Hamiltonian mechanics - Hamilton's equations

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So far, we have seen that all of mechanics can be formulated using the Lagrangian formalism, encapsulated in the principle of least action and the Euler-Lagrange equations. Here, we introduce a new theoretical formulation, called Hamiltonian mechanics, which is distinct (although closely related) to the Lagrangian formalism.

Typically, the Hamiltonian formalism does *not* help to solve practical problems better or more easily than the Lagrangian formalism. However, the Hamiltonian formalism does provide and elegant picture of dynamical motion in the so-called phase space (the space of positions and momenta) and, perhaps more importantly, serves as a starting point for most theoretical physics, especially quantum mechanics. The Lagrangian formalism is often more useful for solving problems, but the Hamiltonian formalism is often more useful for addressing theoretical questions.

Hamilton's equations

Hamiltonian

When studying conserved quantities in the Lagrangian approach, we introduced the Hamiltonian

$$H = \sum_i p_i q_i' - \mathcal{L}(\mathbf{q}, \mathbf{q}', t)\,,$$

where $p_i = \partial\mathcal{L}/\partial q_i'$ is the generalized momentum conjugate to q_i. We saw that, when the Lagrangian does not depend explicitly on time, H is a conserved quantity.

In principle, H is a function of $\mathbf{p}$, $\mathbf{q}$ and $\mathbf{q}'$,[1] but let's see how H changes when these variables change[2]

$$\begin{aligned} dH &= \sum_i \left[\frac{\partial H}{\partial p_i}dp_i + \frac{\partial H}{\partial q_i}dq_i + \frac{\partial H}{\partial q_i'}dq_i'\right] \\ &= \sum_i \left[q_i' dp_i - \frac{\partial L}{\partial q_i}dq_i + \left(p_i - \frac{\partial L}{\partial q_i'}\right)dq_i'\right] \\ &= \sum_i \left[q_i' dp_i - p_i' dq_i\right]\,. \end{aligned} \tag{1}$$

Therefore, changing q_i' alone does not lead to a change in H; in other words **the Hamiltonian $H = H(\mathbf{p}, \mathbf{q})$ is a function of the generalized coordinates q_i and their generalized conjugate momenta p_i** (and time, if the Lagrangian depends explicitly on time), but not of the generalized velocities $\mathbf{q}'$.

[1] For now, we assume that $\mathcal{L}$ does not depend explicityly on time, so we ignore this explicit dependency in the Hamiltonian.

[2] Note that this expression for the variation of H does not require that $\mathbf{p}$, $\mathbf{q}$ and $\mathbf{q}'$ are independent.

Legendre transformation

This is a good point to stop and talk about the Legendre transformation—as we will see, the Hamiltonian can be seen as the Legendre-transformed Lagrangian.[3] The Legendre transformation can be understood as a way to, starting from a function of a variable, obtain a function of a different variable. If the transformation is repeated, it restores the old function of the old variable.

[3] Besides mechanics, Legendre transformations play a key role in thermodynamics.

For now, let's forget about mechanics and consider an arbitrary function $A(x,y)$ of two variables x and y. Then, introduce a third variable z and define a function B of this (initially) independent variables as $B(x,y,z) = yz - A(x,y)$. Infinitesimal changes in x, y and z lead to changes in B that are given by

$$dB = -\frac{\partial A}{\partial x}dx + \left(z - \frac{\partial A}{\partial y}\right)dy + ydz\,.$$

So far, x, y and z have been independent. But we can choose z to be a function of x and y defined by

$$z(x,y) = \left.\frac{\partial A}{\partial y}\right|_x\,. \tag{2}$$

With this, the variation dB is given by

$$dB = -\frac{\partial A}{\partial x}dx + ydz$$

so that $B = B(x,z)$ and, by equating to

$$dB = \frac{\partial B}{\partial x}dx + \frac{\partial B}{\partial z}dz\,,$$

we get

$$\left.\frac{\partial B}{\partial x}\right|_z = -\left.\frac{\partial A}{\partial x}\right|_y \quad \text{and} \quad \left.\frac{\partial B}{\partial z}\right|_x = y\,. \tag{3}$$

For clarity, we have now made explicit the variables that are held constant in each partial derivative.

All in all we have a very symmetric structure in which the derivatives with respect to the *passive* variable x are equal, except for a sign, in $A(x,y)$ and $B(x,z)$, and the *active* variables y and z are given by the active derivatives of the transformed function. It is because of this symmetry that the transformation is reversible.

There is a useful geometrical interpretation of the Legendre transformation. First, we note that the line yz, with $z = \partial A/\partial y$, is the straight line that goes through the origin and is parallel to the tangent of $A(y)$ at y (Fig. 1). Thus, to obtain $B(z)$ we need to identify the point y^* where the slope of $A(y)$ is z, and then measure the distance $yz - A(y)$ (which is also the maximum distance between yz

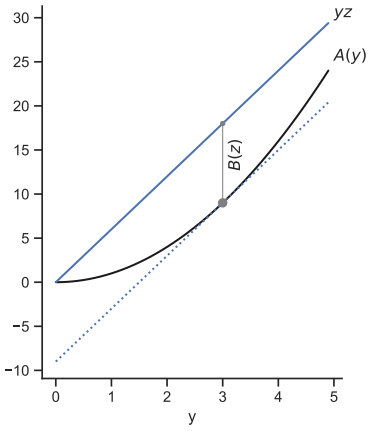

Figure 1: Geometrical interpretation of the Legendre transform $B(z)$ of $A(y)$.

and $A(y)$.[4] This interpretation shows that $A(y)$ needs to be a convex function for the Legendre transformation to be well defined—otherwise, there might be more than one point with the "right slope." This interpretation also illustrates the dual nature of the Legendre transformation.

[4] Why?

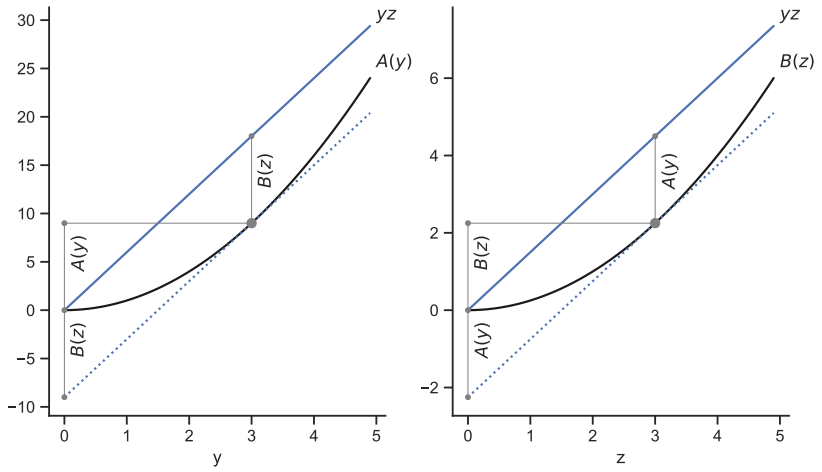

Figure 2: Geometrical interpretation of the Legendre transform $B(z)$ of $A(y)$, and the corresponding Legendre transform $A(y)$ of $B(z)$.

Hamilton's equations of motion

With what we have now seen, it becomes apparent that the Hamiltonian $H(\mathbf{q}, \mathbf{p}, t)$ is the Legendre transform of the Laplacian $L(\mathbf{q}, \mathbf{q}', t)$. Using the relations that we have obtained for the active derivatives, we have

$$\boxed{q'_k = \frac{\partial H}{\partial p_k} \quad \text{and} \quad p'_k = -\frac{\partial H}{\partial q_k}} \tag{4}$$

which are **Hamilton's equations of motion**. Additionally, as we have seen, if the Lagrangian depends explicitly on time (otherwise, H is constant), we have

$$\boxed{\frac{dH}{dt} = -\frac{\partial L}{\partial t}}\,. \tag{5}$$

For a system with N degrees of freedom, Newton's second law led to N second-order differential equations for the positions. Using the Euler-Lagrange equations for the same system, we obtain N first-order differential equations for positions and velocities, which amounts to pretty much the same. Now, with Hamilton's equations, we have $2N$ first-order differential equations for positions and momenta.

In practice, solving Hamilton's equations instead of the Euler-Lagrange equations often makes very little difference in the difficulty

of finding and solving the equations of motion. However, the fact that $\mathbf{p}$ and $\mathbf{q}$ are treated symmetrically allows for the discovery of some important theorems, like the Liouville theorem that we introduce below. Perhaps even more importantly, the Hamiltonian formalism also makes it possible to develop sophisticated analytical tools such as Poisson brackets and canonical transformations, that we discuss in the next chapter.

Solving problems using the Hamiltonian approach

In general, solving problems using the Hamiltonian approach involves the following steps:

1. Write the Lagrangian in some coordinates $\mathbf{q}$.
2. Obtain the generalized conjugate momenta $p_k = \partial L/\partial q'_k$, for all degrees of freedom $k = 1, \ldots, N$. Invert the relationship to obtain q'_k as a function of $\mathbf{q}$ and $\mathbf{p}$.
3. Write the Hamiltonian as
$$H = \sum_i p_i q'_i - \mathcal{L}(\mathbf{q}, \mathbf{q}', t)\,.$$
4. Eliminate the generalized velocities from the Hamiltonian, so that it becomes a function of $\mathbf{q}$ and $\mathbf{p}$ only (and perhaps time).
5. Solve the $2N$ first-order equations given by Hamilton's equations.

EXAMPLE: HARMONIC OSCILLATOR. Consider a simple one-dimensional harmonic oscillator, with Lagrangian
$$\mathcal{L} = \frac{m}{2}x'^2 - \frac{k}{2}x^2\,.$$
Let's now derive Hamilton's equations of motion. The conjugate momentum is $p_x = d\mathcal{L}/dx' = mx'$, so the Hamiltonian is
$$H = p_x x' - \mathcal{L} = \frac{p_x^2}{m} - \frac{p_x^2}{2m} + \frac{k}{2}x^2 = \frac{p_x^2}{2m} + \frac{k}{2}x^2\,,$$
which trivially coincides with the total energy $H = T + V = E$. Now Hamilton's equations of motion are
$$x' = \frac{\partial H}{\partial p_x} = \frac{p_x}{m} \quad \text{and} \quad p'_x = -\frac{\partial H}{\partial x} = -kx\,.$$
The second equation is, as expected, Newton's second law combined with Hooke's law.

Phase space and Liouville's theorem

Phase space

At this point, choosing the Lagrangian $\mathcal{L}(q, q')$ (and the Euler-Lagrange equations) or the Hamiltonian $H(q, p)$ (and Hamilton's equations) seems just a matter of taste. Why should we prefer using the momentum p instead of the velocity q'? As we show next, the key feature of using p is that **the principle of least action holds for independent variations of q and p**, that is, arbitrary variations δp and δq are truly independent at each point in time.[5]

Now, let's calculate the change in the Lagrangian in terms of the variations of q and p

$$\delta\mathcal{L} = q'\delta p + p\delta q' - \delta H\,.$$

Additionally, we have that

$$\delta H = \frac{\partial H}{\partial q}\delta q + \frac{\partial H}{\partial p}\delta p\,.$$

Putting both equations together, we have that

$$\delta\mathcal{L} = \left(q' - \frac{\partial H}{\partial p}\right)\delta p - \left(p' + \frac{\partial H}{\partial q}\right)\delta q + \frac{d}{dt}(p\,\delta q) = \frac{d}{dt}(p\,\delta q)\,,$$

where, in the last step, we have used Hamilton's equations. Since the change in Lagrangian is the total time derivative of some function, then the physics is exactly the same as with the original Lagrangian. Therefore, we have proved that independent infinitesimal variations δq and δp from the physical path in the (q, p) space do not change the action. **The (q, p) space is called the phase space.**

In the formulation of Lagrangian mechanics, we had a trajectory $q(t)$, and proved that the equations of motion follow from making the action extremal for the actual trajectory. We are now plotting the trajectory in phase space,[6] and have shown that infinitesimal variations of q and p also leave the action unchanged. Therefore, **the trajectory in phase space with this extremum property is (equivalently) the solution for the motion (Fig. 3).**

Liouville's theorem

Consider infinitely many copies i of the same system (or equivalently, a bunch of systems i with identical Hamiltonian) but different initial conditions (x_0^i, p_0^i). In particular, suppose that the (infinitely many) points (x_0^i, p_0^i) occupy an area A in phase space. Liouville's theorem tells us about the time evolution of this volume A.

[5] Recall that this was not the case when working with q and q'. There, we defined a variation δq (we also called it η) around the real trajectory that minimizes the action and, thus, satisfies $\delta S = 0$. Given δq, $\delta q'$ was fixed. The condition that δq had to satisfy was that, at the origin and endpoint of the trajectory, $\delta q = 0$ so that (q_1, t_1) and (q_2, t_2) were fixed; again, no mention of q' there—things happen in (q, t) space.

[6] Now, time t just parametrizes the trajectory in phase space.

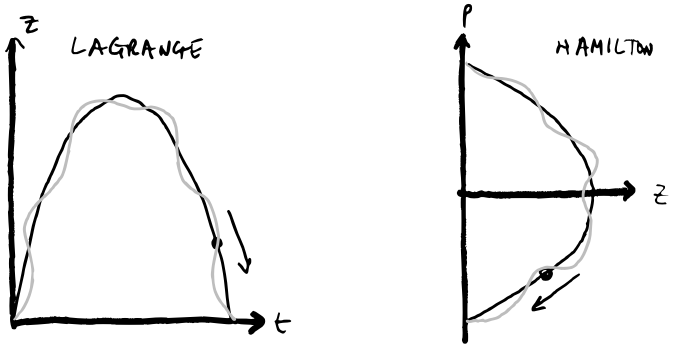

Figure 3: Lagrangian vs Hamiltonian views of the variations on the trajectory of a falling body.

LIOUVILLE'S THEOREM. **The area of any small patch in phase space is preserved as time progresses.**

If the points (x_0^i, p_0^i) in phase space are infinitely many, we can describe them by just talking about the density ρ of points in phase space, just as we talk about the density of molecules in a gas. The *phase space density* is the limit[7]

$$\rho \equiv \lim_{\Delta A \to 0} \frac{\mathcal{N}(\Delta A)}{\Delta A},$$

where $\mathcal{N}(\Delta A)$ is the number of systems in the area $\Delta A = \Delta q \Delta p$. Because we have infinitely many systems (a continuum of systems), we treat the density as a continuous function $\rho(q, p, t)$ that only depends on the phase space variables and, perhaps, time. Liouville's theorem states that ρ flows over phase space like an incompressible fluid, that is, that it cannot be squeezed. More precisely, it means that the phase fluid may change shape but, if we *follow* a point (q^*, p^*) which moves according to Hamilton's equations and measure ρ around the trajectory, the density does not change.[8] Let's see why.

Consider a small area of phase space as depicted in Fig. 4. The number of systems inside the area at some time t is $\mathcal{N} = \rho \Delta q \Delta p$ (top of Fig. 4). How does this number change after some time Δt? We can calculate this by quantifying the flows into and out of the area through the boundaries 1, 2, 3, and 4. Let's consider boundary 1, first (Fig. 4 bottom); the number of systems $\Delta\mathcal{N}_1$ entering the area through 1 is

$$\Delta\mathcal{N}_1 = \left(\rho q'\right)_q \Delta t \Delta p,$$

where the subscript q indicates that the quantities in parentheses are evaluated at q. Similarly, the number of systems entering through boundary 2 is

$$\Delta\mathcal{N}_2 = -\left(\rho q'\right)_{q+\Delta q} \Delta t \Delta p,$$

with a negative sign because positive velocities q' (towards the right in the figure) imply loss of systems, rather than entry. All in all,

[7] In the general case in which phase space has $2N$ dimensions, instead of just 2, we have volumes $\Delta V = \Delta q_1 \Delta p_1 \ldots \Delta q_N \Delta p_N$ instead of areas ΔA, but all arguments below remain the same.

[8] Note that the density at a *fixed* point in phase space can change. So what Liouville's theorem states is that $d\rho/dt = 0$ (total change in ρ, including the change due to the fact that q and p are changing); in general, $\partial\rho/\partial t \neq 0$ (temporal change in ρ at a fixed location).

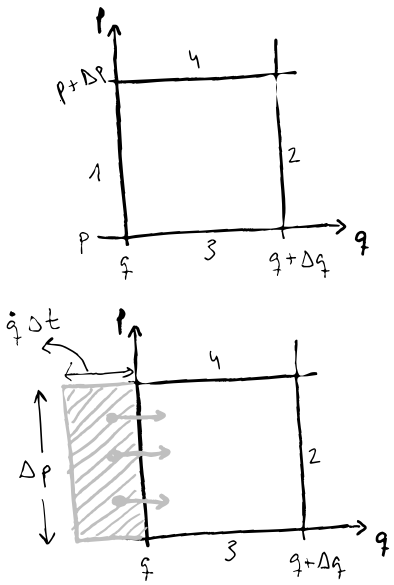

Figure 4: Flows in and out of a small area in phase space.

assuming that Δq is small, the net change due to the flow through the vertical boundaries 1 and 2 is

$$\Delta \mathcal{N}_{12} = -\frac{(\rho q')_{q+\Delta q} - (\rho q')_q}{\Delta q} \Delta t \Delta q \Delta p = -\frac{\partial(\rho q')}{\partial q} \Delta t \Delta q \Delta p \,.$$

Analogously, we have a net flow through the horizontal surfaces 3 and 4

$$\Delta \mathcal{N}_{34} = -\frac{\partial(\rho p')}{\partial p} \Delta t \Delta q \Delta p \,.$$

Finally, the total change in the number of systems inside the area is

$$\Delta \mathcal{N}_{\text{inside}} = \frac{\partial \rho}{\partial t} \Delta t \Delta q \Delta p \,,$$

but this change must come from systems entering and leaving the area[9], so we have that

$$\frac{\partial \rho}{\partial t} = -\frac{\partial(\rho q')}{\partial q} - \frac{\partial(\rho p')}{\partial p} \implies \frac{\partial \rho}{\partial t} + \frac{\partial(\rho q')}{\partial q} + \frac{\partial(\rho p')}{\partial p} = 0 \,.$$

This is a *continuity equation*[10] and it just encodes the fact that systems do not appear or disappear in phase space—so far there is no mechanics in the equation.

Now, we finally use the fact that trajectories obey Hamilton's equations to get[11]

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial q} q' + \frac{\partial \rho}{\partial p} p' = 0$$

or simply

$$\boxed{\frac{d\rho}{dt} = 0} \tag{6}$$

which proves Liouville's theorem. This equation means that the area of any distribution in phase space must be preserved, and it has many practical implications, for example in statistical mechanics or quantum mechanics (where the quantum analog of the theorem describes the evolution of the density matrix of a mixed state).

As a final comment, note that dissipative systems do not obey Hamilton's equations, and therefore they do not obey Liouville's theorem either.[12]

[9] Systems cannot appear out of the blue or disappear inside the area!

[10] Continuity equations occur in many areas of physics and engineering. Can you think an area where you have encountered a continuity equation before?

[11] EXERCISE: Do it!

[12] This should be very clear if you imagine the trajectories of infinitely many damped oscillators in phase space. Where do they all end up after long enough times?