(15) Hamiltonian Dynamics

1 Generalizing F = ma, Take 2

You may recall that back in lecture 2, I said there are many ways to generalize, but few bear fruit. As were generalizing F = ma to find the E-L equations, we took a couple of tricky steps which we justified by the resulting success (and the PLA).

from lecture 2

$$\dot{p} = F = -\frac{\partial U}{\partial q} \text{ (ok)}$$

$$\dot{p} = \frac{d}{dt} \left(\frac{\partial T}{\partial \dot{q}} \right) \text{ for } T = \frac{1}{2}m\dot{q}^2 \text{ (tricky)}$$

$$L(q, \dot{q}) = T(\dot{q}) - U(q)$$

$$\Rightarrow \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) = \frac{\partial L}{\partial q} \text{ (just names?)}$$

OR we could have done this differently

$$T = \frac{1}{2}mv^2 \implies T = \frac{p^2}{2m} \Rightarrow \frac{\partial T}{\partial p} = \frac{p}{m} = \dot{q} \quad \text{(tricky)}$$

with $H(p,q) = T(p) + U(q) \quad \text{(just names?)}$
 $\Rightarrow \dot{q} = \frac{\partial H}{\partial p} , \quad \dot{p} = -\frac{\partial H}{\partial q}$

If we now take these equations as fundamental, rather than F = ma, and allow

$$\begin{array}{rcl} H\left(p,q\right) &=& T\left(p,q\right) + U\left(p,q\right) \\ \Rightarrow & p \neq m\dot{q} \quad \text{in general} \end{array}$$

we break the relationship between momentum and velocity. This leaves us with two sets of N independent state variables rather than N coordinates and their time derivatives (less constrained, more flexible, more complicated to use).

2 Lagrangians vs Newtonian mechanics

We started the course with an alternative formulation of mechanics, derived from the principle of least action and which results in the E-L equations, which are equivalent to Newton's 2nd Law.

PLA to E-L $0 = \delta S = \delta \int_{t_1}^{t_2} dt L (q, \dot{q}, t) \Rightarrow \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) = \frac{\partial L}{\partial q_i}$

where we recognize the above as Newtonian 2nd order differential equations where $L = L(q, \dot{q}, t)$ such that $q = \{q_1, ..., q_N\}$ and $\dot{q} = \{\dot{q}_1, ..., \dot{q}_N\}$.

Central to this formulation is the Lagrangian function, which in general is:

$$L = T - U$$

where T is the kinetic energy, and U is the potential energy.

Simple	General
$T = T\left(\dot{q}\right)$	$=T\left(q,\dot{q},t\right)$
$U = U\left(q\right)$	$=U\left(q,\dot{q},t\right)$

This description has advantages over Newtonian mechanics:

- 1. We work with scalars T and U, rather than vectors.
- 2. It's easy to incorporate constraints, and we can avoid discussing force of constraint (tension, forces normal to surface, etc.)
- 3. We always use the same formula independently of our coordinate choice (E-L equations do not depend on generalized coordinate choice)

However, the Lagrangian formulation of mechanics presupposes that the mechanical state of the system is described by specifying its generalized coordinates and velocities. However, this is not the only possible mode of description.

3 Hamiltonian Mechanics

In Hamiltonian mechanics, we describe the state of the system in terms of the generalized coordinates and momenta. (Unlike Lagrangian mechanics, the connection between coordinates and momenta is not obvious.) Lagrangian and Hamiltonian mechanics are equivalent descriptions for many problems, and while the Lagrangian formulation often provides easier solutions to mechanics problems, the Hamiltonian description is a stepping stone to other areas of modern physics: phase space and Liouville's theorem are useful in statistical mechanics, Poisson brackets and time-translation with the Hamiltonian have analogies in quantum mechanics, and Hamilton-Jacobi theory leads to a more general formulation of mechanics (8.09!).

Lagrangian: $L = L(q, \dot{q}, t)$ Hamiltonian: H = H(p, q, t)

So we have to transform $L(q, \dot{q}, t) \rightarrow H(p, q, t)$ without losing any information! This passage from one set of independent variables to another is done by means of Legendre's transformation.

4 Mathematics of the Legendre Transform

Generally, a function expresses a relation between two parameters: an independent variable or control parameter (x) and a dependent variable or function F. This information is encoded in the functional form of F(x).

In some circumstances, it is useful to encode the information encoded in F(x) in a different way. Two common examples are the Fourier transform and the Laplace transform. These express the function F as sums of exponentials to display the information in F in terms of the amount of each component contained in the function rather than in terms of the value of the function.

Given a function F(x), the LT provides a more convenient way of encoding the information in the function when two conditions are met:

- 1. The function is strictly convex (second derivative never changes sign or is zero and is smooth).
- 2. It is easier to measure, control, or think about the derivative of F with respect to x than it is to measure or think about x itself.

Because of condition 1, the derivative of F(x) with respect to x can serve as a stand-in for x, that is there's a one-to-one mapping between x and $\frac{dF}{dx}$. The LT shows how to create a function that contains the same information as F(x) but as a function of $\frac{dF}{dx}$.

Slope Function

$$s(x) = \frac{dF(x)}{dx} \quad , \quad x \iff s$$

Because F(x) is convex, s(x) is a strictly monotonic function of x. In other words,

there is a unique value of the slope s(x) for each x, and vice versa

The Legendre's Transform of F(x) is a function of x, namely:

$$G(s(x)) = s(x) x - F(x)$$



Furthermore, given the one-to-one relationship between x and s, we invert them and express x(s). In this way, we start with s as the independent variable.

$$G(s) = s x(s) - F(x(s))$$

or $F(x) + G(s) = s x$

This symmetric expression makes it more natural to appreciate that F and G are equivalent, **but** we should be careful with this equation. In reality only one variable is independent, either s or x. So this should read either:

$$F(x) + G(s(x)) = s(x) x$$

or
$$F(x(s)) + G(s) = s x(s)$$

Some properties of the LT

The LT of
$$G(s)$$
 is $F(x)$
 $F(x(s)) = x(s) s - G(s)$
and $x(s) = \frac{dG}{ds}$

Let's prove this. Take $\frac{d}{ds}$ of G(s):

$$\frac{dG(s)}{ds} = x(s) + s\frac{dx(s)}{ds} - \frac{dF(x(s))}{ds}$$
$$= x(s) + s\frac{dx(s)}{ds} - \underbrace{\frac{dF}{dx}}_{s}\frac{dx(s)}{ds} = x(s)$$

For example:

$$F(x) = \frac{1}{2}mx^2 , \quad s(x) = \frac{dF}{dx} = mx \Rightarrow x(s) = \frac{s}{m}$$

$$G(s) = s x(s) - F(x(s))$$

$$= s\frac{s}{m} - \frac{1}{2}m\left(\frac{s}{m}\right)^2 = \frac{s^2}{2m}$$

5 Back to Physics

Take the simple Lagrangian:

Simple Lagrangian

$$L(q,\dot{q}) = \frac{1}{2}m\dot{q}^2 - U(q)$$

The Hamiltonian is the Legendre's Transform of the Lagrangian:

Hamiltonian

$$H(p,q) = p \dot{q}(p) - L(q, \dot{q}(p))$$

$$s(x) = \frac{dF(x)}{dx} \rightarrow p = \frac{\partial L(q, \dot{q})}{\partial \dot{q}} = m\dot{q}$$

$$\Rightarrow \dot{q}(p) = \frac{p}{m} \Rightarrow L(q, \dot{q}(p)) = \frac{p^2}{2m} - U(q)$$

$$H(p,q) = \frac{p^2}{m} - \frac{p^2}{2m} + U(q) = \frac{p^2}{2m} + U(q)$$

In this simple case, H = T + U = E. As noted earlier in the course, this is not always the case. With a somewhat more general Lagrangian, we get

$$L(q, \dot{q}) = \frac{1}{2}m(q)\dot{q}^{2} + T_{R}(q) - U(q)$$
$$H(p, q) = \frac{p^{2}}{2m(q)} - T_{R}(q) + U(q)$$

where $H \neq E$. This sort of thing can happen in a rotating coordinate system (e.g., the flyball governor problem), where H is constant, but energy is not conserved.

Generalizing to a system with N degrees of freedom:

N DoF LT

$$L(q_1, q_2, ..., q_N, \dot{q}_1, ..., \dot{q}_N) \rightarrow H(q_1, ..., q_N, p_1, ..., p_N)$$

$$H(p, q) = \sum_i p_i \dot{q}_i(p) - L(q, \dot{q}(p))$$

We are ready now to follow Landau's derivation of the Hamiltonian and canonical equations:

$$L = L(q_i, \dot{q}_i)$$

$$dL = \sum_i \frac{\partial L}{\partial q_i} dq_i + \sum_i \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i$$

$$= \sum_i \dot{p}_i dq_i + \sum_i p_i d\dot{q}_i$$

since $\dot{p}_i = \frac{\partial L}{\partial q_i}$ and $p_i = \frac{\partial L}{\partial \dot{q}_i}$

by definition and by the E-L equations.

product rule
$$\sum p_i d\dot{q}_i = d\left(\sum p_i \dot{q}_i\right) - \sum \dot{q}_i dp_i$$

 $\Rightarrow d\left(\sum p_i \dot{q}_i - L\right) = -\sum \dot{p}_i dq_i + \sum \dot{q}_i dp_i$

The differential on the right is the Hamiltonian, and the above differential equation gives us Hamilton's equations

Canonical Eqns

$$dH = -\sum \dot{p}_i dq_i + \sum \dot{q}_i dp_i$$

$$\Rightarrow \qquad \dot{q}_i = \frac{\partial H}{\partial p_i} \quad , \qquad \dot{p}_i = \frac{-\partial H}{\partial q_i}$$

also known as the "canonical equations".

These are 2N first order differential equations for the 2N unknown function $p_i(t)$ and $q_i(t)$, i = 1, ..., N. By contrast, in the Lagrangian formulation we had N 2nd order differential equations. Note that the use of the Hamiltonian means putting on an equal footing the coordinates and generalized momenta. It also makes the energy the key quantity to worry about.

Comment: In quantum mechanics, where the concept of velocity of a particle is not well defined, it is advantageous to work with momenta, which are well defined.

The total time derivative of the Hamiltonian is:

$$\frac{d}{dt}H = \frac{\partial H}{\partial t} + \sum \frac{\partial H}{\partial q_i}\dot{q}_i + \sum \frac{\partial H}{\partial p_i}\dot{p}_i$$

$$= \frac{\partial H}{\partial t}$$

That is, if H is not an explicit function of time, then H is constant.

As a final sanity check, let's make sure we recover F = ma for a simple problem.

$$T = \frac{p^2}{2m} , \quad H = \frac{p^2}{2m} + U(q)$$

$$\dot{q} = \frac{\partial H}{\partial p} = \frac{p}{m} , \quad \dot{p} = -\frac{\partial H}{\partial q} = -\frac{\partial U}{\partial q}$$

$$m\ddot{q} = -\frac{\partial U}{\partial q} \Rightarrow F = ma$$

And let's look at how we got the effective potential in the Kepler problem. We start by finding the Lagrangian from the Hamiltonian via the Legendre Transform.

$$\begin{split} L(r,\phi,\dot{r},\dot{\phi}) &= p_{r}\dot{r} + p_{\phi}\dot{\phi} - H(p_{r},p_{\phi},r,\phi) \\ H(p_{r},p_{\phi},r,\phi) &= \frac{p_{r}^{2}}{2\mu} + \frac{p_{\phi}^{2}}{2r^{2}\mu} + U(r) \\ \Rightarrow \dot{r} &= \frac{\partial H}{\partial p_{r}} = \frac{p_{r}}{\mu} , \ \dot{\phi} = \frac{\partial H}{\partial p_{\phi}} = \frac{p_{\phi}}{r^{2}\mu} \\ H(r,\phi,\dot{r},\dot{\phi}) &= \frac{1}{2}\mu\dot{r}^{2} + \frac{1}{2}\mu(r\dot{\phi})^{2} + U(r) \\ L(r,\phi,\dot{r},\dot{\phi}) &= (\mu\dot{r})\dot{r} + (\mu r^{2}\dot{\phi})\dot{\phi} - H \\ &= \frac{1}{2}\mu\dot{r}^{2} + \frac{1}{2}\mu(r\dot{\phi})^{2} - U(r) \end{split}$$

Now, what happens if we only transform r, but leave p_{ϕ} . This seems like a good idea because ϕ does not appear in H, so p_{ϕ} must be constant.

$$H(r, \dot{r}, p_{\phi}) = \frac{1}{2}\mu \dot{r}^{2} + \frac{p_{\phi}^{2}}{2r^{2}\mu} + U(r)$$

$$L(r, \dot{r}) = (\mu \dot{r})\dot{r} - H$$

$$= \frac{1}{2}\mu \dot{r}^{2} - \left(\frac{p_{\phi}^{2}}{2r^{2}\mu} + U(r)\right)$$

$$= \frac{1}{2}\mu \dot{r}^{2} - U_{\text{eff}}(r)$$

Thus the effective potential appears naturally when cyclic coordinates in H are not transformed to make L.

So, we now have a new way of approaching problems in mechanics, a clear means of transforming from one approach to the other (e.g., from Lagrangian to Hamiltonian or vice versa with the Legendre Transform). Next, we will learn about the interesting features of the Hamiltonian formalism.

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