Physics 6010, Fall 2010

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 EL equations. The Hamilton equations determine curves in momentum phase space. Since the Hamilton equation 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, 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*

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

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

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

$$q^i = q^i(t), \quad p_i = p_i(t)$$

in momentum phase space.

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.

More on the Phase Space Action Principle

Although the physical interpretation of the ingredients entering $S[q,p]$ are different, *mathematically* the phase space action $S[q,p]$ can be viewed as the same kind of integral we have used before in discussing the calculus of variations, *i.e.,* it is the integral of a Lagrangian which is a function of some "configuration" variables Q^A and some velocity variables $\dot{Q}^A$ where

$$Q^A = (q^i, p_i)$$

and

$$\dot{Q}^A = (\dot{q}^i, \dot{p}_i).$$

Note that for the phase space variational principle the velocities of the momenta, $\dot{p}_i$, do not actually appear in the phase space "Lagrangian" we are interested in.

Because we can view the integrand of the phase space action as a Lagrangian $\mathbf{L}$ on $(Q, \dot{Q})$ space:

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

it will not surprise you to find that the Hamilton equations are the EL equations of $\mathbf{L}$. We have

$$\frac{\partial \mathbf{L}}{\partial q^i} = -\frac{\partial H}{\partial q^i}, \quad \frac{\partial \mathbf{L}}{\partial p_i} = \dot{q}^i - \frac{\partial H}{\partial p_i},$$

and

$$\frac{\partial \mathbf{L}}{\partial \dot{q}^i} = p_i, \quad \frac{\partial \mathbf{L}}{\partial \dot{p}_i} = 0,$$

so that the EL equations for $\mathbf{L}$ are the Hamilton's equations (exercise).

Although the Hamiltonian form of the variational principle is different than the Lagrangian form. It is not hard to understand the relation between the two. The Lagrangian form of the variational principle arises once one has extremized the Hamiltonian action, $S[q, p]$, with respect to p. To understand this, first recall a basic calculus result. Suppose that we want to compute the critical points of a function $F(x, y)$. Of course we must solve the coupled system of equations

$$\frac{\partial F}{\partial x} = 0,$$
$$\frac{\partial F}{\partial y} = 0$$

for the critical points (x_0, y_0). An equivalent procedure is to (1) solve the x equation first:

$$\frac{\partial F}{\partial x} = 0 \Rightarrow x = g(y),$$

(2) substitute into $F(x, y)$ to get a new function

$$f(y) = F(g(y), y)$$

and then (3) find the critical points of $f(y)$:

$$\frac{df}{dy} = 0.$$

This latter step determines y_0; to determine x_0 we simply substitute into g:

$$x_0 = g(y_0).$$

It is a nice calculus exercise to prove that this procedure does correctly find all the critical points provided one can solve $\frac{\partial F}{\partial x} = 0$ for x as a function of y. If this is not possible, *e.g.,* if F is linear in x, then the procedure described above need not work.

Now, an analogous result is occurring when we find the critical points of the phase space action. Suppose that we first vary p_i – thereby getting the EL equations from $\mathbf{L}$ for the degrees of freedom p_i. As we have seen, this gives

$$\dot{q}^i - \frac{\partial H}{\partial p_i} = 0,$$

which will give a relation between momenta and velocities (exercise), which we always assume can be solved to get

$$p_i = p_i(q, \dot{q}, t).$$

Having solved for p_i as functions of the remaining variables, we substitute this expression for p_i into the phase space action $S[q,p]$ thereby obtaining a reduced action on configuration space (exercise)

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

Finding the critical points of $S[q]$ (with fixed endpoint conditions) then gives the configuration space curves $q^i(t)$. The analogy with our calculus model is that F is the phase space action, x is the momentum, y is the coordinate, and f is the configuration space action. Thus the Lagrangian variational principle can be considered as a consequence of the Hamiltonian variational principle.

Canonical Transformations: What are they?

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 the most elegant form of dynamics: the Hamilton-Jacobi formalism (to be discussed later). 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 tranformations 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 $(Q, \dot{Q})$ variables, but has the special form $p\dot{q} - H$. We thus only consider transformations which preserve this form up to a total time derivative.

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

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

where I used the identity

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

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

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, if $H = p^2/2m + V(q)$, then $K = Q^2/2m + V(P)$. We now verify that the transformation is canonical by examining Hamilton's equations in the new variables. We have

$$\dot{Q} = \frac{\partial K}{\partial P} = -\frac{\partial H}{\partial q} = \dot{p},$$

and

$$\dot{P} = -\frac{\partial K}{\partial Q} = -\frac{\partial H}{\partial p} = -\dot{q}.$$

Perfect.

Note that this canonical transformation interchanges the roles of coordinates and momenta! Evidently, whether or not a variable is from 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.

Canonical Transformations: How they work

Now that we have some idea what a canonical transformation is, it is time to see how they are put together. To get at the structure of the canonical transformations we return to the phase space variational principle, in which the allowed paths satisfying Hamilton's equations are critical points of

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

Equally well, we can use

$$S[Q, P] = \int_{t_0}^{t_1} (P_i \dot{Q}^i - K(Q, P, t))\, dt.$$

In each system of canonical coordinates (q^i, p_i) or (Q^i, P_i) the equations of motion come from a Lagrangian as indicated above. Since the two Lagrangians give the same EL equations, they must differ by a total derivative (exercise):

$$p_i \dot{q}^i - H = P_i \dot{Q}^i - K + \frac{dF}{dt}.$$

Here $F = F(Q, P, t)$. From this formula you can see that the key feature of the canonical transformation is that all time derivatives — the "dots" appearing in the $p\dot{q}$ term — go into the $P\dot{Q}$ term and the total derivative. Any left over "undotted" terms are used to relate K and H.

Note that if the transformation $(q, p) \leftrightarrow (Q, P)$ does not depend explicitly upon time there will be no left over undotted terms. In this case H and K are related by just substitution for one set of variables in terms of the other. The function F will not depend explicitly upon t either. In this case we have

$$p_i\dot{q}^i - P_i\dot{Q}^i = \frac{dF}{dt}.$$

Thus canonical transformations are characterized by a function F, which can be viewed as a function of (q, p, t) or of (Q, P, t). In any case, the function F characterizing the canonical transformation will in general depend upon $2n + 1$ variables (coordinates, momenta, time) and is called the *generating function* of the transformation.

Any set of variables (Q, P) such that the action, up to a total derivative, takes the standard "$p\dot{q} - H$" form , for *some* choice of Hamiltonian, are called a set of *canonical variables*. Sometimes one also calls canonical variables "canonical coordinates and momenta", but this is not a particularly apt designation, as will be seen from the example below.

From our discussion above you can see that the Hamiltonian does not play any role in determining if a transformation is canonical. The canonical nature of a transformation is completely determined by what happens to the "$p\dot{q}$" terms. Canonical transformations are defined by the phase space only. We also see that when a transformation is time independent the respective Hamiltonians are related by simple substitution. If the transformation depends upon time, then there will be "undotted" terms which modify the Hamiltonians beyond simple substitution. This makes sense: a coordinate transformation which depends upon time will inject some new time dependence into the variables. The Hamiltonian, which determines the time evolution of the system, must then be adjusted to account for this newly injected time dependence.

Let us return to one of our simple simple examples. Let (q, p) be a set of canonical variables with Hamiltonian $H(q, p, t)$. Consider the transformation

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

This is a canonical transformation in which

$$K(Q, P, t) = H(-P, Q, t), \quad F(Q, P, t) = -PQ.$$

To see this, write

$$\begin{aligned} p\dot{q} - H(q, p, t) &= -Q\dot{P} - H(-P, Q, t) \\ &= P\dot{Q} - K(Q, P, t) + \frac{d(-QP)}{dt}. \end{aligned}$$

Let us see that the point transformation is canonical. We will even allow for time dependence. The claim is that the following transformation is canonical

$$Q^i = Q^i(q,t), \quad q^i = q^i(Q,t),$$

and

$$P_i = \frac{\partial q^j}{\partial Q_i} p_j, \quad p_i = \frac{\partial Q^j}{\partial q^i} P_j.$$

To verify this we compute

$$P_i \dot{Q}^i = \frac{\partial q^j}{\partial Q^i} p_j \left(\frac{\partial Q^i}{\partial q^k} \dot{q}^k + \frac{\partial Q^i}{\partial t} \right)$$

We have

$$\frac{\partial q^j}{\partial Q^i} \frac{\partial Q^i}{\partial q^k} = \delta^j_k,$$

so

$$P_i \dot{Q}^i = p_i \dot{q}^i + p_j \frac{\partial q^j}{\partial Q^i} \frac{\partial Q^i}{\partial t}.$$

Evidently the transformation is canonical and

$$K = H + p_j \frac{\partial q^j}{\partial Q^i} \frac{\partial Q^i}{\partial t} = H - p_j \frac{\partial q^j}{\partial t}.$$

The last equality here follows from

$$q^i(Q(q,t),t) = q^i \quad \Longrightarrow \quad \frac{\partial q^i}{\partial Q_k} \frac{\partial Q^k}{\partial t} + \frac{\partial q^i}{\partial t} = 0.$$

Note that if the point transformation is time independent, then the two Hamiltonians (H and K) are related by simply substituting for the coordinates and momenta.