Week 10

PHY 305 Classical Mechanics
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4 Hamiltonian mechanics

After Newton's and Lagrange's, Hamiltonian mechanics is yet a third formulation of mechanics. While the motivation to learn Lagrange after Newton was that many calculations get significantly easier in the former, Hamiltonian mechanics does not necessarily provide an advantage in calculations. However we shall see, that it provides powerful new concepts to mechanics, which then have been instrumental in setting up statistical mechanics, quantum mechanics and quantum field theory.

There is a twofold aesthetic motivation for the change from the Lagrangian to Hamiltonian approach: (i) Lagrange equations always end up as ODEs that are second order in time for the coordinates $q_n(t)$, which require us to specify initial conditions for $q_n(0)$ and $\dot{q}_n(0)$. We would rather prefer first order equations, so that the state at any given time completely determines the future. (ii) Lagrange equations deals with $\mathbf{q}$ and $\dot{\mathbf{q}}$ differently, can this be made more "symmetric".

It turns out both aspects can be achieved by treating $\mathbf{q}$ and the generalized momentum $p_n = \frac{\partial \mathcal{L}}{\partial \dot{q}_n}$ (see section 2.5.2) as the dynamical variables. In order to do this, we have to move from the Lagrangian $\mathcal{L}(\mathbf{q}, \dot{\mathbf{q}}, t)$ to a function called Hamiltonian, with variables $\mathcal{H}(\mathbf{q}, \mathbf{p}, t)$. This is achieved by a Legendre transformation.

4.1 Legendre Transformation

The plan above is a little tricky, since we want to change the variables of our function to one that is defined via a derivative. Suppose we have a generic 2D function $f(x, y)$. We can then write the differential of that function as

$$df = \underbrace{\frac{\partial f}{\partial x}}_{\equiv u} dx + \underbrace{\frac{\partial f}{\partial y}}_{\equiv v} dy. \tag{4.1}$$

Let us define a new function $g = ux - f$. Writing down the differential of that function

$$dg = dux + udx - df = dux + udx - udx - vdy = xdu - vdy. \tag{4.2}$$

This no longer depends on dx but instead on du, telling us that we swapped the dependence on x for one on u. In the first equality we used the product rule and in the second (4.1). Based on this we define the

Legendre Transformation of the function $f(x, y)$ as

$$g(u, y) = u \;\; x(u, y) - f(x(u, y), y) \tag{4.3}$$

where $u = \frac{\partial f}{\partial x}$.

- A key point, is that the function g contains the same amount of information as the function f did.
- The Legendre transformation is important in mechanics (as we will see below) and in thermodynamics: Based on the differential definition of the internal energy $dU = dQ - dW$, where dQ is the input heat and dW the work done, and its differential $dU = TdS - PdV$ (for temperature T, entropy S, pressure P and volume V), we can use a Legendre transformation to generate a couple of different differential forms, dependent on some variables that are define via derivatives of U. For example the definition of Enthalpy H

$$H = PV + U, \quad \Leftrightarrow \quad dH = TdS + VdP, \tag{4.4}$$

  takes exactly the form (4.3), since pressure $P = -\partial U/\partial dV$, hence also change the differential through a cancellation such as in Eq. (4.2). The same procedure gives us the Helmholtz free energy $F = U - TS$, and Gibbs free energy $G = H - TS$. See GPS and your favorite thermodynamics or statistical physics book for more details.

4.2 The Hamiltonian

We now apply the Legendre transformation to our Lagrangian, in order to change variables in a function $f = \mathcal{L}$ from $x = \dot{q}$ $y = q$ to $u = \partial\mathcal{L}/\partial\dot{q}$ reaching a function $\mathcal{H}$. We do this for each generalized coordinative and then find the

Hamiltonian (function)

$$\mathcal{H}(\mathbf{q}, \mathbf{p}) = \sum_n p_n \dot{q}_n - \mathcal{L}(\mathbf{q}, \dot{\mathbf{q}}, t). \tag{4.5}$$

where we have used the canonical momentum

$$p_n = \frac{\partial \mathcal{L}}{\partial \dot{q}}. \tag{4.6}$$

- Earlier we had used the name "generalized momentum" for the "canonical momentum".

- In the Hamiltonian, $\dot{q}_n$ is understood to be replaced on the rhs by p_n. For example for a particle in cartesian 3D coordinates, subject to a potential $V(\mathbf{q})$, the Lagrangian is $\mathcal{L} = \frac{1}{2}m\dot{\mathbf{q}}^2 - V(\mathbf{q})$, hence $\mathbf{p} = m\dot{\mathbf{q}}$ and we can write $\mathcal{L} = \frac{\mathbf{p}^2}{2m} - V(\mathbf{q})$. Then the Hamiltonian $\mathcal{H}$ is

$$\mathcal{H} = \mathbf{p}\cdot\dot{\mathbf{q}} - \mathcal{L} = \frac{\mathbf{p}^2}{m} - \left(\frac{\mathbf{p}^2}{2m} - V(\mathbf{q})\right) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{q}). \tag{4.7}$$

  We see that it is equal to the total energy, and shall comment on this again shortly.

From the Hamiltonian we find the equations of motion by taking partial derivatives

$$\begin{aligned}\frac{\partial\mathcal{H}}{\partial q_k} &\overset{Eq.\ (4.5)}{=} \sum_n p_n \frac{\partial\dot{q}_n}{\partial q_k} - \left[\frac{\partial\mathcal{L}(\mathbf{q},\dot{\mathbf{q}},t)}{\partial q_k} + \sum_n \underbrace{\frac{\partial\mathcal{L}(\mathbf{q},\dot{\mathbf{q}},t)}{\partial\dot{q}_n}}_{=p_n}\frac{\partial\dot{q}_n}{\partial q_k}\right] \\ &= -\frac{\partial\mathcal{L}(\mathbf{q},\dot{\mathbf{q}},t)}{\partial q_k} \overset{Eq.\ (2.29)}{=} -\frac{d}{dt}\frac{\partial\mathcal{L}(\mathbf{q},\dot{\mathbf{q}},t)}{\partial\dot{q}_k} = -\dot{p}_k.\end{aligned} \tag{4.8}$$

Now let's do

$$\frac{\partial\mathcal{H}}{\partial p_k} \overset{Eq.\ (4.5)}{=} \sum_n \left[\underbrace{\frac{\partial p_n}{\partial p_k}}_{=\delta_{nk}}\dot{q}_n + p_n\frac{\partial\dot{q}_n}{\partial p_k}\right] - \left[\sum_n \underbrace{\frac{\partial\mathcal{L}(\mathbf{q},\dot{\mathbf{q}},t)}{\partial\dot{q}_n}}_{=p_n}\frac{\partial\dot{q}_n}{\partial p_k}\right] = \dot{q}_k. \tag{4.9}$$

Together we have found

Hamilton's equations for a system of M degrees of freedom:

$$\begin{aligned}\dot{q}_k &= \frac{\partial\mathcal{H}}{\partial p_k}, \qquad k = 1, 2, \cdots, M \\ \dot{p}_k &= -\frac{\partial\mathcal{H}}{\partial q_k}.\end{aligned} \tag{4.10}$$

for the evolution of the canonical momenta p_k and canonical coordinates q_k from the Hamiltonian defined in Eq. (4.5).

- These are now nicely symmetric in q versus p and as desired of first order in time, so the entire solution is specified once you know the initial state $p_k(t=0)$ and $q_k(t=0)$.
- In principle, find the Hamiltonian requires the lengthy sequence of finding generalized coordinates, setting up Lagrangian, doing Legendre transform etc. However it turns out that it many cases usually encountered, the Hamiltonian is in fact the energy in terms of the generalized coordinates. In that case it is possible to write it down directly. Exceptions are e.g. when the link between generalized coordinates and original coordinates involves time explicitly. See GPS for more details.

Example 39, Particle in a central potential:
Let us re-consider the central force problem of section 2.8 in the Hamiltonian approach. We start with the Lagrangian (2.65) which was

$$\mathcal{L}_{=}\frac{1}{2}\mu(\dot{r}^2 + r^2\dot{\varphi}^2) - V(r). \tag{4.11}$$

We stick to our variables r and φ and find their associated canonical momenta $p_r = \partial\mathcal{L}_{/}\partial\dot{r} = \mu\dot{r}$ and $p_\varphi = \partial\mathcal{L}_{/}\partial\dot{\varphi} = mr^2\dot{\phi}$. The latter turns out to be the angular momentum ℓ, by comparison with Eq. (2.66). Either by writing the total energy or by doing a Legendre transformation, we then arrive at the Hamiltonian

$$\mathcal{H}_{=}\frac{1}{2m}\left(p_r^2 + \frac{p_\varphi^2}{r^2}\right) + V(r). \tag{4.12}$$

From this we can now derive the four Hamilton's equations (4.10) which turn out to be:

$$\begin{aligned} \dot{r} &= \frac{\partial\mathcal{H}}{\partial p_r} = \frac{p_r}{m}, \quad & \dot{p}_r &= -\frac{\partial\mathcal{H}}{\partial r} = \frac{p_\varphi^2}{mr^3} \\ \dot{\varphi} &= \frac{\partial\mathcal{H}}{\partial p_\varphi} = \frac{p_\varphi}{mr^2}, \quad & \dot{p}_\varphi &= -\frac{\partial\mathcal{H}}{\partial\varphi} = 0 \end{aligned} \tag{4.13}$$

With the equation for $\dot{p}_\varphi$ we rediscovered that angular momentum is conserved, and we can combine those for $\dot{r}$ and $\dot{p}_r$ easily to reproduce the radial equation of motion for the Kepler problem (2.67). Finally the $\dot{\varphi}$ equation just reproduced the definition of ℓ. Alltogether we just saw that the Hamiltonian approach gives the exact same equations of motions as the Lagrangian one, and the solution thus is as in week5.

Example 40, Particle in an electro-magnetic field:
Consider a particle with mass m and charge q in an electro-magnetic field with scalar potential $\phi(\mathbf{r})$ and vector-potential $\mathbf{A}(\mathbf{r})$. It has a Lagrangian

$$\mathcal{L} = \frac{1}{2}m\dot{\mathbf{r}}^2 - q(\phi - \dot{\mathbf{r}}\cdot\mathbf{A}). \tag{4.14}$$

To understand that this is the right Lagrangian, and as a good advanced exercise, show that the Euler-Lagrange equations (2.29) describe the Coulomb and Lorentz forces:

$$m\ddot{\mathbf{r}} = q(\mathbf{E} + \dot{\mathbf{r}}\times\mathbf{B}), \tag{4.15}$$

with the electric field $\mathbf{E} = -\boldsymbol{\nabla}\phi - \dot{\mathbf{A}}$ and magnetic field[a] $\mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A}$.
The conjugate momentum to $\mathbf{r}$ is

$$\mathbf{p} = \frac{\partial\mathcal{L}}{\partial\dot{\mathbf{r}}} = m\dot{\mathbf{r}} + e\mathbf{A}. \tag{4.16}$$

[a] Use the epsilon-tensor (2.96) to handle the curl of the vector potential

Example continued: Importantly note, that $\mathbf{p}$ is not just the usual momentum, but contains the vector potential! We can now follow the Legendre transformation (exercise) to find the classical Hamiltonian of a charged particle in an electromagnetic field

$$\mathcal{H} = \frac{1}{2m}(\mathbf{p} - e\mathbf{A}(\mathbf{r}))^2 + e\phi(\mathbf{r}). \tag{4.17}$$

4.3 Conservation laws in the Hamilton formalism

It is also relatively straightforward to identify conservation laws in the Hamiltonian formalism (similar to what we had seen for Lagrange in section 2.7). Let us start by calculating the total derivative of the Hamiltonian with respect to time:

$$\frac{d\mathcal{H}(\mathbf{q},\mathbf{p},t)}{dt} = \sum_n \underbrace{\left[\underbrace{\frac{\partial \mathcal{H}(\mathbf{q},\mathbf{p},t)}{\partial q_n}}_{-\dot{p}_n} \frac{dq_n}{dt} + \underbrace{\frac{\partial \mathcal{H}(\mathbf{q},\mathbf{p},t)}{\partial p_n}}_{\dot{q}_n} \frac{dp_n}{dt} \right]}_{=0} + \frac{\partial \mathcal{H}(\mathbf{q},\mathbf{p},t)}{\partial t} = \frac{\partial \mathcal{H}}{\partial t} \tag{4.18}$$

Since we had earlier seen that the Hamiltonian typically is actually the total energy, we have seen that the total energy is conserved as long as the Hamiltonian does not depend on time explicitly. (i.e. there is no "t" in the equation, other than as argument of $\mathbf{q}$ or $\mathbf{p}$).

Even easier is to see (again), that if a coordinate q_n is cyclic/ ignorable, which means that the Hamiltonian does not depend on q_n, the corresponding canonical momentum is conserved:

$$\dot{p}_n = -\frac{\partial \mathcal{H}(\mathbf{q},\mathbf{p},t)}{\partial q_n} = 0. \tag{4.19}$$

4.4 Phase space

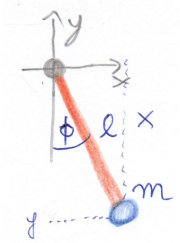
We can now put our earlier preview of the concept of phase space in section 4.4 onto a much firmer footing: Phase-space is chosen to discuss the physical state of a mechanical system, because knowing the variables $\mathbf{q}(t_0)$, $\mathbf{p}(t_0)$ at a certain time t_0 tells us the entire future $t > t_0$ evolution of a physical system, because Hamilton's equation (4.10) are of first order in time.

An important consequence of this, is that

Trajectories in phase-space cannot cross! By a given trajectory or phase-space orbits we refer to the dynamical evolution $\mathbf{p}(t)$ $\mathbf{q}(t)$ at $t > t_0$ of the system starting from some specific initial condition $\mathbf{q}(t_0)$, $\mathbf{p}(t_0)$. Different initial condition will thus refer to different trajectories.

We best see what that means and why it might be useful by looking at extending the earlier example of the phase-space for the harmonic oscillator, to the simple pendulum in example 11 instead.

Example 41, Phase space of simple pendulum:



left: As we had seen earlier, thanks to the constraint $\ell = \sqrt{x^2 + y^2}$ the simple pendulum can be described with the generalised coordinate $q = \phi$.

We start with setting up the Lagrangian

$$\mathcal{L} = \frac{1}{2} m\ell^2 \dot{\phi}^2 - mg\ell(1 - \cos\phi). \tag{4.20}$$

From this we find a canonical momentum $p = \partial\mathcal{L}/\partial\dot{\phi} = m\ell^2\dot{\phi}$. As a result of our Legendre transformation we thus reach the Hamiltonian

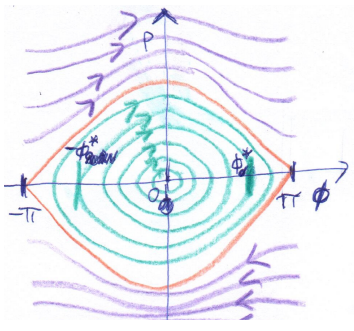
$$\mathcal{H} = \frac{1}{2} m\ell^2 \dot{\phi}^2 + mg\ell(1 - \cos\phi) = \frac{p^2}{2m\ell^2} + 2mg\ell \sin(\phi/2)^2. \tag{4.21}$$

From this we obtain Hamilton's equations

$$\begin{aligned} \dot{p} &= -\frac{\partial\mathcal{H}}{\partial\phi} = mg\ell\sin(\phi), \\ \dot{\phi} &= \frac{\partial\mathcal{H}}{\partial p} = \frac{p}{m\ell^2}. \end{aligned} \tag{4.22}$$

Thanks to the sine the equations are not easy to solve analytically. However we can resort to the idea of a phase-space portrait, shown below: We see that the Hamiltonian above is the total energy, which is conserved according to Eq. (4.18). Hence phase-space trajectories must be lines of constant $\mathcal{H} = E$.
Those are easier to find than the actual time dependent solution of (4.22), and tell us already a lot about the motion. Solving $\mathcal{H} = E$ for $p(\phi)$ gives

$$p = \pm\sqrt{2m\ell^2}\sqrt{E - 2mg\ell\sin^2(\phi/2)}. \tag{4.23}$$



left: Now drawing lines for different E relative to $2mg\ell$ into phase-space on the left, we find three different cases. (i) For $E < 2mg\ell$, p in Eq. (4.25) becomes complex for some finite ϕ^*, so the pendulum does not have enough energy to reach beyond the angle ϕ^*, it performs oscillatory motion (cyan), which for small energies looks just like that of the harmonic oscillator in example 11. (ii) For $E = 2mg\ell$ (orange), we have $\phi^* = \pm\pi$, so the pendulum could reach the inverted position given infinite time.

Example continued: (iii) For $E > 2mg\ell$ p remains positive or negative for all ranges of ϕ (violet). This corresponds to the case where the pendulum has enough energy to go over the top, and hence preserve its direction of rotation. We see also here that no trajectories cross. The case (ii) forms a separatrix between the oscillatory and rotational types of motion.

4.4.1 Liouville theorem

- The mathematics for the proof of the theorem is bonus material, but should be familiar to you from electro-magnetism courses.
- The theorem content is exam relevant.

In statistical mechanics you encounter the idea of an ensemble (a large number of identical replica of your physical system, filling all of phase-space subject to certain constraints). In phase space, we can visualize the evolution of an ensemble as the motion of a cloud of dots, see below. Since different trajectories do not cross, this resembles fluid flow lines in continuum mechanics. Let us define the phase space velocity $\dot{z} = \mathbf{v} = [\dot{\mathbf{q}}, \dot{\mathbf{p}}]^T$. This has nothing to do with a real velocity, it just states how a point in phase-space is moving.

left: (left) Evolution of an ensemble of systems in phase space. How does the volume enclosed in brown change?. (right) The change of a phase-space volume element within a short time interval δt, will depend on the phase space velocity $\mathbf{v}$ at the surface.

Geometrically from the figure above, we realize that the change of the volume V in phase space will be

$$\delta V = \int_S \mathbf{n} \cdot \mathbf{v}\, \delta t\, dA, \tag{4.24}$$

where $\int_S dA$ is a surface integral over the surface enclosing the volume, and $\mathbf{n}$ a normal vector on that surface. You will have encountered these surface integrals in electro-magnetism. Bringing δt on the left side and making it infinitesimally small gives

$$\frac{dV}{dt} = \int_S \mathbf{n} \cdot \mathbf{v}\, dA. \tag{4.25}$$

At this point we can invoke:

Gauss's theorem: The volume integral over the divergence of vector field $\mathbf{v}$ is equal to the flux of that vectorfield through the surface enclosing the volume.

$$\int_S \mathbf{n} \cdot \mathbf{v}\, dA = \int_V \boldsymbol{\nabla} \cdot \mathbf{v}\, dV. \tag{4.26}$$

This works in any number of dimensions. V is a volume in our N dimensional space, S its $N-1$ dimensional surface, $\mathbf{n}$ a normal unit vector on that surface, then $\boldsymbol{\nabla} = \left[\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \cdots, \frac{\partial}{\partial x_N}\right]^T$.

But the divergence of the phase-space flow $\mathbf{v}$ vanishes due to Hamilton's equations:

$$\begin{aligned}\boldsymbol{\nabla} \cdot \mathbf{v} &\overset{\text{def of v}}{=} \left[\frac{\partial \dot{q}_1}{\partial q_1} + \cdots + \frac{\partial \dot{q}_M}{\partial q_M} + \frac{\partial \dot{p}_1}{\partial p_1} + \cdots + \frac{\partial \dot{p}_M}{\partial p_M}\right] \\ &\overset{Eq.\ (4.10)}{=} \left[\frac{\partial}{\partial q_1}\frac{\partial \mathcal{H}}{\partial p_1} + \cdots + \frac{\partial}{\partial q_M}\frac{\partial \mathcal{H}}{\partial p_M} + \frac{\partial}{\partial p_1}\left(-\frac{\partial \mathcal{H}}{\partial q_1}\right) + \cdots + \frac{\partial}{\partial p_M}\left(-\frac{\partial \mathcal{H}}{\partial q_M}\right)\right] = 0. \end{aligned} \tag{4.27}$$

Combining Eq. (4.27), (4.26) and (4.25) we have now shown

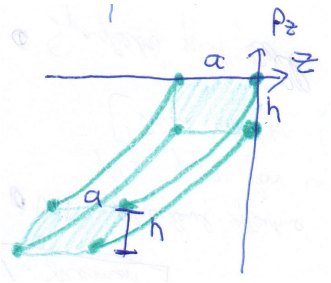
Liouville's theorem Hamiltonian evolution in phase-space is such that the phase-space volume V of an ensemble of trajectories does not change:

$$\frac{dV}{dt} = 0. \tag{4.28}$$

- The number of totally different proofs for this, seems to be near equal to the number of books.
- Liouville's theorem provides a crucial backbone of statistical physics, by allowing us to average quantities over all available phase-space, disregarding time-evolution. In doing those averages, all phase-space elements accessible are given an equal probability. If Liouville's theorem was not true, those probabilities would change in time, because a certain part of the ensemble might increase its phase-space volume at the expense of others.

Example 42, Phase space of object falling under gravity: An easy case to verify the preservation of phase-space volume, is an object falling under gravity, possibly with an initial momentum in the downwards direction. The phase-space coordinates then evolve as:

$$z = z_0 + \frac{p_z}{m}t - \frac{1}{2}gt^2, \quad p_z = p_{z0} - mgt. \tag{4.29}$$



left: We see from Eq. (4.29) that the momentum difference between two phase-space points never changes compared to the initial value. For two trajectories with equal initial momentum, also the position difference never changes. Overall, a phase space volume such as the green one thus changes from rectangular into parallelogram, but the base-width a and height h remain constant, and hence the volume $V = ah$ does not change.

4.4.2 Integrable systems

We had seen in section 4.4 that the phase-space of the simple pendulum attained a simple structure, thanks to energy conservation $E = \mathcal{H}(p, q)$. This equations acts like a constraint, turning the two-dimensions of phase space into one dimension (a line) for eery given trajectory. Since these lines can neither cross nor suddenly terminate, not too many really complicated structures in phase space are possible.

The same holds in higher dimensions and leads us to the following definition.

Integrable system
A mechanical system is called integrable, if it has as many constants of the motion as degrees of freedom.

- As for the pendulum, this means that we can slice up phase-space into lower dimensional subspaces for different values of the conserved quantities. I
- The name "integrable" refers to the possibility to formally solve the equations of motion by integration, which does not necessarily imply that these integrals are practically solvable.
- An important consequence of integrability, is that that the system cannot be chaotic (see later).