Classical Mechanics

Lecture 10

The Principle of least Action:

The principle of least action for the Hamiltonian formulation of classical mechanics involves variation of both $q_i(t)$ and $p_i(t)$ of the action written in terms of the Hamiltonian:

$$S = \int_{t_1}^{t_2} L \, dt$$

$$= \int_{t_1}^{t_2} (p_i \dot{q}_i - H) \, dt$$

And the physical path in phase space $q_i(t), p_i(t)$ extremises S:

$$\delta S = \int_{t_1}^{t_2} \left(\delta p_i \dot{q}_i + p_i \delta \dot{q}_i - \frac{\partial H}{\partial p_i} \delta p_i - \frac{\partial H}{\partial q_i} \delta q_i \right)$$

$$= \int_{t_1}^{t_2} \left\{ \left(\dot{q}_i - \frac{\partial H}{\partial p_i}\right) \delta p_i - \left(\dot{p}_i + \frac{\partial H}{\partial q_i}\right) \delta q_i + \frac{d}{dt}(p_i \delta q_i) \right\}$$

Thus we see if we require $\delta S = 0$ for arbitrary variations δq_i & δp_i, we also need to impose the boundary conditions:

$$\delta q_i(t_1) = \delta q_i(t_2) = 0.$$

$$\Rightarrow \quad \dot{q}_i = \frac{\partial H}{\partial p_i}$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}$$

So we see that the boundary conditions do not involve $\delta p_i(t_1)$ and $\delta p_i(t_2)$.

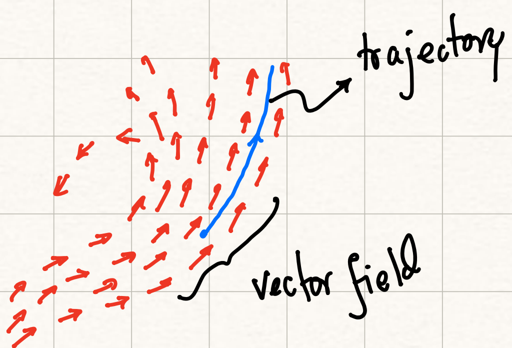
If we further want to impose $\delta p_i(t_1) = \delta p_i(t_2) = 0$, it doesn't affect the equation of motion.

But in that case we allowed to add an extra term in the action that does not affect the equation of motion:

$$S = \int_{t_1}^{t_2} \left(p_i \dot{q}_i - H + \frac{dF(p,q)}{dt} \right)$$

Hamiltonian Flow and Liouville's Theorem:

The Hamiltonian function H defines a flow on phase space. For any point on phase space, the future trajectory is, in principle, defined by the Hamiltonian. Thus, one can imagine this flow as specifying a vector field on phase space.



Comment on the determinism:

The picture that emerges is that given that we are able to solve Hamilton's equations exactly, we can forever predict the future of a system. All we have to do is to start at a specific point on phase space and follow the trajectory determined by the Hamiltonian flow. This is the deterministic view of classical mechanics.

However, there is an important caveat emptor to this deterministic picture! In stating that we can deterministically predict the future of a system we are assuming that we can specify its intitial condition with infinite precision! That is, of course, not true.

In fact, real numbers are dense in irrational numbers — examples of numbers which cannot be speeified with indefinite precision. Moreover, even in the realm of numbers irrational numbers which are algebraic form a vanishing subset. Most numbers are non-computable, i.e., there are no known algorithm with which we can compute them.

And there are many important classical mechanical system where a small indeterminacy $\delta\xi_i(0)$ in the initial condition (by ξ_i we mean a generic phase space coordinate) can grow into a large uncertainty exponentially:

$$\delta\xi_i(t) \sim \delta\xi_i(0)\, e^{\lambda_i t}$$

where λ_i are positive constants ($O(1)$ or large) known as Lyapunov exponents. This remarkable breakdown in predictability in what is essentially a deterministic system is one of the hallmarks of classical chaos. It is known as the butterfly effect.

In quantum mechanics, one limited in how precisely one can specify the positions and momenta of quantal particles by the uncertainty principle. In fact in quantum mechanics, the fundamental state of a system is given by a vector $|\Psi(t)\rangle$ in an abstract complex vector space.

The time evolution of this state is <u>also</u> governed the Hamiltonian but it is now an operator (a linear map on the complex vector space) which we denote by $\hat{H}$. The time evolution of a quantal state is then given by:

$$|\psi(t)\rangle = \exp\left[-\frac{i}{\hbar}\hat{H}(t-t')\right]|\psi(t')\rangle$$

$$= \hat{U}(t-t')|\psi(t')\rangle$$

$\hat{U}(t-t') = \exp\left[-\frac{i}{\hbar}\hat{H}(t-t')\right]$ is called the time-evolution operator and it is a Unitary operator:

$$U^\dagger = U^{-1}.$$

It then follows that $U^{-1}(t-t') = U(t'-t)$.

In quantum mechanics states are usually normalized. I.e., If $|\psi\rangle$ & $|\varphi\rangle$ are two distinct physical states then $\exists$ an inner product $(\,,\,) : |\psi\rangle \times |\varphi\rangle \to (\psi,\varphi)$ s.t.

1. $(\psi,\varphi)^* = (\varphi,\psi)$
2. $(\psi, a_1\varphi_1 + a_2\varphi_2) = a_1(\psi,\varphi_1) + a_2(\psi,\varphi_2)$

for $a_1, a_2 \in \mathbb{C}$.

3. $(\psi, \psi) \geq 0$ with $(\psi,\psi) = 0 \Rightarrow |\psi\rangle = 0$.

The modulus of the inner product is the most obvious measure of distance between two states $|\psi(0)\rangle$ & $|\varphi(0)\rangle$. But the unitarity of the time evolution operator means that

$$|\psi(t)\rangle = U(t)\,|\psi(0)\rangle$$

$$|\varphi(t)\rangle = U(t)\,|\varphi(0)\rangle$$

have inner product st $(\psi, \varphi)(t) = (\psi, \varphi)(0)$. And so the inner product is not a good measure of quantum chaos.

What is a good measure of quantum chaos is still an active field of research.

Liouville's Theorem and Liouville's Equation:

Since we are often unable to exactly specify the initial conditions of a classical system we can ask how a distribution (probability/particle number) evolves under a Hamiltonian flow.

This is addressed by Liouville's Theorem which states that the volume of a region of phase space is preserved under Hamiltonian flow. Note that Liouville's Theorem makes no statement about the shape of the region under the Hamiltonian flow, just its volume.

Let $dV = dq_1 dq_2 \dots dq_n \, dp_1 dp_2 \dots dp_n$ be the volume of a small region in phase space. Under Hamiltonian flow for a small time interval dt the phase space coordinates q_i & p_i evolve to:

$$q_i(t) \rightarrow \tilde{q}_i = q_i + \dot{q}_i \, dt$$
$$p_i(t) \rightarrow \tilde{p}_i = p_i + \dot{p}_i \, dt$$

Now comes the crucial part. Since the flow is due to the Hamiltonian evolution we can use Hamilton's equations to write:

$$\tilde{q}_i = q_i + \frac{\partial H}{\partial p_i} dt$$

$$\tilde{p}_i = p_i - \frac{\partial H}{\partial q_i} dt$$

And so the new volume

$$d\tilde{V} = d\tilde{q}_1 \, d\tilde{q}_2 \dots d\tilde{q}_n \, d\tilde{p}_1 \, d\tilde{p}_2 \dots d\tilde{p}_n$$

$$= (\det J) \, dV$$

where $J = \begin{pmatrix} \frac{\partial \tilde{q}_i}{\partial q_j} & \frac{\partial \tilde{q}_i}{\partial p_j} \\ \frac{\partial \tilde{p}_i}{\partial q_j} & \frac{\partial \tilde{p}_i}{\partial p_j} \end{pmatrix} = \begin{pmatrix} \delta_{ij} + \frac{\partial^2 H}{\partial q_j \partial p_i} dt & \frac{\partial^2 H}{\partial p_j \partial p_i} dt \\ -\frac{\partial^2 H}{\partial q_j \partial q_i} dt & \delta_{ij} - \frac{\partial^2 H}{\partial p_j \partial q_i} dt \end{pmatrix}$

$$\simeq 1 + M \, dt$$

With $M_{ij} = \begin{pmatrix} \frac{\partial^2 H}{\partial q_i \partial p_j} & \frac{\partial^2 H}{\partial p_i \partial p_j} \\ -\frac{\partial^2 H}{\partial q_i \partial q_j} & -\frac{\partial^2 H}{\partial p_i \partial q_j} \end{pmatrix}$

Using the useful matrix identity

$$\log \det J = \mathrm{Tr} \log J$$

We get $\det(1 + M\,dt) \simeq \det e^{M\,dt}$

$$= e^{\mathrm{Tr}\, M\, dt}$$

$$\simeq 1 + (\mathrm{Tr}\, M)\, dt$$

Now $\mathrm{Tr}\, M = \sum_i \left(\frac{\partial^2 H}{\partial q_i \partial p_i} - \frac{\partial^2 H}{\partial p_i \partial q_i} \right) = 0$

and so $\det J = 1$, and so

$$dV = d\tilde{V}.$$

Liouville's Equation:

Liouville's theorem implies that for any distribution on any part of phase space:

$$\int \rho \, dq_1 dq_2 \ldots dq_n dp_1 \ldots dp_n = c$$

$c = 1$ for a probability distribution and N for a number distribution. Since the volume measure is invariant under flow we must have

$$\frac{d\rho}{dt} = 0$$

from probability / particle number conservation. Thus we have for distributions on phase space:

$$\boxed{\frac{\partial \rho}{\partial t} = \frac{\partial \rho}{\partial p_i}\frac{\partial H}{\partial q_i} - \frac{\partial \rho}{\partial q_i}\frac{\partial H}{\partial p_i}}$$

This is Liouville's equation