

Physics 3550, Fall 2011

The Hamiltonian Formalism.

Relevant Sections in Text: §13.1, 13.2

## Introduction to the Hamiltonian Formalism

To finish the semester we return to formal developments: an introduction to the Hamiltonian formulation of mechanics. This formulation of mechanics is in many ways more powerful than the Lagrangian formulation. Among the advantages of Hamiltonian mechanics we note that: it leads to powerful geometric techniques for studying the properties of dynamical systems; it allows a much wider class of coordinates than either the Lagrange or Newtonian formulations; it allows for the most elegant expression of the relation between symmetries and conservation laws; it leads to many structures that can be viewed as the macroscopic (“classical”) imprint of quantum mechanics.

Although the Hamiltonian form of mechanics is logically independent of the Lagrangian formulation, it is convenient and instructive to introduce the Hamiltonian formalism via transition from the Lagrangian formalism, since we have already developed the latter. (In a more advanced course one would eventually give an *ab initio* development of the Hamiltonian formalism.) The most basic change we encounter when passing from Lagrangian to Hamiltonian methods is that the “arena” we use to describe the equations of motion is no longer the configuration space, but rather the *momentum phase space*. Recall that the Lagrangian formalism is defined once one specifies a configuration space  $Q$  (coordinates  $q^i$ ) and then the velocity phase space  $\Omega$  (coordinates  $(q^i, \dot{q}^i)$ ). The mechanical system is defined by a choice of Lagrangian,  $L$ , which is a function on  $\Omega$  (and possibly the time):

$$L = L(q^i, \dot{q}^i, t).$$

Curves in the configuration space  $Q$  – or in the velocity phase space  $\Omega$  – satisfying the Euler-Lagrange (EL) equations,

$$\frac{\partial L}{\partial q^i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} = 0,$$

define the dynamical behavior of the system. The EL equations shown above are second order; each point of  $\Omega$  defines possible initial conditions for the system. Because solutions are uniquely determined by initial conditions there is a unique curve satisfying the EL equations passing through every point of  $\Omega$ .

A simple, geometrically natural way to define the motion of a system is to define the allowed curves directly by specifying the tangent vectors to these curves at each time. Because there is a unique curve satisfying the EL equations passing through every point

of  $\Omega$ , the set of physically possible curves can be characterized by a *vector field* on  $\Omega$ . The “field lines” of this vector field are the physical motions of the system in  $\Omega$ .<sup>\*</sup> So, we can characterize a dynamical system by a vector field on  $\Omega$ . Ideally, we would like a nice way to characterize this vector field for this or that dynamical system. The Lagrangian formulation is not quite designed to do this. There the arena is the space of positions and velocities,  $(q^i, \dot{q}^i)$ . A curve  $(q^i(t), \dot{q}^i(t))$  has tangent vector  $V$  at time  $t$  given by components  $(\frac{dq^i}{dt}, \frac{d\dot{q}^i}{dt})$ . We have, of course,

$$\frac{dq^i}{dt} = \dot{q}^i,$$

but how do we specify  $\frac{d\dot{q}^i}{dt}$ ? Well, the EL equations *implicitly* define this part of the tangent vector to the curve in velocity phase space, of course, since these equations are second-order in time derivatives, coming from

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} = \frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} \ddot{q}^j + \dots$$

We can isolate the  $\ddot{q}^i$  by multiplying the EL equations by the inverse matrix to  $\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j}$  (which we assume exists). Then we will get an expression of the type

$$\ddot{q}^i = F^i(q, \dot{q}, t),$$

so that the vector field  $V$  in  $\Omega$  defining the dynamics has components given by

$$V = (\dot{q}^i, F^i).$$

This is fine, but not terribly explicit.

As we shall show, we can get a much more explicit – and very simple – description of the motion if we work in the *momentum phase space*. This is the idea behind the Hamiltonian formalism. We shall see that the equations of motion of the system are just the specification of a vector field on the momentum phase space, and this vector field is determined in a very simple way by a single function (the Hamiltonian).

The momentum phase space,  $\Gamma$ , is the space of coordinates and canonical momenta,  $(q^i, p_i)$ . Recall that the canonical momenta can be defined from the Lagrangian via

$$p_i(q, \dot{q}, t) = \frac{\partial L}{\partial \dot{q}^i}.$$

In the Lagrangian formalism we view the canonical momenta as some functions on  $\Omega$  and possibly the time (typically of the form  $p_i = m\dot{q}_i$  for a particle). The motion of the system can be described by

$$\frac{dq^i}{dt} = \dot{q}^i, \quad \frac{dp_i}{dt} = \frac{\partial L}{\partial q^i}.$$

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<sup>\*</sup> Mathematicians call this set of curves the *flow* of the vector field.

Thus you can maybe see that the equations of motion “want” to describe the motion of the system by specifying tangents to curves in *momentum* phase space. But we aren’t there yet. This is because  $L$  is a function on velocity phase space and the partial of  $L$  with respect to  $q^i$  is taken holding  $\dot{q}^i$  fixed. We are in a sort of mixed world involving positions, velocities and momenta, and they are not all independent variables. We need to get the velocities out of the picture. If we can do this, the equations of motion will express the physically allowed motions as curves in  $\Gamma$ :

$$q^i = q^i(t), \quad p_i = p_i(t),$$

these curves being defined by specifying their tangents, *i.e.*, via some equations of the form

$$\frac{dq^i}{dt} = F^i(q, p, t), \quad \frac{dp_i}{dt} = G_i(q, p, t).$$

As we shall see,  $F$  and  $G$  — components of a vector field in  $\Gamma$  — cannot be just anything, but must be obtained in a very particular way. Indeed, we shall now show that, once we get rid of the velocities in favor of the momenta, the differential equations that define these curves are obtained from a single function on  $\Gamma$  (and possibly time),

$$H = H(q, p, t),$$

known as the *Hamiltonian*.

Recall that the EL equations are computed from partial derivatives of the Lagrangian, which appear in the differential

$$dL = \frac{\partial L}{\partial q^i} dq^i + \frac{\partial L}{\partial \dot{q}^i} d\dot{q}^i + \frac{\partial L}{\partial t} dt.$$

Here, of course, the partial derivatives with respect to the coordinates are taken while holding the velocity variables and time fixed, the partials with respect to velocities hold coordinates and time fixed, *etc.* We desire to express these quantities in terms of coordinates and momenta only and translate the EL equations, which are differential equations determining curves in  $(q, \dot{q})$  space, into differential equations determining curves in  $(q, p)$  space. We need a way to pass from expressions which involve derivatives with velocities held fixed (Lagrangian formalism) to expressions with momenta held fixed in the various partial derivatives (Hamiltonian formalism). To do this, we use the *Legendre transformation*, which is perhaps familiar to you from thermodynamics.

To begin, we must assume that the relation

$$p_i(q, \dot{q}, t) = \frac{\partial L}{\partial \dot{q}^i}$$

can be solved to express the velocities in terms of  $(q, p)$  variables:\*

$$\dot{q}^i = \dot{q}^i(q, p, t).$$

We define the Hamiltonian via the *Legendre transformation*

$$H(q, p, t) = p_i \dot{q}^i(q, p, t) - L(q, \dot{q}(q, p, t), t).$$

We then have

$$\begin{aligned} dH &= \dot{q}^i dp_i + p_i d\dot{q}^i - \left( \frac{\partial L}{\partial q^i} \right)_{\dot{q}, t} dq^i - \left( \frac{\partial L}{\partial \dot{q}^i} \right)_{q, t} d\dot{q}^i + \left( \frac{\partial L}{\partial t} \right)_{q, \dot{q}} dt \\ &= \dot{q}^i dp_i - \left( \frac{\partial L}{\partial q^i} \right)_{\dot{q}, t} dq^i + \left( \frac{\partial L}{\partial t} \right)_{q, \dot{q}} dt, \end{aligned}$$

where the subscripts on the partial derivatives emphasize what is being held fixed in the derivative process. The key feature of the Legendre transformation  $L \rightarrow H$  is that the differentials  $d\dot{q}^i$  have dropped out of  $dH$ . Therefore we can compute partials of the Hamiltonian (holding various momentum phase space variables fixed) and easily relate the expressions obtained to partial derivatives that appear in the Lagrangian formalism where velocity phase space variables are fixed. In detail, we have

$$\begin{aligned} \left( \frac{\partial H}{\partial q^i} \right)_{p, t} &= - \left( \frac{\partial L}{\partial q^i} \right)_{\dot{q}, t}, \\ \left( \frac{\partial H}{\partial p^i} \right)_{q, t} &= \dot{q}^i, \\ \left( \frac{\partial H}{\partial t} \right)_{q, p} &= - \left( \frac{\partial L}{\partial t} \right)_{q, \dot{q}}. \end{aligned}$$

*Exercise: Show that the Legendre transformation of the Hamiltonian, in which you eliminate  $p$  in favor of  $\dot{q}$  leads back to the Lagrangian. More generally, show that two successive Legendre transformations (with respect to the same pair of variables) is the identity transformation.*

Using the above relations between various partial derivatives, we can express the equations of motion as conditions on curves  $(q^i(t), p_i(t))$  in momentum phase space via (exercise)

$$\begin{aligned} \dot{q}^i(t) &= \frac{\partial H}{\partial p^i}, \\ \dot{p}_i(t) &= - \frac{\partial H}{\partial q^i}. \end{aligned}$$

\* For this to be possible, at least in a small enough region of  $\Omega$ , it is necessary and sufficient for the *Hessian* matrix,  $\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j}$  to be non-singular.

These are *Hamilton's equations* of motion. As an exercise you can check (using the partial derivative relations above) that the EL equations are satisfied *if and only if* Hamilton's equations are satisfied.

### Key features of the Hamilton equations

Note that the coordinates and momenta are treated *almost* symmetrically in the Hamilton equations. There *is* a key difference between coordinates and momenta, though; note the minus sign in the  $\dot{p}$  equation. This minus sign is really all that distinguishes coordinates from momenta in the Hamiltonian formalism.

On curves in  $\Gamma$  *satisfying the Hamilton equations*, the numerical value of the Hamiltonian is the same as the value of the *canonical energy* on the corresponding curves in  $\Omega$ . Note that the condition for conservation of canonical energy,  $\frac{\partial L}{\partial t} = 0$ , corresponds to  $\frac{\partial H}{\partial t} = 0$ . Despite this relation between the Hamiltonian and the (canonical) energy, I must emphasize *the Hamiltonian is always to be thought of as a function on momentum phase space*.

If the dynamical system has  $n$  degrees of freedom, the Hamilton equations are a set of  $2n$  first-order differential equations. Recall that, in general, the EL equations are a system of  $n$  *second-order* equations for  $n$  unknowns. Thus the passage to the Hamilton equations is an instance of the general rule that a system of  $n$  second order differential equations can be expressed as a system of  $2n$  first order equations (exercise) for  $2n$  variables. There are infinitely many ways to turn  $n$  second order equations into  $2n$  first order equations according to how you define the new  $n$  variables in terms of the velocities. In the Hamiltonian formalism the relation between the new variables – the momenta – and the velocities is determined by the choice of Hamiltonian. In particular, the equation

$$\dot{q}^i = \frac{\partial H}{\partial p_i},$$

gives a relation

$$\dot{q}^i = \dot{q}^i(q, p, t),$$

which can be solved to get

$$p_i = p_i(q, \dot{q}, t).$$

Thus this half of the Hamilton equations reconstructs the relationship between the momenta and the velocities. If you solve Hamilton's equations you will get a solution parametrized by  $2n$  initial values, the initial values of the  $q^i$  and  $p_i$  variables. Since we can always express  $p$  in terms of  $\dot{q}$  and *vice versa*, you see that the initial value problem for the EL equations matches up with that for the Hamilton equations.

The key discovery of Hamilton is that there is a special feature of dynamical systems characterized by a variational principle (Hamilton’s principle), namely, the equations of motion always have a standard – or “canonical” – first order form. This canonical form of the equations specifies the tangent vector,  $(\dot{q}^i(t), \dot{p}_i(t))$ , at each point (specified by  $t$ ) of the curve  $q^i = q^i(t)$ ,  $p_i = p_i(t)$  in terms of partial derivatives of a single function  $H$  on  $\Gamma$  (and possibly the time). The Hamiltonian equations are often referred to as the *canonical equations of motion*. The Hamiltonian formalism that we are developing is often called the *canonical formalism*. The variables  $(q^i, p_j)$  are called the *canonical coordinates and momenta*, or sometimes just *canonical variables*, or *canonical coordinates on the momentum phase space*  $\Gamma$ .

Although we derived the Hamilton equations from the EL equations, the Hamiltonian formalism can be viewed as independent of the Lagrangian formalism. In this point of view, we specify a dynamical system by first defining a phase space  $\Gamma$ , which includes a choice of canonical variables  $(q^i, p_i)$ . (We shall see that there is considerable freedom in specifying these coordinates on  $\Gamma$  for any given dynamical system.) Different dynamical systems may have the same phase space, but different dynamics, so the definition of  $\Gamma$  is purely *kinematical*. To characterize the *dynamical* behavior of the system we specify the Hamiltonian  $H$  as a function on  $\Gamma$  (and possibly time). In a nutshell: a dynamical system is defined by the pair  $(\Gamma, H)$ . Granted a dynamical system, *i.e.*, a pair  $(\Gamma, H)$ , we can use Hamilton’s equations to define the allowed time evolutions of the system, *i.e.*, curves  $(q(t), p(t))$ . In particular, the various derivatives of  $H$  define the motion of the system — as represented by curves in phase space — by specifying the tangent vectors to those curves at each time. Equivalently, the allowed curves are the “field lines” of the vector field  $\vec{V}$  on  $\Gamma$  with  $q$ - $p$  components given by

$$\vec{V} = (V^{q^i}, V^{p_i}) = \left( \frac{\partial H}{\partial p_i}, -\frac{\partial H}{\partial q^i} \right).$$

From this point of view, the “art” of the physicist is to take a dynamical system of interest from nature and devise a suitable phase space and Hamiltonian to model it.

## Examples

Let us examine some familiar dynamical systems using the Hamiltonian formalism.

### *Particle in a Force Field*

A particle with position vector  $\vec{r}$  moves in a force field derivable from a potential  $V(\vec{r}, t)$ . The Lagrangian is

$$L = \frac{1}{2}m\dot{\vec{r}}^2 - V(\vec{r}, t).$$

The canonical momentum has Cartesian components given by

$$p_i = \frac{\partial L}{\partial \dot{x}^i} = m\dot{x}_i,$$

so that

$$\vec{p} = m\dot{\vec{r}} \iff \dot{\vec{r}} = \frac{\vec{p}}{m}.$$

The Hamiltonian is

$$\begin{aligned} H &= \vec{p} \cdot \dot{\vec{r}} - L \\ &= \vec{p} \cdot \left( \frac{\vec{p}}{m} \right) - \left[ \frac{p^2}{2m} - V \right] \\ &= \frac{p^2}{2m} + V. \end{aligned}$$

The Hamilton equations are

$$\begin{aligned} \dot{x}^i &= \frac{\partial H}{\partial p_i} = \frac{p_i}{m}, \\ \dot{p}_i &= -\frac{\partial H}{\partial x^i} = -\frac{\partial V}{\partial x^i}, \end{aligned}$$

so that

$$\begin{aligned} \dot{\vec{r}} &= \frac{\vec{p}}{m} \\ \dot{\vec{p}} &= -\nabla V. \end{aligned}$$

These equations are equivalent to the EL equations, *i.e.*, to Newton's second law (exercise). In particular, the first equation gives the relation between velocity and momentum, with this result in hand the second equation gives the law of motion.

Note that if a coordinate is absent from the Hamiltonian (so that  $H$  is translationally invariant with respect to that coordinate), then the corresponding momentum component will be conserved (exercise). This is easily seen to be a general rule since  $n$  of the Hamilton equations are:

$$\dot{p}_i = \frac{\partial H}{\partial q^i}.$$

In the special case of a Newtonian particle the cyclic coordinate simply indicates the component of force in the corresponding direction in configuration space is zero. But, again, the result applies to any Hamiltonian system.

We will later explore the general relation between symmetries and conservation laws from the Hamiltonian point of view.

*Spherical pendulum*

The Lagrangian for a spherical pendulum of mass  $m$  and length  $R$  in a uniform gravitational field takes the form

$$L = \frac{1}{2}mR^2(\dot{\theta}^2 + \sin^2\theta\dot{\phi}^2) - mgR\cos\theta.$$

Here we have oriented the  $z$  axis of spherical coordinates to point upward, *i.e.*, against the gravitational force field. The canonical momenta are

$$\begin{aligned} p_\theta &= mR^2\dot{\theta}, \\ p_\phi &= mR^2\sin^2\theta\dot{\phi}. \end{aligned}$$

The Hamiltonian is

$$\begin{aligned} H &= p_\theta \left( \frac{p_\theta}{mR^2} \right) + p_\phi \left( \frac{p_\phi}{mR^2\sin^2\theta} \right) - \left[ \frac{p_\theta^2}{2mR^2} + \frac{p_\phi^2}{2mR^2\sin^2\theta} - mgR\cos\theta \right] \\ &= \frac{p_\theta^2}{2mR^2} + \frac{p_\phi^2}{2mR^2\sin^2\theta} + mgR\cos\theta. \end{aligned}$$

The Hamilton equations are

$$\begin{aligned} \dot{\theta} &= \frac{p_\theta}{mR^2}, \\ \dot{\phi} &= \frac{p_\phi}{mR^2\sin^2\theta}, \\ \dot{p}_\theta &= \frac{p_\phi^2\cos\theta}{mR^2\sin^3\theta} + mgR\sin\theta, \\ \dot{p}_\phi &= 0. \end{aligned}$$

You can check that this system of equations is equivalent to the equations of motion obtained via Newton's second law or via the EL equations. Note that, because  $\phi$  is absent in  $H$ , we get conservation of  $p_\phi$ . Using the  $\dot{\phi}$  Hamilton equation, you can see that this is conservation the  $z$ -component of angular momentum (exercise).

### Example: Particle in a given electromagnetic field

The Lagrangian for a particle of mass  $m$  and charge  $q$  in a given electromagnetic field  $(\vec{E}(\vec{r}, t), \vec{B}(\vec{r}, t))$  is given by\*

$$L = \frac{1}{2}m\dot{\vec{r}}^2 + \frac{q}{c}\vec{A} \cdot \dot{\vec{r}} - q\phi,$$

where  $(\phi, \vec{A})$  are any set of potentials for the given  $\vec{E}$  and  $\vec{B}$ :

$$\vec{E} = -\frac{1}{c}\frac{\partial\vec{A}}{\partial t} - \nabla\phi,$$

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\* We use Gaussian units.



$$\vec{B} = \nabla \times \vec{A}.$$

The canonical momentum is (exercise)

$$\vec{p} = m\dot{\vec{r}} + \frac{q}{c}\vec{A},$$

The Hamiltonian is (exercise)

$$H = \frac{(\vec{p} - \frac{q}{c}\vec{A})^2}{2m} + q\phi.$$

There are a few things to note here. On solutions to the Hamilton equations (where the momenta and velocities are related as above), the term  $\frac{(\vec{p} - \frac{q}{c}\vec{A})^2}{2m}$  is the mechanical kinetic energy of the particle (exercise). Thus, the vector potential appears in the Hamiltonian as a function on phase space, but the vector potential makes no contribution to the numerical value of the canonical energy. This is a manifestation of the fact that the magnetic field does no work (exercise).

Next, note that the values of the canonical momentum have no immediate physical significance. This is because it differs from the (physically meaningful) mechanical momentum  $m\vec{v}$  by the vector potential, which is not directly observable. In detail, recall that the potentials are not uniquely associated to an electromagnetic field. Any two sets of potentials,  $(\phi, \vec{A})$  and  $(\phi', \vec{A}')$ , related by a gauge transformation:

$$\phi' = \phi - \frac{1}{c} \frac{\partial \Lambda}{\partial t},$$

$$\vec{A}' = \vec{A} + \nabla \Lambda,$$

where  $\Lambda(\vec{r}, t)$  is *any* function of the indicated variables, correspond to the same  $\vec{E}$  and  $\vec{B}$  (exercise). Thus the potentials are not uniquely determined by physical effects: the potentials are not physically measurable. Because the canonical momentum relies upon  $\vec{A}$  for its definition, both the functional relation between canonical momentum, coordinates and velocities and the numerical value of  $\vec{p}$  along any motion of the particle is gauge-dependent, *i.e.*, not physically observable.

The Hamiltonian also suffers from this problem. Even though the *numerical value* of the term  $\frac{(\vec{p} - \frac{q}{c}\vec{A})^2}{2m}$  is gauge invariant when  $\vec{p}$  is related to the velocity via Hamilton's equations, this term renders the functional form of the Hamiltonian to be very much gauge-dependent. Moreover, the presence of the scalar potential also makes the functional form and the value of the Hamiltonian gauge-dependent. Because of this, only in specialized situations does the numerical value of  $H$  have a direct physical meaning. For example, for purely magnetic fields we can choose  $\phi = 0$ ; then the value of  $H$  is the mechanical kinetic

energy, which is observable. Another situation where the value of the Hamiltonian has a physical interpretation arises if we consider static electromagnetic fields. Then we can choose potentials that are time independent and this means that we can only make gauge transformations in which

$$\Lambda = \Lambda(\vec{r}), \quad \text{or} \quad \Lambda = (\text{const.})t.$$

In this case, because  $t$  will not appear explicitly in  $H$ , we know that  $H$  will be a conserved quantity – the energy. The value of the kinetic energy still has gauge invariant meaning, but its functional form is gauge dependent. In the static case the potential  $\phi$  can be constructed in a nearly gauge invariant manner from the electric field via

$$\phi = \int_C \vec{E} \cdot d\vec{l}.$$

where  $C$  is a contour from some arbitrary reference point to the point where we are computing the value of  $\phi$ . For static fields  $\nabla \times \vec{E} = 0$ , so the choice of  $C$  is irrelevant. The choice of reference point reflects the freedom to add a constant to  $\phi$ ; clearly this freedom cannot be avoided. The freedom to add a constant to  $\phi$  is all the gauge freedom left in the static case. Thus,  $H$  is *still* not measurable, but differences in canonical energy are measurable in the static case.

Note that, in any case, the functional form of the Hamiltonian will always be gauge dependent (even if its value has a gauge invariant meaning!). Nevertheless, the Hamilton equations reproduce the Lorentz force law. This means that, while the Hamiltonian is a gauge-dependent function on the phase space, the Hamilton equations are gauge invariant. We will get a deeper understanding of this fact when we study canonical transformations.

### Ignorable coordinates and conservation laws

Our basic results on cyclic coordinates and conservation laws is easily seen to hold in the Hamiltonian formalism. Our Legendre transformation showed us that

$$\frac{\partial L}{\partial q^i} = -\frac{\partial H}{\partial q^i}, \quad \frac{\partial L}{\partial t} = -\frac{\partial H}{\partial t}.$$

Thus, if a particular coordinate or time is absent (ignorable) in the Lagrangian it will also be absent in the Hamiltonian, and conversely. If a coordinate, say  $q^1$  is absent, its Hamilton equations tell us that

$$\dot{p}_1 = -\frac{\partial H}{\partial q^1} = 0.$$

Thus we recover the connection between ignorable coordinates and conservation laws.

Likewise, if  $H$  is explicitly time independent, then we know it will be conserved. This follows in a very nice way from Hamilton's equations. We always have

$$\frac{dH}{dt} = \frac{\partial H}{\partial q^i} \dot{q}^i + \frac{\partial H}{\partial p_i} \dot{p}_i + \frac{\partial H}{\partial t}.$$

Assuming the last term vanishes ("the Hamiltonian has no explicit time dependence"), and restricting this identity to a phase space curve satisfying Hamilton's equation, we get

$$\frac{dH}{dt} = \frac{\partial H}{\partial q^i} \frac{\partial H}{\partial p_i} + \frac{\partial H}{\partial p_i} \left( -\frac{\partial H}{\partial q^i} \right) = 0.$$