translations along the q^k direction.

Equations (22) are the Hamilton equations if one takes $f = H$, and $s = t$ (the time). Then, Eq. (23) reduces to the time-dependent HJ equation for the principal function $S(q^i, t) \equiv W(q^i, t)$,

$$\frac{\partial S}{\partial t} = -H\left(q^i, \frac{\partial S}{\partial q^i}\right),$$

whose solution is given by the well-known relation between the principal function, S, and the characteristic function, W, in the cases considered here, where the Hamiltonians do not depend explicitly on the time,

$$S(q^i, t) = W(q^i) - Et.$$

4. Concluding remarks

The general expressions (13) and (14), as well as the examples given in Sec. 2, show that the effect of an arbitrary canonical transformation on functions defined on the configuration space is somewhat involved, contrasting with the rather trivial effect of a point transformation [Eq. (15)].

As we have shown, under a one-parameter group of canonical transformations that leave the Hamiltonian invariant, a particular solution to the HJ equation is transformed into another solution containing an additional parameter. Hence, expression (14) allows us to add several parameters at the same time, making use of a group of canonical transformations that leave the Hamiltonian invariant, if the dimension of the group is greater than 1.

A Lie group of canonical transformations must have some representation on the functions defined on the configuration space, and the nature of this representation deserves a separate, detailed study.

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