The Hamiltonian

In the Hamiltonian formulation of dynamics each second order ODE given by the Euler-Lagrange equation in terms of the Lagrangian is replaced by two first order ODEs for the coordinate and the conjugate momentum given by derivatives of the Hamiltonian.

The Hamiltonian is defined (as we have seen before) by

$$H(q_i, p_i, t) = \sum_k p_k \dot{q}_k - L(q_i, \dot{q}_i, t), \quad p_k = \frac{\partial L}{\partial \dot{q}_k},$$

where the last equation is inverted to give $\dot{q}_k$ in terms of other coordinates and momentum so that the Hamiltonian is investigated as a function of the independent variables $\{q_i\}, \{p_i\}, t$.

This is an important point: the Lagrangian is considered to be a function of coordinates and velocities (and maybe time) whereas the Hamiltonian is considered to be a function of coordinates and conjugate momenta (and maybe time).

This transformation is invertible; you can go both directions: $L[q, \dot{q}, t] \Leftrightarrow H[q, p, t]$ and $\dot{q} = \dot{q}(q, p) \Leftrightarrow p$. In fact, it is possible to apply the Legendre transform to some of the $\dot{q}_k$'s into $p_k$ for Hamiltonian dynamics, and leave others as $\dot{q}_k$'s for Lagrangian dynamics, and there can be good reasons for doing that; see the discussion of the Routhian, below.

Legendre transformations

The transformation $L(q_i, \dot{q}_i, t) \Rightarrow H(q_i, p_i, t)$ is an example of a Legendre transformation for changing independent variables. Most simply for a function $f(x)$ the Legendre transformation $f(x) \rightarrow B(s)$ takes the form

$$B(s) = xs - f(x) \quad \text{with} \quad s = \frac{df}{dx},$$

where the last equation is inverted to calculate $x(s)$. (This is always possible if $f(x)$ is a convex function, i.e. the curvature is everywhere of the same sign.) Note the geometrical interpretation: $s$ is the slope of the tangent to $f(x)$ at $x$, and $-B$ is the intercept of this tangent with the ordinate — see Hand and Finch, Fig. 5.3. Thus $B(s)$ specifies the same curve in terms of the tangents defined in slope-intercept form. The inverse transformation takes exactly the same form

$$f(x) = sx - B(s) \quad \text{with} \quad x = \frac{dB}{ds},$$

where the last relation can be seen by explicitly differentiating $B(s)$ in Eq. (2). A Legendre transformation (rather than say $C(z) = f(x(z))$ for some arbitrary choice of $z(x)$) has the advantage that for a convex function the inverse can always be found and no information about the function is lost. Legendre transformations are used in thermodynamics, e.g. from Helmholtz to Gibbs free energies

$$F(T, V) \Rightarrow H(T, P) = F + PV \quad \text{with} \quad P = -\frac{\partial F}{\partial V},$$

$$
(the sign differences from Eq. (2) are inessential differences due to conventions in the definitions of the various quantities).

**Hamiltonian equations of motion**

For simplicity, consider only one degree of freedom, so \( k = 1 \) and we drop the subscript \( k \): \( H[q,p,t] = p\dot{q} - L[q,\dot{q},t] \), where we use \( \dot{q}(q,p) \). Everything proceeds the same if you put subscript \( k \) everywhere, because this formalism assumes that the functions can be varied independently. The partial derivatives are:

\[
\frac{\partial H}{\partial q} = p \frac{\partial \dot{q}}{\partial q} - \left( \frac{\partial L}{\partial q} + \frac{\partial L}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial q} \right) = -\frac{\partial L}{\partial q} = -\dot{p},
\]

where we have used the definition of the conjugate momentum \( p \equiv \frac{\partial L}{\partial \dot{q}} \), and the E-L equation \( \dot{p} = \frac{\partial L}{\partial q} \).

\[
\frac{\partial H}{\partial p} = \dot{q} + p \frac{\partial \dot{q}}{\partial p} - \left( \frac{\partial L}{\partial p} + \frac{\partial L}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial p} \right) = \dot{q},
\]

where we have used \( \partial L/\partial p = 0 \) (or equivalently, \( (\partial L/\partial q)(\partial q/\partial p) = 0 \) because \( q \) and \( p \) are independent variables), and \( \partial L/\partial q = p \). Finally, we can compute the partial derivative with respect to \( t \), taking into account only the explicit time dependence of the Lagrangian, not the implicit time dependence associated with \( q(t), p(t), \dot{q}(t) \): \( \partial H/\partial t = -\partial L/\partial t \).

Adding the \( k \) subscripts back in, we have:

\[
\frac{\partial H}{\partial p_k} = \dot{q}_k, \quad \frac{\partial H}{\partial q_k} = -\frac{\partial L}{\partial q_k}, \quad \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}.
\]

Remember in these partials the other independent variables are held fixed, so that \( \partial L/\partial t \) means \( (\partial L/\partial t)_{\{q_k,\dot{q}_k\}} \) whereas \( \partial H/\partial t \) means \( (\partial H/\partial t)_{\{q_k,\dot{p}_k\}} \), etc. Together with the Euler-Lagrange equation, Eq. (7) gives us the *Hamiltonian equations of motion*

\[
\dot{q}_k = \frac{\partial H}{\partial p_k}
\]

\[
\dot{p}_k = -\frac{\partial H}{\partial q_k}
\]

as well as the total derivative, using Hamilton’s equations:

\[
\frac{dH}{dt} = \frac{\partial H}{\partial q} \frac{dq}{dt} + \frac{\partial H}{\partial p} \frac{dp}{dt} + \frac{\partial H}{\partial t} = -\dot{p} \dot{q} + \dot{q} \dot{p} + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t}.
\]

Since \( \partial H/\partial t = -\partial L/\partial t \) we see (again) that the Hamiltonian is a constant of the motion \( (dH/dt = 0 \) so that \( H = \text{constant} = E) \) if \( L \) (and so \( H \)) is not an explicit function of time.

Ignorable coordinates are particularly simple in the Hamiltonian formulation: if the Hamiltonian does not depend on some coordinate \( q_m \) (which via Eqs. (7) corresponds to the Lagrangian not depending on that coordinate) then from Eq. (9) the corresponding momentum \( p_m \) is a constant of the motion. The dynamics of \( q_m \) is then given by Eq. (8).
Hamilton’s Principle

The action is defined in terms of the Lagrangian:  \( S = \int L dt \) and we allow it to vary by varying the path \( q(t) \):  \( \delta S = \int (\delta L/\delta q) \delta q dt = 0 \). Recall from Lecture 2 that \((\delta L/\delta q)\) actually involves both \( q \) and \( \dot{q} \), because when we vary the path \( q(t) \), we are also varying the path \( \dot{q}(t) \) at the same time; they can’t be varied independently.

By contrast, if we re-express Hamilton’s principle of least action in terms of the Hamiltonian instead of the Lagrangian,

\[
S = \int \sum_k [p_k \dot{q}_k - H(\{q_k\}, \{p_k\}, t)] dt, \quad (11)
\]

we can show that \( \delta S = \) for independent variations of either \( q(t) \) or \( p(t) \):

\[
L[q, \dot{q}] = p\dot{q} - H[q, p] \Rightarrow \delta L = p\delta \dot{q} + \dot{q}\delta p - \frac{\partial H}{\partial q} \delta q - \frac{\partial H}{\partial p} \delta p. \quad (12)
\]

Now (as in Lecture 2) we integrate by parts to get rid of \( \delta \dot{q} \), noting that the endpoints of the integral are fixed, so the “surface” term drops out and thus \( p\delta \dot{q} = -q\delta \dot{p} \). Collecting terms:

\[
\delta L = \left( \dot{q} - \frac{\partial H}{\partial p} \right) \delta p + \left( \ddot{p} + \frac{\partial H}{\partial q} \right) \delta q. \quad (13)
\]

Hamilton’s equations tell us that the two terms in the parentheses are zero, so we have that \( \delta L = 0 \) and thus \( \delta S = 0 \) (Hamilton’s principle) for independent variations \( \delta q \) and \( \delta p \), with \( \delta q \) zero at the beginning and end as usual, but no restriction on \( \delta p \) at the beginning and end.

Since \( q(t_0) \) and \( p(t) \) can be varied independently (in contrast to \( q \) and \( \dot{q} \)), it is particularly easy to evolve them in phase space.

Phase space

Plotting the \((\{q_k(t)\}, \{p_k(t)\})\) trajectories in the 2N dimensional phase space for N degrees of freedom \( q_k \) gives a nice picture of the dynamics.

We can (abstractly) denote the dynamical variables (functions of time) in phase space as \( \vec{z} = (\{q_k\}, \{p_k\}) \) where the vector on top of \( z \) lives in that 2N-dimensional phases space. We can also combine the 2N functions \( \partial H/\partial p_k \) and \( \partial H/\partial q_k \) as \( \vec{f}(\vec{z}) \), so that the Hamiltonian dynamics of a point in phase space is given by \( \vec{\dot{z}} = \vec{f}(\vec{z}) \). This system of 2N first-order ODEs expresses all of classical physics in phase space.

Once one has defined a set of \( q \)’s and \( p \)’s in a Hamiltonian \( H \) that describe a physical system (incorporating all symmetries, constraints, and appropriate choice of coordinate system), their initial conditions are a single point in the 2N-dimensional phase space, and Hamilton’s equations tell you exactly how they evolve in time. That evolution is a phase space trajectory (or orbit) \( \vec{z}(t) \), a path in the 2N-dimensional space parametrized by time.

Notice that because they can vary independently (subject only to Hamilton’s equations), there’s a nice symmetry between the \( q \)’s and \( p \)’s in phase space (in contrast to the \( q \)’s and \( \dot{q} \)’s in the Lagrangian). Indeed, you can swap them: \( q \leftrightarrow p \), and still know how they evolve with time. More generally, you can make a broad range of transformations from \((\{q_k\}, \{p_k\})\) to \((\{Q_k(q_k, p_k)\}, \{P_k(q_k, p_k)\})\) (essentially, a rotation in 2N-dimensional phase space), and
preserve the Hamiltonian dynamics. Such Canonical Transformations, and their usefulness, will be discussed next week.

Note that phase space trajectories cannot cross (either at the same time or at different times). If they did, the point at which they cross would have to have two different values of $\dot{z}$, but Hamilton’s equations only give one such unique value.

### Phase space for the SHO, and for the pendulum

A simple example is the $(x,p)$ phase space of the simple harmonic oscillator:

$$L = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} k x^2, \quad \text{with} \quad p = \frac{\partial L}{\partial \dot{x}} = m \dot{x}. \tag{14}$$

$$H = p \dot{x} - L = \frac{1}{2} m \dot{p}^2 + \frac{1}{2} k x^2 \quad \Rightarrow \quad \ddot{x} = \frac{\partial H}{\partial p} = \frac{p}{m}, \quad \dot{p} = -\frac{\partial H}{\partial q} = -kx. \tag{15}$$

$$\Rightarrow \quad \ddot{x} = \frac{\dot{p}}{m} = -\frac{k}{m} x \equiv -\omega^2 x \quad \Rightarrow \quad x(t) = A \cos(\omega t + \phi), \quad p(t) = -m\omega A \sin(\omega t + \phi) \tag{16}$$

$$H = \frac{1}{2} m \dot{x}^2 + \frac{1}{2} k x^2 = \frac{1}{2} m \omega^2 A^2 \equiv \text{constant} = E. \tag{17}$$

The phase space $(x,p)$ is an ellipse, with area proportional to $A$ and therefore $E$, and the trajectory is a clockwise evolution of a point along the ellipse.

You can also redefine what you mean by $x$ and $p$ to turn it into a circle:

$$H \rightarrow H' = \frac{p^2}{(m\omega A)^2} + \frac{x^2}{A^2} = p'^2 + x'^2 = 1. \tag{18}$$

You can also redefine $x$ and $p$ so that $H = (1/2)(p^2 + x^2)$, and Hamilton’s equations then give $\ddot{x} = p$, $\dot{p} = -x$; particularly simple clockwise motion. Of course, different values of $A$ and therefore $E$ will be circles of different radii; the trajectories can never cross!

A pendulum (mass $m$, length $\ell$, with gravity $g$) has a more complicated Hamiltonian and thus a more complicated set of trajectories in $(\theta, p_\theta)$ phase space:

$$L = T - V = \frac{1}{2} m \ell^2 \dot{\theta}^2 - mg\ell(1 - \cos \theta), \quad \text{with} \quad p_\theta = \frac{\partial L}{\partial \dot{\theta}} = m\ell^2 \dot{\theta}. \tag{19}$$

$$H = p_\theta \dot{\theta} - L = \frac{p_\theta^2}{2m\ell^2} + mg\ell(1 - \cos \theta) \quad \Rightarrow \quad \dot{\theta} = \frac{\partial H}{\partial p} = \frac{p}{m\ell^2}, \quad \dot{p} = -\frac{\partial H}{\partial \theta} = -m g \ell \sin \theta. \tag{20}$$

$$\Rightarrow \quad \ddot{\theta} = \frac{\dot{p}}{m\ell^2} = \frac{-m g \ell \sin \theta}{m\ell^2} \equiv -\omega^2 \sin \theta. \tag{21}$$

For small values of $\theta$ and $p_\theta$, we can approximate $\sin \theta \approx \theta$ and $1 - \cos \theta \approx \theta^2/2$, so that $\ddot{\theta} = -\omega^2 \theta$ and $\theta(t) \approx \theta_0 \cos(\omega t + \phi)$.

$$H = \frac{p^2_\theta}{2m\ell^2} + mg\ell(1 - \cos \theta) \approx \frac{1}{2} m \omega^2 \ell^2 \theta_0^2 = \text{constant} = E, \tag{22}$$
and the phase space trajectories are again ellipses, traversed clockwise.

But for larger amplitude oscillations, corresponding to larger \( \theta_0 \) and therefore \( E \), the restoring force becomes anharmonic. The phase space trajectories distort away from ellipses, increasingly so as the energy is raised.

For sufficiently high energy \( (E = 2mg\ell) \), the pendulum bob can make it all the way to the top of its swing, which is an unstable fixed point. It could get stuck there for some time! But even the slightest jiggle will cause the bob to fall back down - in either direction - a bifurcation. It could go back in the direction it came from, completing a full orbit, returning back to the same stable fixed (equilibrium) point (at the bottom, \( \theta = 0 \)); this is called a homoclinic orbit. Or, it could keep going in the same direction through the upper unstable equilibrium point (at \( \theta = \pi \)), and on to a different stable equilibrium point (\( \theta = 2\pi \)); this is called a heteroclinic orbit. However, because of the periodic boundary conditions on \( \theta \in [-\pi, \pi] \), it’s really the same point (that is, \( \theta = 0 \) is the same as \( \theta = 2\pi \)), but the system got there through a different path.

For even higher energies \( (E > 2mg\ell) \), the bob swings around and around, in an unbounded or running orbit.

A sketch of the trajectories for different energies, from small amplitude oscillations to high energy running solutions, is in Fig. 1.

Figure 1: Phase space trajectories for simple non-linear pendulum. From https://upload.wikimedia.org/wikipedia/commons/f/f5/Separatrix_for_a_Simple_Pendulum.png.

Because trajectories cannot cross for a time independent Hamiltonian except at fixed points, there are strong constraints on the possible dynamics: just fixed points, periodic orbits, and homo/heteroclinic orbits) in a two dimensional phase space — the Poincaré-Bendixson theorem.

**Ignorable coordinates and the Routhian**

The Hamiltonian formulation is particularly simple for ignorable coordinates. For an ignorable coordinate \( q_m \) we know \( \partial L/\partial q_m = 0 \) which implies, using Eq. [7], \( \partial H/\partial q_m = 0 \). The
equations of motion for this degree of freedom are
\[ \dot{p}_m = -\frac{\partial H}{\partial q_m} = 0 \quad p_m \text{ a constant of the motion,} \tag{23} \]
\[ \dot{q}_m = \frac{\partial H}{\partial p_m} . \tag{24} \]

This simplicity can be exploited by doing a partial Legendre transformation over the ignorable coordinates to form the Routhian which effectively reduces the number of degrees of freedom that have to be studied. Arrange the order of coordinates so that \( q_{s+1} \ldots q_N \) are ignorable and define
\[ R(q_1, q_2, \ldots, q_s, \dot{q}_1, \dot{q}_2, \ldots, \dot{q}_s, p_{s+1}, \ldots, p_N) = \sum_{i=s+1}^{N} p_i \dot{q}_i - L. \tag{25} \]

Note there is no dependence on \( q_{s+1} \ldots q_N \) since these are ignorable, and the momenta appearing in \( R \) are constant. Thus the Routhian \( R \) acts as the Lagrangian for the remaining \( s \) variables, giving the Euler-Lagrange equations
\[ \frac{d}{dt} \frac{\partial R}{\partial \dot{q}_k} - \frac{\partial R}{\partial q_k} = 0, \quad k = 1 \ldots s. \tag{26} \]

As an example, consider the Kepler problem. We reduced the problem to the Lagrangian for the coordinates \( r, \phi \) in the plane perpendicular to the angular momentum, with the Lagrangian
\[ L = \frac{1}{2} \mu (\dot{r}^2 + r^2 \dot{\phi}^2) + \frac{k}{r}, \tag{27} \]
and \( p_\phi = \mu r^2 \dot{\phi} \) is constant. Remember from [Lecture 7] that I said it is incorrect to eliminate \( \dot{\phi} \) from the Lagrangian in favor of the constant \( p_\phi \); we now know that we should do a Legendre transformation to allow this substitution, i.e. form the Routhian \( R = p_\phi \dot{\phi} - L \) and then eliminate \( \dot{\phi} \) using \( p_\phi \). This gives
\[ R(r, \dot{r}, p_\phi) = -\left[ \frac{1}{2} \mu \dot{r}^2 + V_{\text{eff}} \right] \quad \text{with} \quad V_{\text{eff}} = \frac{k}{r} - \frac{p_\phi^2}{2\mu r^2}, \tag{28} \]
which can now be used as the effective Lagrangian for the \( r \) coordinate. Applying Eq. (26) to the radial coordinate gives
\[ \mu \ddot{r} = -\frac{dV_{\text{eff}}}{dr} = \frac{p_\phi^2}{\mu r^3} - \frac{k}{r^2}. \tag{29} \]
The Hamiltonian equations for \( \phi, p_\phi \) are
\[ \dot{p}_\phi = 0, \quad \dot{\phi} = \frac{p_\phi}{\mu r^2}. \tag{30} \]
The procedure is not much different from what we used before, but perhaps makes the calculation more natural, e.g. the effective potential appears in a straightforward way in Eqs. (28,29).

Hand and Finch mention the Routhian on p23, and then in a number of problems (see the index).