Physics 6010, Fall 2016

Phase Space Variational Principle. Canonical Transformations.

Relevant Sections in Text: §8.5, 8.6, 9.1–9.5

Hamilton's principle and Hamilton's equations

You will recall that the Lagrangian formulation of mechanics arises from a variational principle, known (somewhat confusingly at this point) as *Hamilton's principle.* Hamilton's principle determines physically allowed curves in configuration space. Physically allowed curves are critical points of the *action integral*:

$$S[q] = \int_{t_0}^{t_1} L(q(t), \frac{dq(t)}{dt}, t)\, dt,$$

with fixed endpoint conditions. This means that, if $\hat{q}^i(t)$ defines the physical curve, then for any other path $q^i(t)$, where

$$q^i(t) = \hat{q}^i(t) + \delta q^i(t), \quad \delta q^i(t_0) = \delta q^i(t_1) = 0,$$

we have that $S[q] - S[\hat{q}]$ is zero to first order in the variations δq. We saw that the critical curves in configuration space satisfied the Euler-Lagrange (EL) equations. Now we have introduced the Hamiltonian form of the equations of motion. The Hamilton equations determine curves in momentum phase space. Since the Hamilton equations and EL equations are equivalent (when viewed as differential equations for curves in configurations space) it is natural to wonder if there is a variational principle governing Hamilton's equations. There is such a variational principle – it is *the* Hamilton's principle – and it is defined as follows.

We consider curves $(q^i(t), p_i(t))$ in momentum phase space and define the *phase space action integral* $S[q, p]$ via

$$S[q, p] = \int_{t_0}^{t_1} (p_i \dot{q}^i - H(q, p, t))\, dt.$$

As usual, it is understood that all quantities *in the integral* are evaluated on a curve in momentum phase space:

$$q^i = q^i(t), \quad p_i = p_i(t), \quad \dot{q}^i = \frac{dq^i(t)}{dt}.$$

You can easily see that on paths satisfying the Hamilton equations the numerical value of S is the same as the usual action used in the Lagrangian formulation. This is because $p_i \dot{q}^i - H(q, p, t)$ is the usual Lagrangian in this case (exercise). On the other hand, previously we viewed the action as a functional of curves in the (n-dimensional) configuration space and it was these curves which are varied in the variational principle. Now we are considering curves in the ($2n$-dimensional) phase space in the variational principle. As we evaluate the phase space action on this or that curve, the curves will not in general satisfy the Hamilton equations (the critical point condition – as we shall see) and hence the relation between momentum and velocity does not necessarily hold on the curves in phase space. Thus the phase space variational principle is distinct from the configuration space variational principle.

Let us now consider the conditions placed upon the phase space path by demanding that it provides a critical point of $S[q,p]$. We suppose that the path $q^i(t), p_i(t)$ is a critical point of the action integral. This means that if we substitute

$$q^i(t) \to q^i(t) + \delta q^i(t),$$

$$p_i(t) \to p_i(t) + \delta p_i(t),$$

the first order change in the action integral, δS, with respect to δq and δp vanishes. This condition is (exercise)

$$0 = \delta S = \int_{t_0}^{t_1} \left(\delta p_i \dot{q}^i + p_i \dot{\delta q^i} - \frac{\partial H}{\partial q^i}\delta q^i - \frac{\partial H}{\partial p_i}\delta p_i \right) dt = 0. \quad \forall\ \delta q^i, \delta p_i.$$

If we integrate by parts in the second term, and demand that

$$\delta q^i(t_1) = 0 = \delta q^i(t_2),$$

then we get

$$0 = \int_{t_0}^{t_1} \left[(\dot{q}^i - \frac{\partial H}{\partial p_i})\delta p_i - (\dot{p}_i + \frac{\partial H}{\partial q^i})\delta q^i \right] dt.$$

Because δq and δp are arbitrary in the domain of integration, each of the terms must separately vanish, thus we obtain Hamilton's equations by a variational principle. Note that the coordinates are fixed at the endpoints of the allowed paths (just as in the Lagrangian variational principle), but the momenta are free at the endpoints.

Canonical Coordinates and Momenta

To build the Hamilton equations for a given dynamical system you need two ingredients. The first is pretty obvious – you need the Hamiltonian. This is a function of $2n$ variables (and possibly the time), where n is the number of degrees of freedom. But I if I just hand you a function of, say, 2 variables (for a system with one degree of freedom), you still need another piece of information before you can write the equations of motion. You need to know which variable is "q "and which variable is "p". The reason for this is that minus sign that appears in the Hamilton equations - which distinguishes the q and p variables. The Poisson bracket – which can be used to construct the equations of motion for any observable – knows about this minus sign as well, as you can see from its definition. We shall see that there is a wide variety of choices for coordinates and momenta which permit the Hamiltonian description. Any such system of coordinates on phase is called "canonical", with the q's called "canonical coordinates" and the p's called the corresponding – or "conjugate" – "canonical momenta".

The defining property of canonical coordinates and momenta is that they satisfy the *fundamental Poisson bracket relations*

$$[q^i, q^j] = 0 = [p_i, p_j], \quad [q^i, p_j] = \delta^i_j.$$

You can easily check that it is precisely these relations which guarantee that the Hamilton equations can be expressed as:

$$\dot{q}^i = [q^i, H], \quad \dot{p}_i = [p_i, H].$$

A set of coordinates on phase space satisfies these relations if and only if they define canonical coordinates and momenta.

Given one set of canonical coordinates and momenta, it is easy to construct many others. For example, consider a particle moving in 1-d described with canonical phase space variables (x, p), as usual. It is not too hard to check that the following are also canonical variables:

$$Q = e^x, \quad P = e^{-x} p.$$

To see this, just check that

$$[Q, P] = 1.$$

(Why don't we have to check $[Q, Q] = 0 = [P, P]$?) Let us see how the Hamilton equations look in these new variables. Suppose the Hamiltonian is, say, that of a harmonic oscillator,

$$H(x, p) = \frac{p^2}{2m} + \frac{1}{2} k x^2,$$

with equations of motion

$$\dot{x} = \frac{p}{m}, \quad \dot{p} = -kx.$$

To express the Hamiltonian in terms of the new variables we need to invert the coordinate transformation:

$$x = \ln Q, \quad p = QP.$$

The new Hamiltonian, let's call it $\tilde{H}$, is given by

$$\tilde{H} = \frac{Q^2 P^2}{2m} + \frac{1}{2} k (\ln Q)^2.$$

Here's the punchline: because we are using canonical variables, we can use the same set of Hamilton's equations to compute the equations of motion. Thus:

$$\dot{Q} = \frac{\partial \tilde{H}}{\partial P} = \frac{Q^2 P}{m},$$

$$\dot{P} = -\frac{\partial \tilde{H}}{\partial Q} = -\frac{QP^2}{m} - k\frac{\ln Q}{Q}.$$

As you can see, while the formula for computing the equations is the same as always, the result can be very different depending upon the complexity of the change of variables. It is worth checking that the two systems of equations for the harmonic oscillator are equivalent. You can do that using the original definitions of (Q, P) in terms of (x, p) – I leave it as an exercise. The point is that while the equations turn out differently they are obtained always using the same prescription: Hamilton's equations for canonical coordinates and momenta.

A change of variables on phase space which maps one set of canonical variables into another (such as we just explored) is called a *canonical transformation.*

More about Canonical Transformations

You will recall that the Lagrangian formulation of mechanics allowed for a large class of generalized coordinates. In particular, let q^i be a system of coordinates so that the EL equations of the Lagrangian $L(q, \dot{q}, t)$ give the desired equations of motion. Then if

$$q'^i = q'^i(q, t)$$

is any other system of coordinates, the Lagrangian

$$L' = L(q(q', t), \dot{q}(q', \dot{q}', t), t),$$

where

$$\dot{q}^i(q', \dot{q}', t) = \frac{\partial q^i}{\partial q'^j}\dot{q}'^j$$

will give, *by the same EL equation formulas*, the correct — *i.e.,* equivalent — equations in the new variables. This kind of transformation, in which the new coordinates are functions of the old coordinates and time only, is called a *point transformation.* The fact that the same EL formula works in all coordinates related by a point transformation can be understood from the variational principle point of view. The fact that a configuration space curve is a critical point will not depend upon the choice of generalized coordinates used to compute the action integral.

More general changes of variables in which the new coordinates involve the old velocities are not allowed; the EL equations will, in general, be wrong. This stems from the fact that the variational principle is dealing with curves in configuration space only. As a very simple example of this, consider a free particle with Lagrangian in 1-d

$$L = \frac{1}{2}m\dot{x}^2,$$

and EL equations

$$m\ddot{x} = 0.$$

Let us define a new variable q via

$$q = \dot{x},$$

which is *not* a point transformation. The new Lagrangian, $\tilde{L}$ is given by

$$\tilde{L} = \frac{1}{2}mq^2.$$

The EL equations from $\tilde{L}$ are

$$mq = 0,$$

which are clearly not equivalent to $m\ddot{x} = 0$.

The Hamilton equations, since they come from a variational principle in *phase space*, allow for a much wider class of allowed coordinate transformations, the *canonical transformations*, and this feature is at the heart of many of the powerful aspects of the Hamiltonian formalism. For example, one can view time evolution as a canonical transformation. The link between symmetries and conservation laws is given its fullest expression via canonical transformations. Canonical transformations are at the heart of a very elegant form of dynamics: the Hamilton-Jacobi formalism (which provide the classical analog of the Schrödinger equation). Canonical transformations are the classical analog of unitary transformations in quantum mechanics and give a classical interpretation of the different quantum mechanical representations.

The idea of canonical transformations is that one can perform point transformations in *phase space*, in which the coordinates and momenta get mixed up. However, the key feature that has to be dealt with is that the phase space Lagrangian $\mathbf{L}$ is not just any function of the phase space variables and their time derivatives. The phase space Lagrangian has a special form:

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

We thus may only consider point transformations in phase space which preserve this form up to a total time derivative. This turns out to be a very large class of transformations compared to the point transformations of Lagrangian mechanics.

Example: Point transformations in configuration space

We now consider all invertible transformations

$$Q^i = Q^i(q, p, t)$$

$$P_i = P_i(q, p, t)$$

such that the original Hamilton equations, when expressed in terms of the new variables (Q, P), become

$$\dot{Q}^i = \frac{\partial K}{\partial P_i}$$

$$\dot{P}_i = -\frac{\partial K}{\partial Q^i}$$

for some choice of $K = K(Q, P, t)$. If we can do this, then we say that the transformation $(q, p) \leftrightarrow (Q, P)$ is a canonical transformation since it preserves the canonical form of the equations of motion. From the point of view of the Hamiltonian formulation of mechanics, any set of variables for which the equations of motion are in Hamiltonian form are equally viable for the description of the system.

Let us look at a simple example: time-independent point transformations for a system with one degree of freedom. Let $f(q)$ be a function with inverse $g(q)$:

$$f(g(q)) = q, \quad g(f(q)) = q.$$

Given a phase space (q, p) and Hamiltonian $H(q, p, t)$, the following transformation is a canonical transformation

$$Q = f(q), \quad P = \left.\frac{dg(Q)}{dQ}\right|_{Q=f(q)} p$$

with new Hamiltonian

$$K(Q, P, t) = H(g(Q), \left.\frac{df(q)}{dq}\right|_{q=g(Q)} P, t).$$

To see this, we compute (nice exercise)

$$\dot{Q} = \frac{df(q)}{dq}\dot{q} = \frac{df(q)}{dq}\frac{\partial H}{\partial p} = \frac{\partial K}{\partial P},$$

and

$$\begin{aligned}\dot{P} &= \left.\frac{d^2g(Q)}{dQ^2}\right|_{Q=f(q)} \frac{df(q)}{dq}\dot{q}p + \left.\frac{dg(Q)}{dQ}\right|_{Q=f(q)} \dot{p} \\ &= \left.\frac{d^2g(Q)}{dQ^2}\right|_{Q=f(q)} \frac{df(q)}{dq}\frac{\partial H}{\partial p}p - \left.\frac{dg(Q)}{dQ}\right|_{Q=f(q)} \frac{\partial H}{\partial q} \\ &= -\frac{\partial K}{\partial Q},\end{aligned}$$

where I used the identity

$$\frac{d^2g(Q)}{dQ^2}\frac{df(q)}{dq} = -\frac{d^2f}{dq^2}\frac{dg}{dQ},$$

which comes from differentiating the relation expressing that f and g are inverses.

As an exercise you can see that our previous example of a canonical transformation (in the context of our discussion of canonical coordinates and momenta) is a special case of this one. Indeed, it is possible to show that *a transformation is canonical if and only if it preserves the fundamental Poisson bracket relations.*

Example: Interchanging coordinates and momenta

Here is another, more amusing example. Define

$$Q = p, \quad P = -q.$$

Given $H(q, p, t)$, let

$$K(Q, P, t) = H(-P, Q, t).$$

For example, suppose

$$H = \frac{p^2}{2m} + V(q)$$

so that

$$K = \frac{Q^2}{2m} + V(-P).$$

We now verify that the transformation is canonical by examining Hamilton's equations in the new variables. We have

$$\dot{Q} = \frac{\partial K}{\partial P} = -V'(-P), \quad \dot{P} = -\frac{\partial K}{\partial Q} = -\frac{Q}{m}$$

Using the definitions of Q, P in terms of q, p we then get

$$\dot{p} = -V'(q), \quad -\dot{q} = -\frac{p}{m},$$

which are equivalent to the Hamilton equations in terms of q, p and H.

Note that this canonical transformation interchanges the roles of coordinates and momenta! Evidently, whether or not a variable is deemed a coordinate on the configuration space is not preserved by a canonical transformation. Thus the use of the words "coordinates" or "momenta" is often merely a convenient habit. The Hamilton equations do not require any distinction between coordinates and momenta aside from knowing which set of variables gets the minus sign in the Hamilton equations.

You can check that this transformation is canonical in two additional ways. One is to simply verify that Q and P define a canonical coordinate and momentum:

$$[Q, Q] = 0 = [P, P], \quad [Q, P] = 1.$$

The only non-trivial thing to check is the Poisson bracket between Q and P:

$$[Q, P] = \frac{\partial Q}{\partial q}\frac{\partial P}{\partial p} - \frac{\partial Q}{\partial p}\frac{\partial P}{\partial q} = \frac{\partial p}{\partial q}\frac{\partial(-q)}{\partial p} - \frac{\partial p}{\partial p}\frac{\partial(-q)}{\partial q} = 1.$$

The other way to check the transformation is canonical is to consider the transformation of the phase space Lagrangian. We have:

$$P\dot{Q} - \left[\frac{Q^2}{2m} + V(-P)\right] = -q\dot{p} - \frac{p^2}{2m} - V(q) \;= p\dot{q} - \left[\frac{p^2}{2m} + V(q)\right] + \frac{d}{dt}(-pq).$$

From this relation you can see that the phase space Lagrangian's form is preserved up to a total derivative and with the appropriate relationship between Hamiltonians in two different coordinate systems.

Time evolution as a canonical transformation

We can view time evolution itself as a canonical transformation! Let (q, p) be canonical with Hamiltonian $H = \frac{p^2}{2m}$. This system is the free particle in one dimension. Consider the time-dependent canonical transformation: $(q, p) \longleftrightarrow (Q, P)$ is

$$q = Q + \frac{P}{m}t, \quad p = P$$

with inverse

$$Q = q - \frac{p}{m}t, \quad P = p.$$

Note the physical meaning of the old and new variables: (q, p) represent the values of the coordinates and momenta at time t given that they had values (Q, P) at time $t = 0$. Thus $q(t)$ and $p(t)$ can be viewed as solutions of the Hamilton equations with Hamiltonian $H = \frac{p^2}{2m}$ and initial conditions $q(0) = Q$, $p(0) = P$. With $H(q, p) = \frac{p^2}{2m}$, the canonical nature of the transformation can be checked using Poisson brackets, which I leave to you as an exercise. We will check the canonical transformation here by computing the change in the phase space Lagrangian since this will show us something interesting about the relationship between the Hamiltonians in the different variables. We find (exercise)

$$p\dot{q} - \frac{p^2}{2m} = P\dot{Q} + \frac{d}{dt}\left(\frac{P^2 t}{2m}\right).$$

We see that the transformation is indeed canonical, and that Hamiltonian describing time evolution of the (Q, P) variables *vanishes*! This is because (Q, P) are playing the role of initial data; initial conditions don't change in time. Alterntatively, we have made a change of variables which already implements the dynamics, so the Hamilton equations are simply:

$$\dot{Q} = 0 = \dot{P}.$$

Summary

Canonical transformations are coordinate transformations on phase space such that (with an appropriate redefinition of the Hamiltonian) the equations of motion can still be constructed via the Hamilton equations. Aside from explicitly verifying the definition, we have seen two ways to check whether a transformation is canonical. One way is to check that the canonical transformation preserves the fundamental Poisson bracket relations.

The second way to check that a transformation is canonical is to verify that the phase space Lagrangian changes only up to a total derivative. This latter method also shows how the Hamiltonians in the different coordinate systems are related. If the transformation is time-independent, the Hamiltonians are related simply by substitution according to the change of variables. If the transformation is time-dependent, the Hamiltonian changes by substitution *and* by the sddition of new terms to account for the time dependence which was injected by hand.