

Lecture 18: March 13

Instructor: Veit Elser

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18.1 The Hamiltonian formalism

18.1.1 Hamiltonian equations of motion for Cartesian coordinates

We have already encountered the Hamiltonian \mathcal{H} in connection with energy conservation in the Lagrangian formulation of mechanics (lecture 9). Let's review the Lagrangian equations of motion for the special case that all the generalized coordinates are just the Cartesian particle coordinates (*i.e.* no constraints):

$$\mathcal{L} = T - V = \sum_{i=1}^N \frac{1}{2} m_i \dot{x}_i^2 - V(x_1, \dots, x_N). \quad (18.1)$$

We are using the symbol x for all components of the particle positions to keep the notation simpler. For a 3D system N will be a multiple of three, and $m_1 = m_2 = m_3$ is the mass of the particle with 3D coordinates (x_1, x_2, x_3) , *etc.* The equations of motion are the Euler-Lagrange equations for \mathcal{L} :

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{x}_i} \right) = \frac{\partial \mathcal{L}}{\partial x_i} \quad (18.2)$$

$$\frac{d}{dt} (m_i \dot{x}_i) = - \frac{\partial V}{\partial x_i}. \quad (18.3)$$

The Hamiltonian for this system is

$$\mathcal{H} = \sum_i \dot{x}_i \frac{\partial \mathcal{L}}{\partial \dot{x}_i} - \mathcal{L} = \sum_{i=1}^N \frac{1}{2} m_i \dot{x}_i^2 + V(x_1, \dots, x_N). \quad (18.4)$$

In the Hamiltonian formalism the conjugate momenta

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{x}_i} = m_i \dot{x}_i, \quad (18.5)$$

are treated as independent variables rather than the velocities. Using (18.5) we can rewrite \mathcal{H} in terms of x 's and p 's:

$$\mathcal{H}(x_1, \dots, x_N; p_1, \dots, p_N) = \sum_{i=1}^N \frac{p_i^2}{2m_i} + V(x_1, \dots, x_N). \quad (18.6)$$

The key observation that forms the basis of the Hamiltonian formalism is that the partial derivatives of \mathcal{H} have a very simple structure. There are derivatives of two kinds: derivatives with respect to x 's and

derivatives with respect to p 's. Starting with the x derivatives we obtain

$$\frac{\partial \mathcal{H}}{\partial x_i} = \frac{\partial V}{\partial x_i} = -m_i \frac{d}{dt}(\dot{x}_i) = -\dot{p}_i, \quad (18.7)$$

where we have used the equations of motion (18.3) and remembered to use (18.5) for expressing velocities (their time derivatives) in terms of p 's. The p partial derivatives have the following form:

$$\frac{\partial \mathcal{H}}{\partial p_i} = \frac{p_i}{m_i} = \dot{x}_i. \quad (18.8)$$

The two kinds of equations, when written together,

$$\dot{p}_i = -\frac{\partial \mathcal{H}}{\partial x_i} \quad (18.9)$$

$$\dot{x}_i = +\frac{\partial \mathcal{H}}{\partial p_i} \quad (18.10)$$

have an appealing anti-symmetrical structure. They form a system of $2N$ first-order differential equations that evolve the x 's and p 's in time. The Lagrangian equations of motion (18.2), while they accomplish the same thing, are a system of N second-order differential equations. It would be nice if the Hamiltonian equations of motion always had the structure above, just as the Lagrangian equations of motion always have the form (18.2) no matter what generalized coordinates we chose to use. This fact will be verified in the next section.

18.1.2 Hamiltonian equations of motion for generalized coordinates

For a system described by Lagrangian

$$\mathcal{L}(q_1, \dots, q_N; \dot{q}_1, \dots, \dot{q}_N; t), \quad (18.11)$$

the conjugate momenta are defined by

$$p_k = \frac{\partial \mathcal{L}}{\partial \dot{q}_k} = F_k(q_1, \dots, q_N; \dot{q}_1, \dots, \dot{q}_N; t). \quad (18.12)$$

The functions F_k we get upon taking the partial derivative have the N generalized velocities among their arguments. There are N equations $p_k = F_k(\dots)$ that will in principle enable us to express the N \dot{q} 's in terms of only q 's, p 's and t . We can then express the Hamiltonian

$$\mathcal{H} = \sum_{k=1}^N \dot{q}_k p_k - \mathcal{L} \quad (18.13)$$

purely in terms of q 's, p 's and t . We will have to be mindful of this functional dependence in our derivation below.

Let's start by taking partial derivatives with respect to p 's:

$$\frac{\partial \mathcal{H}}{\partial p_l} = \sum_{k=1}^N \frac{\partial \dot{q}_k}{\partial p_l} p_k + \dot{q}_l - \frac{\partial \mathcal{L}}{\partial p_l}. \quad (18.14)$$

For the indicated partial derivatives on the right we need to think of the \dot{q} 's as expressed in terms of q 's, p 's and t . In particular, in the last term there is only one kind of argument of \mathcal{L} (the generalized velocities) that can have p dependence when we use the multi-variable chain rule:

$$\frac{\partial \mathcal{L}}{\partial p_l} = \sum_{k=1}^N \frac{\partial \mathcal{L}}{\partial \dot{q}_k} \frac{\partial \dot{q}_k}{\partial p_l} = \sum_{k=1}^N p_k \frac{\partial \dot{q}_k}{\partial p_l}. \quad (18.15)$$

Substituting this into (18.14), the simple result

$$\frac{\partial \mathcal{H}}{\partial p_l} = \dot{q}_l \quad (18.16)$$

is exactly the generalization of (18.10) we were hoping to find.

For the other kind of partial derivative of \mathcal{H} we begin with

$$\frac{\partial \mathcal{H}}{\partial q_l} = \sum_{k=1}^N \frac{\partial \dot{q}_k}{\partial q_l} p_k - \frac{\partial \mathcal{L}}{\partial q_l}. \quad (18.17)$$

We have to be careful with the last term, which is a partial derivative of \mathcal{L} where p 's and not \dot{q} 's are held fixed. That is, we have to allow for the fact that also the \dot{q} arguments of \mathcal{L} have a q dependence after the \dot{q} 's have been expressed in terms of q 's, p 's and t :

$$\left. \frac{\partial \mathcal{L}}{\partial q_l} \right|_p = \left. \frac{\partial \mathcal{L}}{\partial q_l} \right|_{\dot{q}} + \sum_{k=1}^N \left. \frac{\partial \mathcal{L}}{\partial \dot{q}_k} \right|_q \frac{\partial \dot{q}_k}{\partial q_l}. \quad (18.18)$$

On all the partial derivatives of \mathcal{L} we have added notation to clarify what arguments are being held fixed. The term on the left, with p held fixed, is what we need in the calculation of (18.17) for the Hamiltonian choice of independent variables. The two terms on the right correspond to the usual partial derivatives of \mathcal{L} we calculate in the Lagrangian formalism. Both of these are already known to us in terms of other quantities:

$$\left. \frac{\partial \mathcal{L}}{\partial \dot{q}_k} \right|_q = p_k \quad (18.19)$$

$$\left. \frac{\partial \mathcal{L}}{\partial q_l} \right|_{\dot{q}} = \frac{d}{dt} \left(\left. \frac{\partial \mathcal{L}}{\partial \dot{q}_l} \right|_q \right) = \dot{p}_l. \quad (18.20)$$

In the second of these we used the Lagrangian equations of motion. Substituting these into (18.18) and (18.17), we obtain

$$\frac{\partial \mathcal{H}}{\partial q_l} = \sum_{k=1}^N \frac{\partial \dot{q}_k}{\partial q_l} p_k - \dot{p}_l - \sum_{k=1}^N p_k \frac{\partial \dot{q}_k}{\partial q_l} = -\dot{p}_l. \quad (18.21)$$

This is the generalization of (18.9) we were hoping to find.

Summarizing, the Hamiltonian equations of motion for a system described by N arbitrary generalized coordinates and their corresponding conjugate momenta are

$$\dot{p}_k = -\frac{\partial \mathcal{H}}{\partial q_k} \quad (18.22)$$

$$\dot{q}_k = +\frac{\partial \mathcal{H}}{\partial p_k}. \quad (18.23)$$

The signs are the only thing that might challenge your memory. However, even that is easily reconstructed when you think of the coordinate dependent part of \mathcal{H} being the potential energy V , so that the first equation is just a generalization of the familiar $\dot{\mathbf{p}} = \mathbf{F} = -\nabla V$ from freshman physics.