# Properties of the Hamiltonian

Monday, 23 September 2013

When is the hamiltonian equal to the total energy?

### Practice with Summation Notation

Recall that Einstein summation notation means that when an index is repeated within a product, it is summed over (unless stated otherwise). For a little practice, let's introduce two more (familiar) symbols, the Kronecker delta

$$\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

and a partial derivative with respect to one of the coordinates (in abbreviated notation)

$$\partial_i \equiv \frac{\partial}{\partial x_i}$$

With these definitions in mind, rewrite in more traditional vector notation and/or interpret the following expressions (a)  $\delta_{ij}v_j$  (b)  $\delta_{ik}v_k$  (c)  $\delta_{lm}x_lv_m$  (d)  $\partial_ix_i$  (e)  $\delta_{ij}\partial_i\partial_j\phi$ 

Answers: (a)  $v_i$  (b)  $v_i$  (same) (c)  $\mathbf{x} \cdot \mathbf{v}$  (d)  $\nabla \cdot \mathbf{x}$  (e)  $\nabla^2 \phi$ 

#### The Hamiltonian

On Friday, you showed that for a function of several dependent variables  $y_i(x)$  and their first derivatives,  $y'_i(x)$ , that satisfy Euler's equation,

$$\frac{\partial f}{\partial y_i} - \frac{d}{dx} \left( \frac{\partial f}{\partial y'_i} \right) = 0$$

that

$$\frac{\partial f}{\partial x} - \frac{d}{dx} \left[ f - y_i' \frac{\partial f}{\partial y_i'} \right] = 0$$

where we employ the summation convention. The proof just requires us to differentiate the term in brackets:

$$\frac{d}{dx}\left[f - y_i'\frac{\partial f}{\partial y_i'}\right] = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y_i}y_i' + \frac{\partial f}{\partial y_i'}y_i'' - y_i''\frac{\partial f}{\partial y_i'} - y_i'\frac{d}{dx}\left(\frac{\partial f}{\partial y_i'}\right)$$
$$= \frac{\partial f}{\partial x} + y_i'\left[\frac{\partial f}{\partial y_i} - \frac{d}{dx}\left(\frac{\partial f}{\partial y_i'}\right)\right]$$

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I hope!

If the dependent variables  $y_i$  satisfy Euler's equation, the term in brackets vanishes, completing the proof.

For dynamics, we have recast the Euler equation to use time as the independent variable and generalized coordinates  $q_i$  as the dependent variables, in which case the same statement is  $\frac{\partial L}{\partial t} - \frac{d}{dt} \left[ L - \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} \right] = 0$ 

We define the hamiltonian as

$$H = \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L \tag{1}$$

from which we deduce that

 $\frac{dH}{dt} = -\frac{\partial L}{\partial t}$ That is, when the Lagrangian is not an explicit function of time, the hamiltonian is conserved—it is a first-integral of motion.

### Other Properties of the Hamiltonian

We have built the lagrangian from the independent variables t,  $q_i$ , and  $\dot{q}_i$ . We now show that the hamiltonian is *not* a natural function of these same variables, but rather of t,  $q_i$ and  $p_i$ , where the generalized momenta are defined by

$$p_i \equiv \frac{\partial L}{\partial \dot{q}_i} \tag{3}$$

Start from Eq. (1)

 $H = \dot{q}_i p_i - L$ 

and take the total differential:

$$dH = \mathbf{p}_i d\dot{q}_i + \dot{q}_i dp_i - \left(\frac{\partial L}{\partial t} dt + \frac{\partial L}{\partial q_i} dq_i + \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i\right)$$
$$= \dot{q}_i dp_i - \frac{\partial L}{\partial q_i} dq_i - \frac{\partial L}{\partial t} dt$$

where the terms in red cancel. On the other hand, if we were to treat the hamiltonian as a function of t,  $q_i$ , and  $p_i$ , then we would write

$$dH = \frac{\partial H}{\partial p_i} dp_i + \frac{\partial H}{\partial q_i} dq_i + \frac{\partial H}{\partial t} dt$$

Comparing these two expressions for dH allows us to identify

$$\frac{\partial H}{\partial p_i} = \dot{q}_i$$

$$\frac{\partial H}{\partial q_i} = -\frac{\partial L}{\partial q_i}$$

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

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Remember, we are using the summation convention.

Definition of generalized momenta.

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Furthermore, for a system that obeys Lagrange's equations of motion, we have two simplifications. First,

$$\frac{\partial L}{\partial q_i} = \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_i} \right) = \frac{dp_i}{dt} = \dot{p}_i$$

so that the canonical equations are

$$\frac{\partial H}{\partial q_i} = -\dot{p}_i \qquad \frac{\partial H}{\partial p_i} = \dot{q}_i \tag{4}$$

These are first-order differential equations in the time for the 2*N* variables  $q_i$  and  $p_i$ . We will talk more later about the implications thereof. Meanwhile, it is nice to look at a very simple example to see if we should salute. Let's pick on the simple harmonic oscillator (mass *m*, spring constant *k*). Then  $T = \frac{1}{2}m\dot{x}^2$ ,  $U = \frac{1}{2}kx^2$  and  $L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2$ .

From the lagrangian we may compute the hamiltonian:

$$H = \dot{x}\frac{\partial L}{\partial \dot{x}} - L = \dot{x}(m\dot{x}) - \frac{1}{2}m\dot{x}^{2} + \frac{1}{2}kx^{2} = \frac{1}{2}m\dot{x}^{2} + \frac{1}{2}kx^{2}$$

However, we really should re-express *H* in terms of *x* and  $p = m\dot{x}$ . This is not hard. We get

$$H = \frac{1}{2}kx^2 + \frac{p^2}{2m}$$

which looks very much like the total energy of the oscillator. That's interesting.

Do the canonical equations work? They are

$$\frac{\partial H}{\partial x} = -\dot{p}$$
 and  $\frac{\partial H}{\partial p} = \dot{x}$ 

or

$$kx = -\dot{p}$$
 and  $\frac{p}{m} = \dot{x}$ 

The first of these is Hooke's law, if we equate  $-\dot{p}$  with the force of the spring. The second is roughly a tautology: mv/m = v. So, Hamilton's canonical equations do indeed describe the motion of this simple system and the hamiltonian seems to be a fancy way of computing the total energy. Is that always the case?

#### When is H = E?

To answer this question, we tear apart carefully the expression that defines the hamiltonian: 2I = 2(T - I)

$$H \equiv \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L = \dot{q}_i \frac{\partial (T - U)}{\partial \dot{q}_i} - (T - U)$$

Now, we have assumed that the potential has no dependence on the velocities, so we may simplify this expression to

$$H = \dot{q}_i \frac{\partial T}{\partial \dot{q}_i} - T + U \tag{5}$$

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One equation has a minus sign. You can remember which by noting that the second equation is really just saying that the derivative of the kinetic energy with respect to momentum is the velocity, which certainly has no negative sign about it. and the question turns on the value of the first term. This term may be expressed in terms of the equation of transformation as

$$T = \frac{1}{2}m\left(\frac{\partial \mathbf{r}}{\partial t} + \frac{\partial \mathbf{r}}{\partial q_j}\dot{q}_j\right) \cdot \left(\frac{\partial \mathbf{r}}{\partial t} + \frac{\partial \mathbf{r}}{\partial q_k}\dot{q}_k\right)$$

where we assume that there is no *explicit* dependence of **r** on the generalized velocities,  $\dot{q}_i$ . When we take a partial derivative of this expression with respect to  $\dot{q}_i$ , we will get nonzero values only when i = j or i = k. That is,

$$\frac{\partial T}{\partial \dot{q}_i} = \frac{m}{2} \left[ \frac{\partial \mathbf{r}}{\partial t} \cdot \frac{\partial \mathbf{r}}{\partial q_i} + \frac{\partial \mathbf{r}}{\partial q_i} \cdot \frac{\partial \mathbf{r}}{\partial t} + \frac{\partial \mathbf{r}}{\partial q_i} \cdot \frac{\partial \mathbf{r}}{\partial q_k} \dot{q}_k + \frac{\partial \mathbf{r}}{\partial q_j} \dot{q}_j \cdot \frac{\partial \mathbf{r}}{\partial q_i} \right]$$
$$= m \left[ \frac{\partial \mathbf{r}}{\partial t} \cdot \frac{\partial \mathbf{r}}{\partial q_i} + \frac{\partial \mathbf{r}}{\partial q_i} \cdot \frac{\partial \mathbf{r}}{\partial q_j} \dot{q}_j \right]$$

Multiplying by  $\dot{q}_i$ , the first term in Eq. (5) is

$$\dot{q}_i \frac{\partial T}{\partial \dot{q}_i} = m \left[ \frac{\partial \mathbf{r}}{\partial t} \cdot \frac{\partial \mathbf{r}}{\partial q_i} \dot{q}_i + \frac{\partial \mathbf{r}}{\partial q_i} \dot{q}_i \cdot \frac{\partial \mathbf{r}}{\partial q_j} \dot{q}_j \right]$$

whereas

$$2T = m \left[ \frac{\partial \mathbf{r}}{\partial t} \cdot \frac{\partial \mathbf{r}}{\partial t} + 2 \frac{\partial \mathbf{r}}{\partial t} \cdot \frac{\partial \mathbf{r}}{\partial q_i} \dot{q}_i + \frac{\partial \mathbf{r}}{\partial q_i} \dot{q}_i \cdot \frac{\partial \mathbf{r}}{\partial q_j} \dot{q}_j \right]$$

The difference is clearly one factor of the blue term and one of the black. That is,

$$\dot{q}_i \frac{\partial T}{\partial \dot{q}_i} = 2T - m \left[ \frac{\partial \mathbf{r}}{\partial t} \cdot \frac{\partial \mathbf{r}}{\partial t} + \frac{\partial \mathbf{r}}{\partial t} \cdot \frac{\partial \mathbf{r}}{\partial q_i} \dot{q}_i \right] = 2T - m \frac{\partial \mathbf{r}}{\partial t} \cdot \left[ \frac{\partial \mathbf{r}}{\partial t} + \frac{\partial \mathbf{r}}{\partial q_i} \dot{q}_i \right]$$

Finally, the term in square brackets is just  $\dot{\mathbf{r}}$ , the total derivative of the position with respect to time. So, the right hand side may be expressed  $2T - \mathbf{p} \cdot \frac{\partial \mathbf{r}}{\partial t}$ . Substituting into Eq. (5) gives

$$H = T + U - \mathbf{p} \cdot \frac{\partial \mathbf{r}}{\partial t}$$

which shows that the Hamiltonian is equal to the total energy only when the equation of transformation has no explicit dependence on the time.

**Exercise 1** Consider once again our typical example of a mass point *m* moving on a parabolic wire,  $z = \alpha \rho^2$ , which is forced to rotate at  $\omega$  about the vertical *z* axis.

- (a) Is the lagrangian an explicit function of time? If not, what can you deduce?
- (b) Write down the equations of transformation,  $\mathbf{r} = \mathbf{r}(t, \rho, \phi, z)$ .
- (c) Compute the hamiltonian. Is it conserved?
- (d) Is the hamiltonian equal to the total energy of the mass point, T + U?
- (e) Compute explicitly the quantity  $\mathbf{p} \cdot \frac{\partial \mathbf{r}}{\partial t}$  and interpret its physical significance.

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Note that I have used a different dummy index of summation for the second term in each parenthesized expression. Why couldn't I use the same one? Because if I used the same one then I could only get terms like  $\dot{q}_1 \frac{\partial \mathbf{r}}{\partial q_1} \cdot \frac{\partial \mathbf{r}}{\partial q_1} \dot{q}_1$ , never  $\dot{q}_1 \frac{\partial \mathbf{r}}{\partial q_1} \cdot \frac{\partial \mathbf{r}}{\partial q_2} \dot{q}_2$ . But the product as written clearly has terms in which the first group has one index and the second a different index.

## Summary

• The motion of a conservative system with *N* degrees of freedom is determined by Lagrange's equations, which take the form

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0 \qquad i = 1, 2, 3, \dots, N$$

where the lagrangian is defined by

$$L(t, q_i, \dot{q}_i) \equiv T(t, q_i, \dot{q}_i) - U(t, q_i)$$

• We can exchange the variables  $\dot{q}_i$  for  $\frac{\partial L}{\partial \dot{q}_i}$  using a Legendre transformation:

$$-H = L - \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} \implies H = \dot{q}_i p_i - L$$

where *H* is the hamiltonian, which is a function of  $(t, q_i, p_i)$ .

- When the lagrangian does not depend *explicitly* on the time, the hamiltonian is a constant of the motion.
- · Hamilton's equations of motion are

$$\frac{\partial H}{\partial q_i} = -\dot{p}_i$$
 and  $\frac{\partial H}{\partial p_i} = \dot{q}_i$ 

They are 2*N* first-order differential equations for the *N* generalized coordinates  $q_i$  and the *N* generalized momenta,  $p_i \equiv \frac{\partial L}{\partial \dot{q}_i}$ .

• When the equations of transformation do not depend explicitly on the time,  $\frac{\partial \mathbf{r}}{\partial t} = 0$ , the hamiltonian is the sum of the kinetic and potential energy (the total energy of the system).

Legendre transformations are ubiquitous in thermodynamics. For example, for a reversible infinitesimal transformation, the internal energy *U* of a compressible system is given by dU = TdS - pdV, which implies that U = U(S, V). Subtracting the total differential of *TS* from both sides yields d(U - TS) = -SdT - pdV, which shows that F = U - TS is a function not of the entropy *S* and *V*, but the temperature *T* and volume *V*.