Hamiltonian Mechanics

January 12, 2016

Perhaps the most beautiful formulation of classical mechanics, and the one which ties most closely to quantum mechanics, is the canonical formulation. In this approach, the position and velocity velocity variables of Lagrangian mechanics are replaced by the position and conjugate momentum, $p_i \equiv \frac{\partial L}{\partial \dot{q}_i}$. It turns out that by doing this the coordinates and momenta are put on an equal footing, giving the equations of motion a much larger symmetry. Here we provide an overview of some of the principal results. More detail, with examples, may be found in my notes on classical mechanics HERE.

1 Hamilton's equations

To make the change of variables, we use a Legendre transformation. This may be familiar from thermodynamics, where the internal energy, Gibb's energy, free energy and enthalpy are related to one another by making different choices of the independent variables. Thus, for example, if we begin with the change in internal energy U with changes in entropy S and volume, V,

$$dU = TdS - PdV$$

where temperature T and pressure P are regarded as functions of S and V, we can define the *enthalpy*,

$$H \equiv U + VP$$

and compute

$$\begin{aligned} dH &= dU + PdV + VdP \\ &= TdS - PdV + PdV + VdP \\ &= TdS + VdP \end{aligned}$$

to achieve a formulation in which T and V are treated as functions of S and P. Similarly, defining the Gibbs free energy as $G(P,T) = U + VP - TU$ interchanges both V with P and S with T.

The same technique works to express Lagrangian mechanics in terms of position and momentum. We have the Lagrangian, $L(q_i, \dot{q}_i)$, dependent on N positions and N velocities, and wish to find a function $H(q_i, p_i)$ by exchanging the velocities for the corresponding momenta, $p_i \equiv \frac{\partial L}{\partial \dot{q}_i}$. Therefore, set

$$H(q_i, p_i) \equiv \sum_{i=1}^{N} p_i \dot{q}_i - L \tag{1}$$

Then, with the differential of L given by

$$dL = \sum_{i=1}^{N} \frac{\partial L}{\partial q_i} dq_i + \sum_{i=1}^{N} \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i$$

the differential of the Hamiltonian, H is

$$\begin{aligned} dH &= \sum_{i=1}^{N} \dot{q}_i dp_i + \sum_{i=1}^{N} p_i d\dot{q}_i - dL \\ &= \sum_{i=1}^{N} \dot{q}_i dp_i + \sum_{i=1}^{N} p_i d\dot{q}_i - \sum_{i=1}^{N} \frac{\partial L}{\partial q_i} dq_i - \sum_{i=1}^{N} \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i \\ &= \sum_{i=1}^{N} \dot{q}_i dp_i - \sum_{i=1}^{N} \frac{\partial L}{\partial q_i} dq_i + \sum_{i=1}^{N} \left(p_i d\dot{q}_i - \frac{\partial L}{\partial \dot{q}_i} \right) d\dot{q}_i \end{aligned}$$

so that using the equations of motion and the definition of the conjugate momentum,

$$dH = \sum_{i=1}^{N} \dot{q}_i dp_i - \sum_{i=1}^{N} \dot{p}_i dq_i \tag{2}$$

and therefore a function of the p_i and q_i. Notice that, as it happens, H is of the same form as the energy. To see that we have really eliminated the dependence on velocity we may compute directly,

$$\begin{aligned} \frac{\partial H}{\partial \dot{q}_j} &= \frac{\partial}{\partial \dot{q}_j} \left(\sum_{i=1}^{N} p_i \dot{q}_i - L(q_i, \dot{q}_i) \right) \\ &= \sum_{i=1}^{N} p_i \delta_{ij} - \frac{\partial L}{\partial \dot{q}_j} \\ &= p_j - \frac{\partial L}{\partial \dot{q}_j} \\ &= 0 \end{aligned}$$

The full $2N$-dimensional space of all q_i and p_i is called *phase space*, with coordinates $\xi_A = (q_i, p_j)$.

The equations of motion are already built into the expression above for dH. Since the differential of H may always be written as

$$dH = \sum_{i=1}^{N} \frac{\partial H}{\partial q_j} dq_i + \sum_{i=1}^{N} \frac{\partial H}{\partial p_j} dp_i$$

we can simply equate the two expressions for dH,

$$dH = \sum_{i=1}^{N} dp_i \dot{q}_i - \sum_{i=1}^{N} \dot{p}_i dq_i = \sum_{i=1}^{N} \frac{\partial H}{\partial q_i} dq_i + \sum_{i=1}^{N} \frac{\partial H}{\partial p_i} dp_i$$

Then, since the differentials dq_i and dp_i are all independent, we can equate their coefficients,

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \tag{3}$$

$$\dot{q}_i = \frac{\partial H}{\partial p_j} \tag{4}$$

These are *Hamilton's equations.*

2 Poisson brackets

Suppose we are interested in the time evolution of some function of the coordinates, momenta and time, $f(q_i, p_i, t)$. Such a function is called a *dynamical variable.* A dynamical variable may any function – the area of the orbit of a particle, the period of an oscillating system, or one of the coordinates. The total time derivative of f is

$$\frac{df}{dt} = \sum \left(\frac{\partial f}{\partial q_i} \frac{dq_i}{dt} + \frac{\partial f}{\partial p_i} \frac{dp_i}{dt} \right) + \frac{\partial f}{\partial t}$$

Using Hamilton's equations we may write this as

$$\frac{df}{dt} = \sum \left(\frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right) + \frac{\partial f}{\partial t}$$

If we define the *Poisson bracket* of H and f to be

$$\{H, f\} = \sum_{i=1}^{N} \left(\frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right)$$

Then the total time derivative is given by

$$\frac{df}{dt} = \{H, f\} + \frac{\partial f}{\partial t} \tag{5}$$

If f has no explicit time dependence, so that $\frac{\partial f}{\partial t} = 0$, then the time derivative is given completely by the Poisson bracket,

$$\frac{df}{dt} = \{H, f\}$$

We generalize the Poisson bracket to two arbitrary dynamical variables,

$$\{f, g\} \equiv \sum_{i=1}^{N} \left(\frac{\partial g}{\partial q_i} \frac{\partial f}{\partial p_i} - \frac{\partial g}{\partial p_i} \frac{\partial f}{\partial q_i} \right) \tag{6}$$

The importance of the Poisson bracket stems from the underlying invariance of Hamiltonian dynamics. Just as Newton's second law holds in any inertial frame, there is a class of *canonical coordinates* which preserve the form of Hamilton's equations. One central result of Hamiltonian dynamics is that any transformation that preserves *certain* fundamental Poisson brackets is canonical, and that such transformations preserve *all* Poisson brackets. Since the properties we regard as physical cannot depend on our choice of coordinates, this means that essentially all truly physical properties of a system can be expressed in terms of Poisson brackets.

In particular, we can write Hamilton's equations as Poisson bracket relations. Using the general relation above we have

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

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 list some properties of Poisson brackets. Bracketing with a constant always gives zero

$$\{f, c\} = 0 \tag{7}$$

The Poisson bracket is *linear*

$$\{af_1 + bf_2, g\} = a\{f_1, g\} + b\{f_2, g\} \tag{8}$$

and *Leibnitz*

$$\{f_1 f_2, g\} = f_2\{f_1, g\} + f_1\{f_2, g\} \tag{9}$$

These three properties are the defining properties of a *derivation,* the formal generalization of differentiation. The action of the Poisson bracket with any given function f on the class of all functions, $\{f, \cdot\}$ is therefore a derivation. Indeed, if we define the $2N$-dimensional phase space vector

$$n_A = \left(\frac{\partial f}{\partial p_i}, -\frac{\partial f}{\partial q_j}\right)$$

then the definition of the bracket, eq.(6), shows that $\{f, \cdot\}$ is just the directional derivative in the n_A direction,

$$\{f, g\} = n_A \frac{\partial g}{\partial \xi^A}$$

If we take the time derivative of a bracket, we can easily show

$$\frac{\partial}{\partial t}\{f, g\} = \{\frac{\partial f}{\partial t}, g\} + \{f, \frac{\partial g}{\partial t}\}$$

The bracket is antisymmetric

$$\{f, g\} = -\{g, f\}$$

and satisfies the Jacobi identity,

$$\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0$$

for all dynamical variables f, g and h. These properties are two of the three defining properties of a Lie algebra (the third defining property of a Lie algebra is that the set of objects considered, in this case the space of functions, be a finite dimensional vector space, while the space of functions is infinite dimensional).

Poisson's theorem is of considerable importance not only in classical physics, but also in quantum theory. Suppose f and g are constants of the motion. Then Poisson's theorem states that thier Poisson bracket, $\{f, g\}$, is also a constant of the motion. To prove this result, we start with f and g constant:

$$\frac{df}{dt} = \frac{dg}{dt} = 0$$

Then it follows that

$$\begin{aligned}\frac{df}{dt} &= \{H, f\} + \frac{\partial f}{\partial t} = 0 \\ \frac{dg}{dt} &= \{H, g\} + \frac{\partial g}{\partial t} = 0\end{aligned}$$

Now consider the time derivative of the bracket,

$$\frac{d}{dt}\{f, g\} = \{H, \{f, g\}\} + \frac{\partial}{\partial t}\{f, g\}$$

Using the Jacobi identity on the first term on the right, and the expression for time derivatives on the second term, we have

$$\begin{aligned}
\frac{d}{dt}\{f,g\} &= \{H,\{f,g\}\}+\frac{\partial}{\partial t}\{f,g\} \\
&= -\{f,\{g,H\}\}-\{g,\{H,f\}\}+\frac{\partial}{\partial t}\{f,g\} \\
&= \{f,\{H,g\}\}-\{g,\{H,f\}\}+\left\{\frac{\partial f}{\partial t},g\right\}+\left\{f,\frac{\partial g}{\partial t}\right\} \\
&= \left\{f,-\frac{\partial g}{\partial t}\right\}-\left\{g,-\frac{\partial f}{\partial t}\right\}+\left\{\frac{\partial f}{\partial t},g\right\}+\left\{f,\frac{\partial g}{\partial t}\right\} \\
&= 0
\end{aligned}$$

We now use Poisson brackets to characterize canonical transformations.

3 Canonical transformations

A canonical transformation is a coordinate transformation of phase space, $\xi_A(\chi_B)$ that preserves Hamilton's equations.

Suppose $\xi_A = (x_i, p_j)$ is a set of coordinates in which Hamilton's equations hold. We define fundamental Poisson brackets to be the brackets $\{\xi_A, \xi_B\}$, that is

$$\begin{aligned}
\{x_i,x_j\}_{xp} &= \sum_{k=1}^{N}\left(\frac{\partial x_i}{\partial x_k}\frac{\partial x_j}{\partial p_k}-\frac{\partial x_j}{\partial x_k}\frac{\partial x_i}{\partial p_k}\right) \\
&= 0 \\
\{x_i,p_j\}_{xp} &= \sum_{k=1}^{N}\left(\frac{\partial x_i}{\partial x_k}\frac{\partial p_j}{\partial p_k}-\frac{\partial x_j}{\partial x_k}\frac{\partial p_i}{\partial p_k}\right) \\
&= \sum_{k=1}^{N}\left(\delta_{ik}\delta_{jk}-0\right) \\
&= \delta_{ij} \\
\{p_i,p_j\}_{xp} &= \sum_{k=1}^{N}\left(\frac{\partial p_i}{\partial x_k}\frac{\partial p_j}{\partial p_k}-\frac{\partial p_j}{\partial x_k}\frac{\partial p_k}{\partial p_k}\right) \\
&= 0
\end{aligned}$$

The xp subscript on the bracket indicates that the derivatives are taken with respect to x_i and p_i. Brackets $\{f,g\}_{q\pi}$ taken with respect to the new variables (q_i, π_j) are identical to those $\{f,g\}_{xp}$ with respect to (x_i, p_j) if and only if the transformation is canonical. In particular, replacing f by H and g by any of the coordinate functions (x_i, π_i), we see that Hamilton's equations are preserved by canonical transformations.

The transformation from $\xi_A = (x_i, p_j)$ to $\chi_B = (q_i, \pi_j)$ is canonical if and only if

$$\begin{aligned}
\{q_i,q_j\}_{xp} &= 0 \\
\{q_i,\pi_j\}_{xp} &= \delta_{ij} \\
\{\pi_i,\pi_j\}_{xp} &= 0
\end{aligned} \tag{10}$$

For the proof and examples, see the classical mechanics Notes HERE.

Working with the Hamiltonian formulation of classical mechanics, we are allowed more transformations of the variables than with the Newtonian, or even the Lagrangian, formulations. We are now free to redefine our coordinates according to

$$\begin{aligned} q_i &= q_i(x_i, p_i, t) \\ \pi_i &= \pi_i(x_i, p_i, t) \end{aligned}$$

as long as Hamilton's equations still hold. It is straightforward to show that given any function $f = f(x_i, q_i, t)$ there is a canonical transformation defined by

$$\begin{aligned} p_i &= \frac{\partial f}{\partial x_i} \\ \pi_i &= -\frac{1}{\lambda}\frac{\partial f}{\partial q_i} \\ H' &= \frac{1}{\lambda}\left(H + \frac{\partial f}{\partial t}\right) \end{aligned}$$

The first equation

$$p_i = \frac{\partial f(x_i, q_i, t)}{\partial x_i}$$

gives q_i implicitly in terms of the original variables, while the second determines π_i. Notice that once we pick a function $q_i = q_i(p_i, x_i, t)$, the form of π_i is fixed. The third equation gives the new Hamiltonian in terms of the old one.

Another set of canonical transformations is given by an arbitrary function $g = g(x_i, \pi_i, t)$. In this case, g satisfies

$$\begin{aligned} p_i &= \frac{\partial g}{\partial x_i} \\ q_i &= \frac{1}{\lambda}\frac{\partial g}{\partial \pi_i} \\ H' &= \frac{1}{\lambda}\left(H + \frac{\partial g}{\partial t}\right) \end{aligned} \tag{11}$$

Since canonical transformations can interchange or mix up the roles of x and p, they are called *canonically conjugate*. Within Hamilton's framework, position and momentum lose their independent meaning except that variables always come in conjugate pairs. Notice that this is also a property of quantum mechanics.

4 Hamilton-Jacobi theory

4.1 The action for Hamilton's equations

It is possible to write the action in terms of x_i and p_i and vary these independently to arrive at Hamilton's equations of motion. Starting with $S = \int Ldt$, we replace L with its relationship to H,

$$\begin{aligned} S &= \int Ldt \\ &= \int (p_i\dot{x}_i - H)\,dt \\ &= \int (p_i\mathbf{d}x_i - H\mathbf{d}t) \end{aligned}$$

Since S depends on position and momentum (rather than position and velocity), it is these we vary, and we vary them independently. Thus:

$$\delta S = \delta \int (p_i\dot{x}_i - H)\,dt$$

$$
\begin{aligned}
&= \int \left(\delta p_i \dot{x}_i + p_i \delta \dot{x}_i - \frac{\partial H}{\partial x_i} \delta x_i - \frac{\partial H}{\partial p_i} \delta p_i \right) dt \\
&= p_i \delta x_i \big|_{t_1}^{t_2} + \int \left(\delta p_i \dot{x}_i - \dot{p}_i \delta x_i - \frac{\partial H}{\partial x_i} \delta x_i - \frac{\partial H}{\partial p_i} \delta p_i \right) dt \\
&= \int \left(\left(\dot{x}_i - \frac{\partial H}{\partial p_i} \right) \delta p_i - \left(\dot{p}_i + \frac{\partial H}{\partial x_i} \right) \delta x_i \right) dt
\end{aligned}
$$

and since δp_i and δx_i are independent we conclude

$$
\begin{aligned}
\dot{x}_i &= \frac{\partial H}{\partial p_i} \\
\dot{p}_i &= -\frac{\partial H}{\partial x_i}
\end{aligned}
$$

as required.

4.2 Hamilton's principal function and the Hamilton-Jacobi equation

Properly speaking, the action is a functional, not a function. That is, the action is a function of *curves* rather than a function of *points* in space or phase space. We define *Hamilton's principal function* $\mathcal{S}$ in the following way. Pick an initial point of space and an initial time, and let $\mathcal{S}(x_i^{(f)}, t)$ be the value of the action evaluated along the actual path that a physical system would follow in going from the initial time and place to $x_i^{(f)}$ at time t :

$$
\mathcal{S}(x_i^{(f)}, t) = S \mid_{physical} = \int_{t_0}^{t} L(x_i(t), \dot{x}_i(t), t) dt
$$

where $x_i(t)$ is the solution to the equations of motion and $x_i^{(f)}$ is the final position at time t. This specification of a single curve for each final point gives us a function, not a functional.

Now consider the variation of the action. In general,

$$
\begin{aligned}
\delta S &= \int_{t_0}^{t} \left(\frac{\partial L}{\partial x_i} \delta x_i + \frac{\partial L}{\partial \dot{x}_i} \delta \dot{x}_i \right) dt \\
&= \left[\frac{\partial L}{\partial \dot{x}_i} \delta x_i \right]_{t_0}^{t} + \int_{t_0}^{t} \left(\frac{\partial L}{\partial x_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}_i} \right) \delta x_i dt
\end{aligned}
$$

but we require the equations of motion to hold, we have simply

$$
\delta S \mid_{physical} = \frac{\partial L}{\partial \dot{x}_i} \delta x_i(t) = p_i \delta x_i
$$

This means that the change in the $function$ $\mathcal{S}$, when we change x_i by dx_i is $d\mathcal{S} = \delta S \mid_{physical} = p_i dx_i$ so that $\frac{\partial \mathcal{S}}{\partial x_i} = p_i$.

To find the dependence of $\mathcal{S}$ on t, we write $\mathcal{S} = S \mid_{physical} = \int L dt$ as

$$
\frac{d\mathcal{S}}{dt} = L
$$

But we also have

$$
\frac{d\mathcal{S}}{dt} = \frac{\partial \mathcal{S}}{\partial x_i} \dot{x}_i + \frac{\partial \mathcal{S}}{\partial t}
$$

Equating these and using $\frac{\partial \mathcal{S}}{\partial x_i} = p_i$ gives

$$
\begin{aligned}
L &= \frac{\partial \mathcal{S}}{\partial x_i} \dot{x}_i + \frac{\partial \mathcal{S}}{\partial t} \\
&= p_i \dot{x}_i + \frac{\partial \mathcal{S}}{\partial t}
\end{aligned}
$$

so that the partial of $\mathcal{S}$ with respect to t is

$$\frac{\partial \mathcal{S}}{\partial t} = L - p_i \dot{x}_i = -H$$

Combining the results for the derivatives of $\mathcal{S}$ we may write the differential of $\mathcal{S}$ as

$$\begin{aligned} d\mathcal{S} &= \frac{\partial \mathcal{S}}{\partial x_i} dx_i + \frac{\partial \mathcal{S}}{\partial t} dt \\ &= p_i dx_i - H dt \end{aligned} \tag{12}$$

This is a nontrivial condition on the solution of the classical problem. It means that form $p_i dx_i - H dt$ must be a total differential, which cannot be true for arbitrary p_i and H.

We conclude by stating the crowning theorem of Hamiltonian dynamics: for any Hamiltonian dynamical system there exists a canonical transformation to a set of variables on phase space such that the paths of motion reduce to single points. Clearly, this theorem shows the power of canonical transformations! The theorem relies on describing solutions to the Hamilton-Jacobi equation, which we introduce first.

We have the following equations governing Hamilton's principal function:

$$\begin{aligned} \frac{\partial \mathcal{S}}{\partial p_i} &= 0 \\ \frac{\partial \mathcal{S}}{\partial x_i} &= p_i \\ \frac{\partial \mathcal{S}}{\partial t} &= -H \end{aligned}$$

These equations have the form of eq.(11), and we can show that Hamilton's principal function does generate a canonical transformation. Since the Hamiltonian is a given function of the phase space coordinates and time, $H = H(x_i, p_i, t)$, we combine the last two equations:

$$\frac{\partial \mathcal{S}}{\partial t} = -H(x_i, p_i, t) = -H(x_i, \frac{\partial \mathcal{S}}{\partial x_i}, t) \tag{13}$$

This first order differential equation in $s + 1$ variables $(t, x_i; i = 1, \dots s)$ for the principal function $\mathcal{S}$ is the *Hamilton-Jacobi equation.* Notice that the Hamilton-Jacobi equation has the same general form as the Schrödinger equation (and is equally difficult to solve!). It is this similarity that underlies Dirac's canonical quantization procedure.

It is not difficult to show that once we have a solution to the Hamiltonian-Jacobi equation, we can immediately solve the entire dynamical problem. Such a solution may be given in the form

$$\mathcal{S} = g(t, x_1, \dots, x_s, \alpha_1, \dots, \alpha_s) + A$$

where the α_i are the s constants of integration describing the solution. Now consider a canonical transformation from the variables (x_i, p_i) using the solution $g(t, x_i, \alpha_i)$ as the generating function. We treat the α_i as the new momenta, and introduce new coordinates β_i. Since g depends on the old coordinates x_i and the new momenta α_i, we have the relations

$$\begin{aligned} p_i &= \frac{\partial g}{\partial x_i} \\ \beta_i &= \frac{\partial g}{\partial \alpha_i} \\ H' &= \left(H + \frac{\partial g}{\partial t} \right) \equiv 0 \end{aligned}$$

where the new Hamiltonian vanishes because g satisfies the Hamiltonian-Jacobi equation! With $H' = 0$, Hamilton's equations in the new canonical coordinates are simply

$$\begin{aligned} \frac{d\alpha_i}{dt} &= \frac{\partial H'}{\partial \beta_i} = 0 \\ \frac{d\beta_i}{dt} &= -\frac{\partial H'}{\partial \alpha_i} = 0 \end{aligned}$$

with solutions

$$\begin{aligned} \alpha_i &= const. \\ \beta_i &= const. \end{aligned}$$

The system remains at the phase space point (α_i, β_i). To find the motion in the original coordinates as functions of time and the $2s$ constants of motion, $x_i = x_i(t; \alpha_i, \beta_i)$, we can algebraically invert the s equations $\beta_i = \frac{\partial g(x_i, t, \alpha_i)}{\partial \alpha_i}$. The momenta may be found by differentiating the principal function, $p_i = \frac{\partial \mathcal{S}(x_i, t, \alpha_i)}{\partial x_i}$. This provides a complete solution to the mechanical problem.