

## HAMILTONIAN FORMALISM AND LEGENDRE TRANSFORMATIONS

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 2.5; Exercise 2.5.1.

The Lagrangian formulation of classical mechanics is one of two principal formalisms used to obtain equations of motion for a system. The other method is the Hamiltonian formalism. The main difference between the two methods is that the Lagrangian treats the generalized coordinates  $q_i$  and their respective velocities  $\dot{q}_i$  as the independent variables, while in the Hamiltonian formalism, the coordinates and their associated momenta are the independent variables. The momentum  $p_i$  corresponding to a coordinate  $q_i$  is defined by

$$(1) \quad p_i \equiv \frac{dL}{d\dot{q}_i}$$

The Lagrangian is replaced by a function  $H(q, p)$  (where we're using unsubscripted variables  $q$  and  $p$  to represent the sets of coordinates and momenta) with the property that

$$(2) \quad \dot{q}_i = \frac{\partial H}{\partial p_i}$$

The method for transforming from the Lagrangian picture to the Hamiltonian picture is known as a *Legendre transformation* and works as follows. Suppose we start with a function  $f(x_1, x_2, \dots, x_n)$  (here, the  $x_i$  can be any independent variables; we're not considering coordinates explicitly yet) and we want to replace a subset  $\{x_i, i = 1 \dots, j\}$  with different variables  $u_i$ , where

$$(3) \quad u_i \equiv \frac{\partial f}{\partial x_i}$$

We now construct the function

$$(4) \quad g(u_1, \dots, u_j, x_{j+1}, \dots, x_n) \equiv \sum_{i=1}^j u_i x_i - f(x_1, \dots, x_n)$$

We're assuming that all the  $x_i$  in the set  $\{x_i, i = 1 \dots, j\}$  can be written as functions of  $\{u_1, \dots, u_j, x_{j+1}, \dots, x_n\}$ . In other words, when written out in full, 4 contains only the variables  $\{u_1, \dots, u_j, x_{j+1}, \dots, x_n\}$ . We can now take the derivative:

$$(5) \quad \frac{\partial g}{\partial u_i} = x_i + \sum_{k=1}^j \left[ u_k \frac{\partial x_k}{\partial u_i} - \frac{\partial f}{\partial x_k} \frac{\partial x_k}{\partial u_i} \right]$$

$$(6) \quad = x_i + \sum_{k=1}^j \left[ u_k \frac{\partial x_k}{\partial u_i} - u_k \frac{\partial x_k}{\partial u_i} \right]$$

$$(7) \quad = x_i$$

where the second line follows from the definition 3.

To move from the Lagrangian formalism to the Hamiltonian formalism, the Lagrangian plays the role of  $f$ , the generalized velocities  $\dot{q}_i$  are the variables  $\{x_i, i = 1 \dots, j\}$  to be replaced, and the Hamiltonian is the new function  $g$ . That is, we have

$$(8) \quad H(q, p) = \sum_{i=1}^n p_i \dot{q}_i - L(q, \dot{q})$$

There are a total of  $n$  momenta  $p_i$  and  $n$  coordinates  $q_i$ , for a total of  $2n$  independent coordinates. In 8, it is assumed that we can express all the velocities  $\dot{q}_i$  as functions of  $q_i$  and  $p_i$ . With these definitions, we can see by following through the derivation of 7 that 2 is satisfied.

We can get another equation by considering the derivative

$$(9) \quad \frac{\partial H}{\partial q_i} = \sum_{j=1}^n p_j \frac{\partial \dot{q}_j}{\partial q_i} - \frac{\partial L}{\partial q_i} - \sum_{j=1}^n \frac{\partial L}{\partial \dot{q}_j} \frac{\partial \dot{q}_j}{\partial q_i}$$

$$(10) \quad = \sum_{j=1}^n \left[ p_j \frac{\partial \dot{q}_j}{\partial q_i} - \frac{\partial L}{\partial \dot{q}_j} \frac{\partial \dot{q}_j}{\partial q_i} \right] - \frac{\partial L}{\partial q_i}$$

$$(11) \quad = \sum_{j=1}^n \left[ p_j \frac{\partial \dot{q}_j}{\partial q_i} - p_j \frac{\partial \dot{q}_j}{\partial q_i} \right] - \frac{\partial L}{\partial q_i}$$

$$(12) \quad = - \frac{\partial L}{\partial q_i}$$

$$(13) \quad = - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i}$$

$$(14) \quad = - \dot{p}_i$$

In the third line, we used 1, in the fifth line we used the Euler-Lagrange equation

$$(15) \quad \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0$$

and in the last line, we used 1 again. We thus get Hamilton's canonical equations:

$$(16) \quad \frac{\partial H}{\partial p_i} = \dot{q}_i$$

$$(17) \quad -\frac{\partial H}{\partial q_i} = \dot{p}_i$$

[As an aside at this point, I was (and still am) unsure exactly what the term 'canonical' means in this, or in almost any other, context. Google is not very helpful in this respect, as it appears that nobody else really knows where the term came from. According to Wikipedia, the term 'canonical' is used to describe equations in several areas of mathematics, physics and even computer science, but ultimately the term appears to originate in religion, as in 'canon law', which is a system of laws created by the Catholic church. Presumably the term in physics is used to describe some equation or principle which is widely applicable and general. Any other thoughts are welcome in the comments.]

In cases where the potential energy doesn't depend on velocity, the Lagrangian is  $T - V$ , where  $T$  is the kinetic energy. The Hamiltonian (as you've probably guessed) can be interpreted as the total energy of such a system, as we can see as follows.

Using rectangular coordinates, where each mass  $m_i$  has a kinetic energy  $T_i = \frac{1}{2}m_i\dot{x}_i^2$  (this is true in one dimension; to extend to 3 dimensions, we write  $T_i = \frac{1}{2}m_i(\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2)$  and the same argument follows). Thus the momentum is

$$(18) \quad p_i = \frac{\partial L}{\partial \dot{x}_i} = \frac{\partial T}{\partial \dot{x}_i} = m_i\dot{x}_i$$

Thus the first term in 8 is

$$(19) \quad \sum_{i=1}^n p_i\dot{q}_i = \sum_{i=1}^n m_i\dot{x}_i^2 = 2T$$

and the Hamiltonian is

$$(20) \quad H = 2T - L = 2T - T + V = T + V$$

Now consider a more general kinetic energy defined as

$$(21) \quad T = \sum_i \sum_j T_{ij}(q) \dot{q}_i \dot{q}_j$$

That is,  $T$  is a matrix that depends on the positions of the various masses. We have

$$(22) \quad p_k = \frac{\partial L}{\partial \dot{q}_k} = \frac{\partial T}{\partial \dot{q}_k}$$

$$(23) \quad = \sum_i \sum_j T_{ij}(q) \frac{\partial \dot{q}_i}{\partial \dot{q}_k} \dot{q}_j + \sum_i \sum_j T_{ij}(q) \dot{q}_i \frac{\partial \dot{q}_j}{\partial \dot{q}_k}$$

$$(24) \quad = \sum_i \sum_j T_{ij}(q) \delta_{ik} \dot{q}_j + \sum_i \sum_j T_{ij}(q) \dot{q}_i \delta_{jk}$$

$$(25) \quad = \sum_j T_{kj}(q) \dot{q}_j + \sum_i T_{ik}(q) \dot{q}_i$$

$$(26) \quad = \sum_j (T_{kj} + T_{jk}) \dot{q}_j$$

The first term in 8 now becomes

$$(27) \quad \sum_k p_k \dot{q}_k = \sum_k \sum_j (T_{kj} + T_{jk}) \dot{q}_j \dot{q}_k$$

$$(28) \quad = 2T$$

where the last line follows because the RHS of the first line is symmetric under the exchange of  $j$  and  $k$ .

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