Canonical transformations

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Recall that we have defined a symplectic transformation to be any linear transformation $M^A{}_B$ leaving the symplectic form invariant,

$$\Omega^{AB} \equiv M^A{}_C M^B{}_D \Omega^{CD}$$

Coordinate transformations, $\chi^A\left(\xi^B\right)$ which are symplectic transformations at each point are called *canonical.* Specifically, those functions $\chi^A(\xi)$ satisfying

$$\Omega^{CD} \equiv \frac{\partial \chi^C}{\partial \xi^A} \Omega^{AB} \frac{\partial \chi^D}{\partial \xi^B}$$

are canonical transformations. Canonical transformations preserve Hamilton's equations.

1 Poisson brackets

We may also write Hamilton's equations in terms of Poisson brackets between *dynamical variables.* By a dynamical variable, we mean any function $f = f\left(\xi^A\right)$ of the canonical coordinates used to describe a physical system.

We define the Poisson bracket of any two dynamical variables f and g by

$$\{f, g\} = \Omega^{AB} \frac{\partial f}{\partial \xi^A} \frac{\partial g}{\partial \xi^B}$$

The importance of this product is that it is preserved by canonical transformations. We see this as follows.

Let ξ^A be any set of phase space coordinates in which Hamilton's equations take the form

$$\frac{d\xi^A}{dt} = \Omega^{AB} \frac{\partial H}{\partial \xi^B} \tag{1}$$

and let f and g be any two dynamical variables. Denote the Poisson bracket of f and g in the coordinates ξ^A be denoted by $\{f, g\}_\xi$. In a different set of coordinates, $\chi^A(\xi)$, we have

$$\begin{aligned}
\{f, g\}_\chi &= \Omega^{AB} \frac{\partial f}{\partial \chi^A} \frac{\partial g}{\partial \chi^B} \\
&= \Omega^{AB} \left(\frac{\partial \xi^C}{\partial \chi^A} \frac{\partial f}{\partial \xi^C}\right) \left(\frac{\partial \xi^D}{\partial \chi^B} \frac{\partial g}{\partial \xi^D}\right) \\
&= \left(\frac{\partial \xi^C}{\partial \chi^A} \Omega^{AB} \frac{\partial \xi^D}{\partial \chi^B}\right) \frac{\partial f}{\partial \xi^C} \frac{\partial g}{\partial \xi^D}
\end{aligned}$$

Therefore, if the coordinate transformation is canonical so that

$$\frac{\partial \xi^C}{\partial \chi^A} \Omega^{AB} \frac{\partial \xi^D}{\partial \chi^B} = \Omega^{CD}$$

we have

$$\{f,g\}_\chi = \Omega^{AB}\frac{\partial f}{\partial \xi^C}\frac{\partial g}{\partial \xi^D} = \{f,g\}_\xi$$

and the Poisson bracket is unchanged. We conclude that canonical transformations preserve all Poisson brackets.

Conversely, a transformation which preserves all Poisson brackets satisfies

$$\begin{aligned}
\{f,g\}_\chi &= \{f,g\}_\xi \\
\left(\frac{\partial \xi^C}{\partial \chi^A}\Omega^{AB}\frac{\partial \xi^D}{\partial \chi^B}\right)\frac{\partial f}{\partial \xi^C}\frac{\partial g}{\partial \xi^D} &= \Omega^{CD}\frac{\partial f}{\partial \xi^C}\frac{\partial g}{\partial \xi^D}
\end{aligned}$$

for all f,g and must therefore be canonical.

An important special case of the Poisson bracket occurs when one of the functions is the Hamiltonian. In that case, we have

$$\begin{aligned}
\{f,H\} &= \Omega^{AB}\frac{\partial f}{\partial \xi^A}\frac{\partial H}{\partial \xi^B} \\
&= \frac{\partial f}{\partial x^i}\frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p^i}\frac{\partial H}{\partial x_i} \\
&= \frac{\partial f}{\partial x^i}\frac{dx^i}{dt} - \frac{\partial f}{\partial p^i}\left(-\frac{dp_i}{dt}\right) \\
&= \frac{df}{\partial t} - \frac{\partial f}{\partial t}
\end{aligned}$$

or simply,

$$\frac{df}{\partial t} = \{f,H\} + \frac{\partial f}{\partial t}$$

This shows that as the system evolves classically, the total time rate of change of any dynamical variable is the sum of the Poisson bracket with the Hamiltonian and the partial time derivative. If a dynamical variable has no explicit time dependence, $\frac{\partial f}{\partial t} = 0$, then the total time derivative is just the Poisson bracket with the Hamiltonian.

The coordinates provide another important special case. Since neither x^i nor p_i has any explicit time dependence, we have

$$\begin{aligned}
\frac{dx^i}{dt} &= \left\{H, x^i\right\} \\
\frac{dp_i}{dt} &= \{H, p_i\} \qquad (2)
\end{aligned}$$

or simply $\dot{\xi}^A = \left\{H, \xi^A\right\}$, and we can check this directly that this reproduces Hamilton's equations,

$$\begin{aligned}
\frac{dq_i}{dt} &= \left\{H, x^i\right\} \\
&= \sum_{j=1}^{N}\left(\frac{\partial x^i}{\partial x^j}\frac{\partial H}{\partial p_j} - \frac{\partial x^i}{\partial p_j}\frac{\partial H}{\partial x^j}\right) \\
&= \sum_{j=1}^{N}\delta_{ij}\frac{\partial H}{\partial p_j} \\
&= \frac{\partial H}{\partial p_i}
\end{aligned}$$

and

$$\begin{aligned}
\frac{dp_i}{dt} &= \{H, p_i\} \\
&= \sum_{j=1}^{N} \left(\frac{\partial p_i}{\partial q_j} \frac{\partial H}{\partial p_j} - \frac{\partial p_i}{\partial p_j} \frac{\partial H}{\partial q_j} \right) \\
&= -\frac{\partial H}{\partial q_i}
\end{aligned}$$

Notice that since q_i, p_i and are all independent, and do not depend explicitly on time, $\frac{\partial q_i}{\partial p_j} = \frac{\partial p_i}{\partial q_j} = 0 = \frac{\partial q_i}{\partial t} = \frac{\partial p_i}{\partial t}$.

We also have the commutator of the Hamiltonian with the Hamiltonian itself,

$$\begin{aligned}
\frac{dH}{dt} &= \{H, H\} + \frac{\partial H}{\partial t} \\
&= \frac{\partial H}{\partial t}
\end{aligned}$$

so if the Hamiltonian is not explicitly time-dependent, then it is a constant of the motion.

More generally, a dynamical variable with no explicit time dependence, $\frac{\partial f}{\partial t} = 0$, is a constant of the motion if and only if it has vanishing Poisson bracket with the Hamiltonian, $\{H, f\} = 0$.

2 Canonical transformations

We now define the *fundamental Poisson brackets.* Suppose x^i and p_j are a set of coordinates on phase space such that Hamilton's equations hold. Since they themselves are functions of (x^m, p_n) they are dynamical variables and we may compute their Poisson brackets with one another. With $\xi^A = (x^m, p_n)$ we have

$$\begin{aligned}
\left\{x^i, x^j\right\}_\xi &= \Omega^{AB} \frac{\partial x^i}{\partial \xi^A} \frac{\partial x^j}{\partial \xi^B} \\
&= \sum_{m=1}^{N} \left(\frac{\partial x^i}{\partial x^m} \frac{\partial x^j}{\partial p_m} - \frac{\partial x^i}{\partial p_m} \frac{\partial x^j}{\partial x^m} \right) \\
&= 0
\end{aligned}$$

for x^i with x^j,

$$\begin{aligned}
\left\{x^i, p_j\right\}_\xi = -\left\{p_j, x^i\right\}_\xi &= \Omega^{AB} \frac{\partial x^i}{\partial \xi^A} \frac{\partial p_j}{\partial \xi^B} \\
&= \sum_{m=1}^{N} \left(\frac{\partial x^i}{\partial x^m} \frac{\partial p_j}{\partial p_m} - \frac{\partial x^i}{\partial p_m} \frac{\partial p_j}{\partial x^m} \right) \\
&= \sum_{m=1}^{N} \delta^i_m \delta^m_j \\
&= \delta^i_j
\end{aligned}$$

for x^i with p_j and finally

$$\begin{aligned}
\left\{p_i, p_j\right\}_\xi &= \Omega^{AB} \frac{\partial p_i}{\partial \xi^A} \frac{\partial p_j}{\partial \xi^B} \\
&= \sum_{m=1}^{N} \left(\frac{\partial p_i}{\partial x^m} \frac{\partial p_j}{\partial p_m} - \frac{\partial p_i}{\partial p_m} \frac{\partial p_j}{\partial x^m} \right) \\
&= 0
\end{aligned}$$

for p_i with p_j. The subscript ξ on the bracket indicates that the partial derivatives are taken with respect to the coordinates $\xi^A = \left(x^i, p_j\right)$. We summarize these relations as

$$\left\{\xi^A, \xi^B\right\}_\xi = \Omega^{AB}$$

However, since Poisson brackets are preserved by canonical transformations, this will hold in any canonical coordinates, $\left\{\xi^A, \xi^B\right\}_\chi = \Omega^{AB}$.

We summarize the results of this subsection with a theorem: Let the coordinates ξ^A be canonical. Then a coordinate transformation $\chi^A(\xi)$ is canonical if and only if it satisfies the fundamental bracket relation

$$\left\{\chi^A, \chi^B\right\}_\xi = \Omega^{AB}$$

For proof, note that the bracket on the left is defined by

$$\left\{\chi^A, \chi^B\right\}_\xi = \Omega^{CD} \frac{\partial \chi^A}{\partial \xi^C} \frac{\partial \chi^B}{\partial \xi^D}$$

so in order for χ^A to satisfy the canonical bracket relation we must have

$$\Omega^{CD} \frac{\partial \chi^A}{\partial \xi^C} \frac{\partial \chi^B}{\partial \xi^D} = \Omega^{AB} \tag{3}$$

which is just the condition shown above for the coordinate transformation $\chi^A(\xi)$ to be canonical. Conversely, suppose the transformation $\chi^A(\xi)$ is canonical, so that eq.(3) holds. Then, computing the Poisson bracket

$$\left\{\chi^A, \chi^B\right\}_\xi = \Omega^{CD} \frac{\partial \chi^A}{\partial \xi^C} \frac{\partial \chi^B}{\partial \xi^D} = \Omega^{AB}$$

so χ^A satisfies the fundamental bracked relation.

In summary, each of the following statements is equivalent:

1. $\chi^A(\xi)$ is a canonical transformation.
2. $\chi^A(\xi)$ is a coordinate transformation of phase space that preserves Hamilton's equations.
3. $\chi^A(\xi)$ preserves the symplectic form, according to

$$\Omega^{AB} \frac{\partial \xi^C}{\partial \chi^A} \frac{\partial \xi^D}{\partial \chi^B} = \Omega^{CD}$$

4. $\chi^A(\xi)$ satisfies the fundamental bracket relations

$$\left\{\chi^A, \chi^B\right\}_\xi = \Omega^{AB}$$

These bracket relations represent a set of integrability conditions that must be satisfied by any new set of canonical coordinates. When we formulate the problem of canonical transformations in these terms, it is not obvious what functions $q^i\left(x^j, p_j\right)$ and $\pi_i\left(x^j, p_j\right)$ will be allowed. Fortunately there is a simple procedure for generating canonical transformations, which we develop in the next section.

We end this section with three examples of canonical transformations.

2.1 Example 1: Coordinate transformations

Let $\left(x^i, p_j\right)$ be one set of canonical variables. Suppose we define new configuration space variables, q^i, be an arbitrary invertible function of the spatial coordinates:

$$q^i = q^i\left(x^j\right)$$

We seek a set of momentum variables π_j such that $\left(q^i, \pi_j\right)$ are canonical. For this they must satisfy the fundamental Poisson bracket relations:

$$\begin{aligned}\left\{q^i, q^j\right\}_{x,p} &= 0 \\ \left\{q^i, \pi_j\right\}_{x,p} &= \delta^i_j \\ \left\{\pi_i, \pi_j\right\}_{x,p} &= 0\end{aligned}$$

Check each:

$$\begin{aligned}\left\{q^i, q^j\right\}_{x,p} &= \sum_{m=1}^{N}\left(\frac{\partial q^i}{\partial x^m}\frac{\partial q^j}{\partial p_m} - \frac{\partial q^i}{\partial p_m}\frac{\partial q^j}{\partial x^m}\right) \\ &= 0\end{aligned}$$

since $\frac{\partial q^j}{\partial p_m} = 0$. For the second bracket,

$$\begin{aligned}\delta^i_j &= \left\{q^i, \pi_j\right\}_{x,p} \\ &= \sum_{m=1}^{N}\left(\frac{\partial q^i}{\partial x^m}\frac{\partial \pi_j}{\partial p_m} - \frac{\partial q^i}{\partial p_m}\frac{\partial \pi_j}{\partial x^m}\right) \\ &= \sum_{m=1}^{N}\frac{\partial q^i}{\partial x^m}\frac{\partial \pi_j}{\partial p_m}\end{aligned}$$

Since q^i is independent of p_m, we can satisfy this only if

$$\frac{\partial \pi_j}{\partial p_m} = \frac{\partial x^m}{\partial q^j}$$

Integrating gives

$$\pi_j = \frac{\partial x^n}{\partial q^j}p_n + c_j\left(x\right)$$

with the c_j an arbitrary functions of x^i. Choosing $c_j = 0$, we compute the final bracket:

$$\begin{aligned}\left\{\pi_i, \pi_j\right\}_{x,p} &= \frac{\partial \pi_i}{\partial x^m}\frac{\partial \pi_j}{\partial p_m} - \frac{\partial \pi_i}{\partial p_m}\frac{\partial \pi_j}{\partial x^m} \\ &= \frac{\partial}{\partial x^m}\left(\frac{\partial x^n}{\partial q^i}p_n\right)\frac{\partial}{\partial p_m}\left(\frac{\partial x^s}{\partial q^j}p_s\right) - \frac{\partial}{\partial p_m}\left(\frac{\partial x^n}{\partial q^i}p_n\right)\frac{\partial}{\partial x^m}\left(\frac{\partial x^s}{\partial q^j}p_s\right) \\ &= \frac{\partial x^m}{\partial q^j}\frac{\partial}{\partial x^m}\left(\frac{\partial x^n}{\partial q^i}\right)p_n - \frac{\partial x^m}{\partial q^i}\frac{\partial}{\partial x^m}\left(\frac{\partial x^n}{\partial q^j}\right)p_n \\ &= \left(\frac{\partial^2 x^n}{\partial q^j \partial q^i}p_n - \frac{\partial^2 x^n}{\partial q^i \partial q^j}\right)p_n \\ &= 0\end{aligned}$$

Exercise: Show that the final bracket, $\left\{\pi_i, \pi_j\right\}_{x,p}$ still vanishes provided $c_i = \frac{\partial f}{\partial q^i}$ for some function $f\left(q\right)$.

Therefore, the transformations

$$\begin{aligned} q^j &= q^j(x^i) \\ \pi_j &= \frac{\partial x^n}{\partial q^j} p_n + \frac{\partial f}{\partial q^j} \end{aligned}$$

is a canonical transformation for any functions $q^i(x)$. This means that the symmetry group of Hamilton's equations is at least as big as the symmetry group of the Euler-Lagrange equations.

2.2 Example 2: Interchange of x and p.

The transformation

$$\begin{aligned} q^i &= p_i \\ \pi_i &= -x^i \end{aligned}$$

is canonical. We easily check the fundamental brackets:

$$\begin{aligned} \left\{q^i, q^j\right\}_{x,p} &= \{p_i, p_j\}_{x,p} = 0 \\ \left\{q^i, \pi_j\right\}_{x,p} &= \left\{p_i, -x^j\right\}_{x,p} \\ &= \left\{x^j, p_i\right\}_{x,p} \\ &= \delta_i^j \\ \{\pi_i, \pi_j\}_{x,p} &= \left\{-x^i, -x^j\right\}_{x,p} = 0 \end{aligned}$$

Interchange of x^i and p_j, with a sign, is therefore canonical. The use of generalized coordinates in Lagrangian mechanics does not include such a possibility, so Hamiltonian dynamics has a larger symmetry group than Lagrangian dynamics.

For our next example, we first show that the composition of two canonical transformations is also canonical. Let $\psi(\chi)$ and $\chi(\xi)$ both be canonical. Defining the composition transformation, $\psi(\xi) = \psi(\chi(\xi))$, we compute

$$\begin{aligned} \Omega^{CD} \frac{\partial \psi^A}{\partial \xi^C} \frac{\partial \psi^B}{\partial \xi^D} &= \Omega^{CD} \left(\frac{\partial \psi^A}{\partial \chi^E} \frac{\partial \chi^E}{\partial \xi^C} \right) \left(\frac{\partial \psi^B}{\partial \chi^F} \frac{\partial \chi^F}{\partial \xi^D} \right) \\ &= \left(\frac{\partial \chi^E}{\partial \xi^C} \frac{\partial \chi^F}{\partial \xi^D} \Omega^{CD} \right) \frac{\partial \psi^A}{\partial \chi^E} \frac{\partial \psi^B}{\partial \chi^F} \\ &= \Omega^{EF} \left(\frac{\partial \psi^A}{\partial \chi^E} \right) \left(\frac{\partial \psi^B}{\partial \chi^F} \right) \\ &= \Omega^{AB} \end{aligned}$$

so that $\psi(\xi)$ is canonical.

2.3 Example 3: Momentum transformations

By the previous results, the composition of an arbitratry coordinate change with x, p interchanges is canonical. Consider the effect of composing (a) an interchange, (b) a coordinate transformation, and (c) an interchange.

For (a), let

$$\begin{aligned} \tilde{q}^i &= p_i \\ \tilde{\pi}_i &= -x^i \end{aligned}$$

Then for (b) we choose an arbitrary function of $\tilde{q}^i$:

$$\begin{aligned} Q^i &= F^i\left(\tilde{q}^j\right) \\ P_i &= \frac{\partial \tilde{q}^n}{\partial Q^i}\tilde{\pi}_n \end{aligned}$$

Finally, for (c), another interchange:

$$\begin{aligned} q^i &= P_i \\ \pi_i &= -Q^i \end{aligned}$$

Combining all three, we have

$$\begin{aligned} q^i &= P_i = \frac{\partial \tilde{q}^n}{\partial Q^i}\tilde{\pi}_n = -\frac{\partial p^n}{\partial \pi_i}x_n \\ \pi_i &= -Q^i = F^i\left(\tilde{q}^j\right) = F^i\left(p_j\right) \end{aligned}$$

so that π_i is replaced by an arbitrary function of the original momenta. This establishes that replacing the momenta by any independent functions of the momenta, preserves Hamilton's equations as long as we choose the proper coordinates q^i.

3 Generating functions

There is a systematic approach to canonical transformations using generating functions. We will give a simple example of the technique. Given a system described by a Hamiltonian $H(x^i, p_j)$, we seek another Hamiltonian $H'(q^i, \pi_j)$ such that the equations of motion have the same form, namely

$$\begin{aligned} \frac{dx^i}{dt} &= \frac{\partial H}{\partial p_i} \\ \frac{dp_i}{dt} &= -\frac{\partial H}{\partial x^i} \end{aligned}$$

in the original system and

$$\begin{aligned} \frac{dq^i}{dt} &= \frac{\partial H'}{\partial \pi_i} \\ \frac{d\pi_i}{dt} &= -\frac{\partial H'}{\partial q^i} \end{aligned}$$

in the transformed variables. The principle of least action must hold for each pair:

$$\begin{aligned} S &= \int \left(p_i dx^i - H dt\right) \\ S' &= \int \left(\pi_i dq^i - H' dt\right) \end{aligned}$$

where S and S' differ by at most a constant. Correspondingly, the integrands may differ by the addition of a total differential, $df = \frac{df}{dt}dt$, since this will integrate to a surface term and therefore will not contribute to the variation.

In general we may therefore write

$$p_i dx^i - H dt = \pi_i dq^i - H' dt + df$$

and solve for the differential df

$$df = p_i dx^i - \pi_i dq^i + (H' - H)\, dt$$

For the differential of f to take this form, it must be a function of x^i, q^i and t, $f = f(x^i, q^i, t)$. Therefore, the differential of f is

$$df = \frac{\partial f}{\partial x^i} dx^i + \frac{\partial f}{\partial q^i} dq^i + \frac{\partial f}{\partial t} dt$$

Equating the expressions for df we match up terms to require

$$\begin{aligned} p_i &= \frac{\partial f}{\partial x^i} && (4) \\ \pi_i &= -\frac{\partial f}{\partial q^i} && (5) \\ H' &= H + \frac{\partial f}{\partial t} && (6) \end{aligned}$$

The first equation

$$p_i = \frac{\partial f(x^j, q^j, t)}{\partial x^i} \tag{7}$$

gives q^i implicitly in terms of the original variables, while the second determines π_i. This choice fixes the form of π_i by eq.(5), while eq.(6) gives the new Hamiltonian in terms of the old one. The function f is the generating function of the transformation.

There are other types of generating functions. By making a Legendre transformation, we can change the independent variables. For example, setting

$$f = p_i x^i + f_2 (p_i, q_i, t)$$

we have

$$\begin{aligned} p_i dx^i - H dt &= \pi_i dq^i - H' dt + df \\ &= \pi_i dq^i - H' dt + dp_i x^i + p_i dx^i + df_2 (p_i, q_i, t) \\ -H dt &= \pi_i dq^i - H' dt + dp_i x^i + df_2 (p_i, q_i, t) \end{aligned}$$

so that the independent variables are now (p_i, q_i), satisfying

$$\begin{aligned} x^i &= -\frac{\partial f}{\partial p_i} \\ \pi_i &= \frac{\partial f}{\partial q^i} \\ H' &= H + \frac{\partial f}{\partial t} \end{aligned}$$

We may also define

$$\begin{aligned} f &= -\pi_i q^i + f_3 \left(x^i, \pi_j, t\right) \\ f &= p_i x^i - \pi_i q^i + f_4 \left(p^i, \pi_j, t\right) \end{aligned}$$

so that the independent variables may be taken as either of the new coordinates with either of the old coordinates.

3.1 Example 1

Let f_2 be a general quadratic,

$$f_2\left(p_i, q^j, t\right) = \frac{1}{2}\left(a_{ij}\left(t\right) q^i q^j + b^i{}_j\left(t\right) p_i q^j + c^{ij}\left(t\right) p_i p_j\right)$$

Then

$$\begin{aligned}
x^i &= -\frac{\partial}{\partial p_i}\left(\frac{1}{2}\left(a_{ij} q^i q^j + 2b^i{}_j p_i q^j + c^{ij} p_i p_j\right)\right) \\
&= -\left(b^i{}_j q^j + c^{ij} p_j\right) \\
\pi_i &= \frac{\partial}{\partial q^i}\left(\frac{1}{2}\left(a_{ij} q^i q^j + 2b^i{}_j p_i q^j + c^{ij} p_i p_j\right)\right) \\
&= a_{ij} q^j + b^i{}_j p_i \\
H' &= H + \frac{1}{2}\left(\dot{a}_{ij}\left(t\right) q^i q^j + \dot{b}^i{}_j\left(t\right) p_i q^j + \dot{c}^{ij}\left(t\right) p_i p_j\right)
\end{aligned}$$

3.2 Example 2

Let

$$f_2\left(p_i, q^j, t\right) = g\left(p, t\right) + g_i\left(p\right) q^i + \frac{1}{2} f_{ij}\left(p\right) q^i q^j + \frac{1}{3!} f_{ijk}\left(p\right) q^i q^j q^k$$

Then

$$\begin{aligned}
x^i &= -\frac{\partial}{\partial p_i}\left(g\left(p, t\right) - g_i\left(p\right) q^i - \frac{1}{2} f_{ij}\left(p\right) q^i q^j - \frac{1}{3!} f_{ijk}\left(p\right) q^i q^j q^k\right) \\
\pi_i &= g_i\left(p\right) - f_{ij}\left(p\right) q^j - \frac{1}{2} f_{ijk}\left(p\right) q^j q^k \\
H' &= H + \frac{\partial}{\partial t} g\left(p, t\right)
\end{aligned}$$