Canonical Transformations

Instead of finding the equations of motion and then working hard to solve them, we can try to change variables to simplify the Hamiltonian and so equations of motion, and perhaps even make them trivially solvable. Historically this has been an important tool in attempts to solve hard problems such as the three body problem (3 masses interacting by gravity, e.g. the earth, moon, sun system). It is a useful approach in advanced calculations in mechanics, such as perturbation calculations, and in formal proofs. It is also widely used in quantum mechanics, where it is harder to solve for the motion specified by a Hamiltonian.

A transformation to a new set of coordinates and momenta for which Hamilton's equations of motion also apply is called a *canonical transformation*

$$\{q_k, p_k\} \Rightarrow \{Q_k, P_k\}, \quad H \Rightarrow \bar{H}$$
 (1)

such that

$$\dot{Q}_k = \frac{\partial \bar{H}}{\partial P_k}, \qquad \dot{P}_k = -\frac{\partial \bar{H}}{\partial Q_k}.$$
 (2)

A particular type of canonical transformation is a transformation of coordinates $\{q_k\} \to \{Q_j\}$, called a *point* transformation. There would then be some new momenta $\{P_j(\{q_k\}, \{p_k\}, t)\}$ that could be derived from the transformed the Lagrangian. The Hamiltonian approach allows to consider more general *contact* transformations that mix coordinates and momenta.

We would like:

- a formal way to generate canonical transformations,
- a way to test that a proposed transformation is canonical.

Generating functions

What is a generating function?

I will look at problems with 1 degree of freedom (2-dimensional phase space) — the results may be generalized to higher dimensions (see Goldstein, Poole and Safko).

For a general transformation from q, p to Q, P, we need to specify two functions Q(q, p, t), P(q, p, t). The restriction to a canonical transformation means that only one function of two variables is needed: the *generating function*. The generating function is a function of one old coordinate or momentum and one new coordinate or momentum. The other pair is then giving by \pm partial derivatives of the generating function with respect to the conjugate variable (coordinate by partial with respect to momentum, etc.).

One approach to the formulation is via Hamilton's principle, which applies in each system of variables:

$$\delta \int (p \, dq - H \, dt) = 0, \qquad \delta \int (P \, dQ - \bar{H} \, dt) = 0, \tag{3}$$

for any path variation (represented by δq , δp or δQ , δP) with fixed coordinates at the endpoints. The first implies the second if

$$P dQ - \bar{H} dt = p dq - H dt - dF_1(q, Q, t)$$
 (4)

since $\delta \int dF_1 = 0$ because of the endpoint restrictions. (This is not "if and only if": it is possible to include an overall scale factor, which turns out to be uninteresting, so we restrict to the form given.) Rewrite

$$dF_1 = p \, dq - P \, dQ + (\bar{H} - H)dt, \tag{5}$$

and read off the derivatives

$$p = \frac{\partial F_1}{\partial q}, \quad P = -\frac{\partial F_1}{\partial Q}, \quad \bar{H} = H + \frac{\partial F_1}{\partial t}.$$
 (6)

The first of these equations must be solved for Q(q, p) (remember F_1 is a function of q, Q). This can only be done, even locally, if $\partial F_1/\partial q$ does depend on Q, i.e.

$$\frac{\partial^2 F_1}{\partial Q \partial q} \neq 0. \tag{7}$$

After we have found Q(q, p), the second equation gives P(q, p). With the condition Eq. (7) satisfied, any function $F_1(q, Q)$ generates a canonical transformation.

Alternative motivations for the generating function are given in the Appendix.

Example 1: Consider $F_1 = qQ$. This generates

$$Q = p, \quad P = -q \tag{8}$$

and so interchanges what we call the coordinate and momentum.

This is an example of "guess a generating function and see what you get". More commonly, we want to find the generating function to do a specific task, as in the next example.

Example 2: Consider the Hamiltonian for a simple harmonic oscillator

$$H = \frac{1}{2}(p^2 + q^2) \tag{9}$$

which gives the equations of motion

$$\dot{q} = p, \quad \dot{p} = -q. \tag{10}$$

The solution is a circle in phase space, and the phase space point travels uniformly around the circle. We might want to simplify the description by using the angle around the circle $Q = \tan^{-1} q/p$ as the new coordinate. What is the conjugate momentum? We have

$$p = q \cot Q = \left(\frac{\partial F_1}{\partial q}\right)_Q \quad \Rightarrow \quad F_1(q, Q) = \frac{1}{2}q^2 \cot Q$$
 (11)

(leaving out possible integration "constant" f(Q) to find the simplest possibility). Then

$$P = -\frac{\partial F_1}{\partial Q} = \frac{1}{2}q^2 \csc^2 Q = \frac{1}{2}(p^2 + q^2). \tag{12}$$

Also $\bar{H} = H = P$ (i.e. the Hamiltonian in the new variables is just given by substitution in the old Hamiltonian), so that

$$\dot{Q} = 1, \quad \dot{P} = 0 \tag{13}$$

and we have solved the problem. This approach can be generalized to other periodic systems, giving *actionangle* variables (see below).

Note that the fact that the transformation is canonical does not depend on the form of the Hamiltonian, although in this example I used the desire to simplify the Hamiltonian to motivate a particular choice of canonical transformation.

Legendre transformations give other generating functions

 F_1 was derived as a function of old-position, new-position. We can derive three other generating functions for the same transformation, so that each is a function of one old variable (position or momentum) and one new variable (position or momentum). This is done using Legendre transforms in the usual way, using "slope - intercept" variables.

Define
$$F_2(q, P, t) = F_1(q, Q, t) + PQ$$
 implies $Q = \frac{\partial F_2}{\partial P}, p = \frac{\partial F_2}{\partial q}$ (14)

Define
$$F_3(p, Q, t) = F_1(q, Q, t) - pq$$
 implies $q = -\frac{\partial F_3}{\partial p}, P = -\frac{\partial F_3}{\partial Q}$ (15)

Define
$$F_4(p, P, t) = F_3(p, Q, t) + PQ$$
 implies $q = -\frac{\partial F_4}{\partial p}$, $Q = \frac{\partial F_4}{\partial P}$ (16)

For time dependent transformations the new Hamiltonian \bar{H} is given in each case by

$$\bar{H} = H + \frac{\partial F_j}{\partial t}.\tag{17}$$

These are all results of pure algebraic manipulations, no physics: just evaluate e.g. dF_2 using what we know about dF_1

$$dF_2 = dF_1 + PdQ + QdP = pdq + QdP + (\bar{H} - H)dt, \tag{18}$$

and read off derivatives. Note these new generating functions in general give the *same* canonical transformation. In some cases though, one or more of the forms may not give results, because conditions analogous to Eq. (7) are not satisfied.

Example 3: Consider $F_2 = qP$. This gives

$$Q = q, \quad p = P \tag{19}$$

the identity transformation. This is useful as a starting point for perturbation expansions.

Example 4: Return to the simple harmonic oscillator example, transforming to the angle variable $Q = \tan^{-1} q/p$. This can be written

$$q = p \tan Q = -\left(\frac{\partial F_3(p, Q)}{\partial p}\right)_Q \quad \Rightarrow \quad F_3(p, Q) = -\frac{1}{2}p^2 \tan Q. \tag{20}$$

Then

$$P = -\frac{\partial F_3}{\partial Q} = \frac{1}{2}p^2 \sec^2 Q = \frac{1}{2}(p^2 + q^2),\tag{21}$$

as before.

Proofs of results

Many elegant results on canonical transformations can be proved using generating functions. Here are a couple of examples:

Time evolution is a canonical transformation Consider an F_2 type transformation using the identity transformation plus a small added piece of the Hamiltonian, evaluated as a function of q, P

$$F_2 = qP + dt H(q, P). \tag{22}$$

This gives

$$Q = q + dt \frac{\partial H}{\partial P},\tag{23}$$

$$p = P + dt \frac{\partial H}{\partial q}.$$
 (24)

For small dt and to O(dt) we can replace H(q, P) by H(q, p) since this appears in terms multiplied by dt. This gives (rearranging the second one)

$$Q = q + dt \frac{\partial H}{\partial p} \simeq q(t + dt), \tag{25}$$

$$P = p - dt \frac{\partial H}{\partial q} \simeq p(t + dt), \tag{26}$$

using the equations of motion for q, p. Thus time evolution is a sequence of infinitesimal canonical transformations, or q(t), p(t) is a canonical transformation of q(0), p(0).

2d canonical transformations are area preserving If we use Eq. (5) at some fixed time we can write

$$\oint p \, dq - \oint P \, dQ = \oint dF = 0.$$
(27)

The quantities $\oint p \, dq$, $\oint P \, dQ$ are the areas of a closed loop in phase space evaluated in the two coordinate-momentum systems. Thus canonical transformations are *area preserving*.

An alternative approach is to relate areas via the Jacobian (determinant) ¹

$$\iint dQdP = \iint \left| \left| \frac{\partial(Q, P)}{\partial(q, p)} \right| \right| dqdp \quad \text{with} \quad \left| \frac{\partial(q, p)}{\partial(Q, p)} \right| = \left| \frac{\frac{\partial q}{\partial Q}}{\frac{\partial p}{\partial Q}} \frac{\frac{\partial q}{\partial P}}{\frac{\partial p}{\partial P}} \right| = \frac{\partial q}{\partial Q} \frac{\partial p}{\partial P} - \frac{\partial q}{\partial P} \frac{\partial p}{\partial Q}. \quad (28)$$

Using the intuitive-looking properties of the Jacobian that can be proven from the definition

$$\left| \frac{\partial(Q, P)}{\partial(q, p)} \right| = \left| \frac{\partial(Q, P)}{\partial(q, Q)} \right| \left| \frac{\partial(q, Q)}{\partial(q, p)} \right| = \left| \frac{\partial(Q, P)}{\partial(q, Q)} \right| \left[\left| \frac{\partial(q, p)}{\partial(q, Q)} \right| \right]^{-1} = -\left(\frac{\partial P}{\partial q} \right)_Q \left[\left(\frac{\partial p}{\partial Q} \right)_q \right]^{-1}. \tag{29}$$

Now using the F_1 generating function, each of the partials in the last expression of Eq. (29) is $\partial^2 F_1/\partial q \partial Q$ and so

$$\left| \frac{\partial(Q, P)}{\partial(q, p)} \right| = 1 \qquad \text{for canonical transformation.}$$
 (30)

The generalization to any dimension is that the transformation is *symplectic* meaning that the sum of projected areas on the coordinate-momentum planes is preserved.

¹Texts differ in their use of the $\partial(q, p)/\partial(Q, P)$ symbol: I'm following Hand and Finch in using the symbol for the Jacobian *matrix*, whereas some texts use it for the *determinant* of the Jacobian matrix.

Poisson brackets

You will recognize the last expression in Eq. (28) as the Poisson bracket $[q, p]_{Q,P}$, introduced in discussing the time dependence of phase space functions. Poisson brackets also provide a way to test whether a transformation is canonical. I'll present the results for general dimension, but only remark on the proofs for a two dimensional phase space. Goldstein, Poole, and Safko provide a detailed discussion, albeit rather heavy on the algebra. First I'll remind you of the definition from Lecture 10.

Definition For functions $A(\{q_k\}, \{p_k\}, t)$, $B(\{q_k\}, \{p_k\}, t)$, the Poisson bracket is defined as

$$[A, B]_{q,p} = \sum_{k=1}^{N} \left(\frac{\partial A}{\partial q_k} \frac{\partial B}{\partial p_k} - \frac{\partial A}{\partial p_k} \frac{\partial B}{\partial q_k} \right)$$
(31)

Results

(a) For a canonical transformation $\{q_k, p_k\} \rightarrow \{Q_k, P_k\}$

$$[Q_j, P_k]_{q,p} = \delta_{j,k}, \quad [Q_j, Q_k]_{q,p} = 0, \quad [P_j, P_k]_{q,p} = 0.$$
 (32)

The first condition is the area preserving condition for the one degree of freedom system. It is a necessary and sufficient condition for the transformation to be canonical and gives a test whether a given transformation is canonical. For higher dimensional phase spaces the first condition gives the preservation of the projection of areas on the q, p planes (the symplectic condition). The second pair of conditions says that any pair of coordinates or pair of momenta must give zero Poisson bracket. One example is that the component of the angular momentum \vec{L}_x , \vec{L}_y cannot both be canonical momenta, since the Poisson bracket is non-zero. Any one component (often chosen to be L_z) and the magnitude or its square $L^2 = L_x^2 + L_y^2 + L_z^2$ do however have zero Poisson bracket and can be used as canonical momenta.

(b) The Poisson bracket is unchanged by canonical transformation

$$[A, B]_{q,p} = [A, B]_{Q,P}. (33)$$

Therefore we can leave off the q,p subscript. In 2d this follows directly from the product rule for Jacobians.

(c) Review Lecture 10 for properties connected with time dependence and constants of the motion, and the connection to quantum mechanics.

Appendix A: More motivation for generating functions

Here are other motivations for the use of generating functions. One, perhaps confusing, point, is that although in the end we are going to consider Q, P as the new variables to describe a phase space point, during the proof we might choose some other pair e.g. q, P as the variables to define the point — except in degenerate cases, any pair out of q, p, Q, P can be used as the "independent variables".

Motivation 1: Most direct but messy

I'll only do this assuming $\bar{H} = H$ (true for time independent transformations) We want Q, P and q, p to satisfy Hamilton's equation of motion with the same Hamiltonian (i.e. given by substitution to get the dependence on the new variables). We can derive the equations of motion for Q, P from those from q, p by two paths.

$$(\dot{Q}, \dot{P}) \Leftarrow (\dot{q}, \dot{p}) \Leftarrow H(q, p)$$
 (34)

$$(\dot{Q}, \dot{P}) \Leftarrow H(Q, P) \Leftarrow H(q, p)$$
 (35)

As an example of what this shorthand means consider \dot{Q} : in Eq. (34) the sequence of operations is

$$\dot{Q} = \frac{\partial Q}{\partial q}\dot{q} + \frac{\partial Q}{\partial p}\dot{p} = \frac{\partial Q}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial Q}{\partial p}\frac{\partial H}{\partial q},\tag{36}$$

and in Eq. (35) the sequence is

$$\dot{Q} = \frac{\partial H}{\partial P} = \frac{\partial H}{\partial p} \frac{\partial p}{\partial P} + \frac{\partial H}{\partial q} \frac{\partial q}{\partial P}.$$
 (37)

Repeating the argument for \dot{P} and equating the two routes in each case gives

$$\begin{pmatrix}
\frac{\partial Q}{\partial q} & -\frac{\partial Q}{\partial p} \\
-\frac{\partial P}{\partial q} & \frac{\partial P}{\partial p}
\end{pmatrix}_{(Q,P)} \begin{pmatrix}
\frac{\partial H}{\partial p} \\
\frac{\partial H}{\partial q}
\end{pmatrix} = \begin{pmatrix}
\frac{\partial p}{\partial P} & \frac{\partial q}{\partial P} \\
\frac{\partial p}{\partial Q} & \frac{\partial q}{\partial Q}
\end{pmatrix}_{(q,p)} \begin{pmatrix}
\frac{\partial H}{\partial p} \\
\frac{\partial H}{\partial q}
\end{pmatrix}.$$
(38)

(The subscripts on the matrix brackets indicate what is being held constant in the partials.) Since we want this to be true for any H we assume that the matrices are equal element by element.

Consider the first elements. We then have

$$\frac{\partial Q}{\partial q} = \frac{\partial p}{\partial P} \tag{39}$$

For this equation, it makes sense to think of q, P as the independent variables. The equation is guaranteed to be true if there exists a function F(q, P) such that $Q = \partial F/\partial P$ and $p = \partial F/\partial q$ for then each side of the equation is the second derivative $\partial^2 F/\partial q \partial P$. Alternatively, think of the equation as $\nabla_{q,P} \times (p,Q) = 0$ with $\nabla_{q,P}$ the gradient operator in q, P space. This implies $(p,Q) = \nabla_{q,P} F(q,P)$. This has given us a type 2 generating function $F_2(q,P)$.

The same can be done for the other three elements, giving the other three type of generating functions.

Motivation 2: Area preserving via Jacobian

For this approach we need to first show that a canonical transformation is area preserving, rather than using generating functions to prove this result! This follows since if the dynamics is area preserving in each of q, p and Q, P as we showed in deriving Liouville's theorem, then up to an uninteresting constant scale factor, the transformation between the two systems must be area preserving. Then equations (28,29) show

$$\left| \frac{\partial(Q, P)}{\partial(q, p)} \right| = 1 \quad \Rightarrow \quad \left(\frac{\partial P}{\partial q} \right)_Q = -\left(\frac{\partial p}{\partial Q} \right)_q \tag{40}$$

and then we proceed as in the previous method.

Method 3: Area preserving via integral

As in the previous method, we first show that a canonical transformation is area preserving. This means

$$\oint p \, dq = \oint P \, dQ. \tag{41}$$

Take q, Q as the independent variables and write the equation as

$$\oint [p(q, Q) \, dq - P(q, Q) \, dQ] = 0.$$
(42)

Since this is true for all closed paths the integrand must be a perfect differential

$$p(q, Q) dq - P(q, Q) dQ = dF(q, Q)$$
 (43)

and so $p = \partial F/\partial q$, $P = -\partial F/\partial Q$. Other types of generating functions are obtained by noting that, for example

$$\oint [p(q, Q) dq - P(q, Q) dQ + d(PQ)] = 0,$$
(44)

so that

$$\oint [p \, dq + Q \, dP] = 0.$$
(45)

Now we think of (q, P) as the independent variables, and proceed as before. This is just a Legendre transformation in disguise.

Appendix B: Canonical perturbation theory

This is a problem that I've set in previous years that illustrates solving a hard problem using perturbation theory formulated in terms of canonical transformations. In such problems the generating function can be systematically calculated, rather than guessed.

The problem is to find the solutions for a slightly anharmonic oscillator with Hamiltonian

$$H(q, p) = \frac{1}{2}(p^2 + \omega^2 q^2) + \epsilon \beta q^4, \tag{46}$$

with ϵ small. We will just keep $O(\epsilon)$ terms - if you find a term with an ϵ^2 , throw it out! The identity generating function is the type-2 function $F_2(P,q) = Pq$. Since the extra term in the Hamiltonian involves two more powers of q we look for a generating function with quadratic corrections too

$$F_2(P,q) = Pq + \epsilon Pq(aq^2 + bP^2) \tag{47}$$

where a, b are constants to be determined.

(a) Show, using the generating function to calculate p and Q and inverting as necessary, that

$$q = Q - 3\epsilon bQP^2 - \epsilon aQ^3 + O(\epsilon^2), \tag{48}$$

$$p = P + \epsilon b P^3 + 3\epsilon a Q^2 P + O(\epsilon^2). \tag{49}$$

(b) Find the values of a, b that reduce the Hamiltonian to the form

$$H(Q, P) = \frac{1}{2}(P^2 + \omega^2 Q^2) + \epsilon c(P^2 + \omega^2 Q^2)^2 + O(\epsilon^2)$$
 (50)

with c a constant that you should also evaluate.

(c) Now, following the method we used for a harmonic oscillator, perform a canonical transformation to θ , p_{θ} coordinates where $\tan \theta = \omega Q/P$, and p_{θ} is derived from a type-1 generating function. You should find the Hamiltonian reduces to

$$H(\theta, p_{\theta}) = \omega p_{\theta} + 4\epsilon c\omega^2 p_{\theta}^2 + O(\epsilon^2), \tag{51}$$

independent of θ (so these are action-angle variables).

(d) Hence show to this order in ϵ the solution is

$$Q = A\sin(\Omega t + \delta), \quad P = \omega A\cos(\Omega t + \delta), \quad \Omega = \omega + 3\epsilon \beta A^2/2\omega,$$
 (52)

with δ an arbitrary constant.

(e) Find q(t) to $O(\epsilon)$. Note that the frequency of the motion is changed. This will not appear in a "conventional" perturbation theory where we write $q(t) = A\cos\omega t + \epsilon q_1(t) + O(\epsilon^2)$ with $A\cos\omega t$ the zeroth order solution, and then try to find the small correction term $\epsilon q_1(t)$: since the frequency is changed, at long times the correction to $A\cos\omega t$ is *not* small.

The algebra is not *too* messy if you throw out higher order terms as quickly as possible. For example

$$\epsilon \beta q^4 = \epsilon \beta Q^4 + O(\epsilon^2)$$

and

$$Q = q + 3\epsilon bq P^2 + \epsilon aq^3 \Rightarrow Q = q + 3\epsilon bQP^2 + \epsilon aQ^3 + O(\epsilon^2)$$

(just substituting the zeroth order expression in the $O(\epsilon)$ terms) giving q in terms of Q, P to the order required.

Solution

(a) From the generating function we have

$$Q = \frac{\partial F_2}{\partial P} = q + \epsilon a q^3 + 3\epsilon b q P^2, \tag{53}$$

$$p = \frac{\partial F_2}{\partial q} = P + 3\epsilon a q^2 P + \epsilon b P^3. \tag{54}$$

To $O(\epsilon)$ Eq. (54) gives

$$q = \frac{\partial F_2}{\partial P} = Q - 3\epsilon b Q P^2 - \epsilon a Q^3.$$
 (55)

(b) To $O(\epsilon)$

$$\epsilon \beta q^4 = \epsilon \beta Q^4 + O(\epsilon^2), \tag{56}$$

$$\frac{1}{2}(p^2 + \omega^2 q^2) = \frac{1}{2}(P^2 + \omega^2 Q^2) + \epsilon P(3\epsilon a q^2 P + \epsilon b P^3) - \epsilon \omega^2 (3\epsilon b Q P^2 + \epsilon a Q^3). \tag{57}$$

Collecting terms

$$H = \frac{1}{2}(P^2 + \omega^2 Q^2) + \epsilon[(\beta - \omega^2 a)Q^4 + (3a - 3\omega^2 b)Q^2 P^2 + bP^4) + O(\epsilon^2).$$
 (58)

To get to the desired form we need

$$b = c, (59)$$

$$3(a - \omega^2 b) = 2\omega^2 c,\tag{60}$$

$$\beta - \omega^2 a = \omega^4 c,\tag{61}$$

which can be solved to give

$$a = \frac{5\beta}{8\omega^2},\tag{62}$$

$$b = c = \frac{3\beta}{8\omega^4}. ag{63}$$

(c) To simplify the Hamiltonian we transform to θ , p_{θ} using $\tan \theta = \omega Q/P$. The generating function is

$$F_1(Q,\theta) = \frac{1}{2}\omega Q^2 \cot \theta, \tag{64}$$

from which we find

$$p_{\theta} = \frac{1}{2\omega} (P^2 + \omega^2 Q^2), \tag{65}$$

so that the Hamiltonian is

$$H = \omega p_{\theta} + 4\epsilon \omega^2 c p_{\theta}^2. \tag{66}$$

(c) The frequency is

$$\Omega = \dot{\theta} = \frac{\partial H}{\partial p_{\theta}} = \omega + 8\epsilon \omega^2 c p_{\theta} = \omega + \frac{3\beta \epsilon}{\omega^2} p_{\theta}$$
 (67)

and p_{θ} is constant. From Eq. (65) and the definition of θ we derive

$$Q = \sqrt{\frac{2p_{\theta}}{\omega}} \sin \theta = A \sin(\Omega t + \delta)$$
 (68)

with $A = \sqrt{2p_{\theta}/\omega}$ and δ an integration constant. Then

$$P = \omega Q \cot \theta = A \cos(\Omega t + \delta). \tag{69}$$

Finally, writing the frequency in terms of the amplitude A

$$\Omega = \omega + \frac{3\epsilon\beta A^2}{2\omega}.\tag{70}$$

(d) Now substitute back into Eq. (55)

$$q = A\sin(\Omega t + \delta) - \frac{\epsilon \beta A^3}{8\omega^2} [9\sin(\Omega t + \delta)\cos^2(\Omega t + \delta) + 5\sin^3(\Omega t + \delta)]$$
 (71)

$$= A\sin(\Omega t + \delta) - \frac{\epsilon \beta A^3}{8\omega^2} \{6\sin(\Omega t + \delta) + \sin[3(\Omega t + \delta)]\}$$
 (72)

$$\simeq A\sin(\Omega t + \delta) - \frac{\epsilon \beta A^3}{8\omega^2}\sin[3(\Omega t + \delta)] \tag{73}$$

showing a third harmonic is generated as well as the frequency shift. The small change to the amplitude of the first harmonic can be absorbed into a redefinition of A without changing any of the other results to $O(\epsilon)$, although we would need to keep it if going to higher order.

Michael Cross: November 5, 2013