Phase space

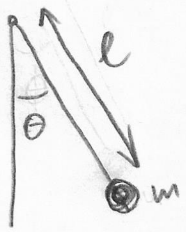
We already introduced the concept of 2n-dimensional (n is the number of degrees of freedom) in the Hamiton's formalism. Unlike a point in the configuration space

$$\vec{q} = (q_1, \dots q_n),$$

or a point in the momentum space

$$\vec{p} = (p_1, \dots, p_n),$$

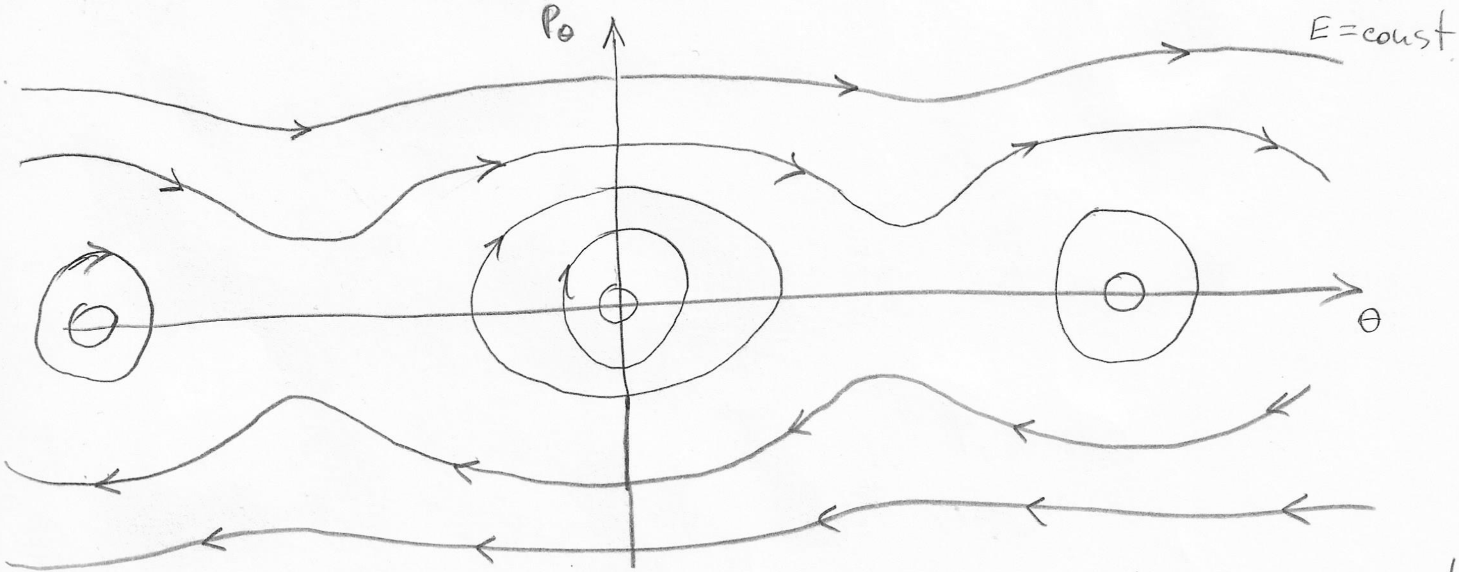
a point in the phase space $\vec{u} = (q_1, \dots q_n, p_1, \dots p_n)$ or $\vec{u} = (q_1, p_1, q_2, p_2, \dots q_n, p_n)$ (the exact order in which we arrage q_i's and p_i's is not important as long as we are consistent) fully determines a mechanical state of our system. For illustarion, let us consider the phase space diagram of a plane pendulum:



$$p_\theta = ml^2\dot{\theta}$$

$$H = \frac{1}{2}m(l\dot{\theta})^2 - mgl\cos\theta = \frac{p_\theta^2}{2ml^2} - mgl\cos\theta = E$$

$$p_\theta = \pm\sqrt{2ml^2(E + mgl\cos\theta)}$$



For energies $E < mgl$ the phase trajectories are closed (ellipse-like) curves. In this case the pendulum oscillates forth and back. For energies $E > mgl$ the pendulum still has non-zero kinetic energy at the highest point $\theta = \pm\pi$ and continues its motion without reversal of direction.

If the Hamiltonian is known then the entire phase trajectory can be unambigously determined from the coordinates of one point. Moreover, when the Hamitonian does not depend on t explicitly each point belongs to one trajectory only and two different trajectories cannot intersect. Indeed if they intersected we would not be able to uniquely describe the time evolution of a system given its initial conditions.

Liouville's theorem

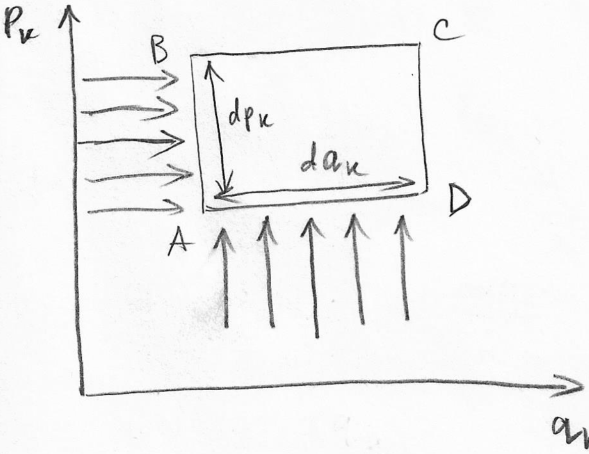
One of the most interesting things about the Hamiltonian dynamics and phase space is the Liouville theorem. It is of great importance in classical statistical mechanics. The Liouville theorem basically states that a system of independent particles in phase space (i.e. a statistical ensemble) flows like an incompressible fluid (see animation in Wikipedia). Before we attempt to prove the Liouville theorem, let us make a few comments and introduce a density in the phase space.

While in principle we can always solve for $\{q_i(t)\}$ and $\{p_i(t)\}$ given their initial values $\{q_i(0)\}$ and $\{p_i(0)\}$ in reality the system of equations can be too complex. As an example consider a macroscopic quantity of gas (atoms or molecules). Therefore we must resort to some alternative and tractable approach. The Hamiltonian formulation of dynamics is very suitable for that.

For sophisticated system with a macroscopic number of degrees of freedom it is difficult to pinpoint its exact location in the phase space. Instead we can introduce the notion of an ensemble — a very large set of equivalent systems. Each single system in the ensemble corresponds to a point/trajectory in the phase space. We can consider a situation in which the number of representative points occupied by the members of the ensemble is so large that it allows us to introduce a density of these points in the phase space, $\rho(q_1, \dots q_n, p_1, \dots p_n)$. The element of volume $du = dq_1 dq_2 \cdots dq_n dp_1 dp_2 \cdots dp_n$ contains a large enough points so that their density can be treated as a continuous function. The number of points in $d\vec{u}$ is given by

$$dN = \rho(q_1, \dots q_n, p_1, \dots, p_n)\, d\vec{u} \qquad \rho = \frac{dN}{du}$$

Now let us consider the components of particle flux along q_k and p_k direction. The rectangle ABCD represents the projection of $2n$-dimensional volume du onto the q_k, p_k-plane.



The number of points entering this volume element per unit time through side AB is

$$\rho \dot{q}_k\, dp_k\, du_k$$

where $du_k = \prod_{\substack{i=1 \\ i \neq k}}^{n} dq_i dp_i$

Similarly the flux in the p_k direction (through AD)

$$\rho \dot{p}_k\, dq_k\, du_k$$

Now the number of representative points leaving through sides CD and BC is

$$\left(\rho \dot{q}_k + \frac{\partial}{\partial q_k}(\rho \dot{q}_k)\, dq_k\right) dp_k\, du_k$$

$$\left(\rho \dot{p}_k + \frac{\partial}{\partial p_k}(\rho \dot{p}_k)\, dp_k\right) dq_k\, du_k$$

where we used the Taylor expansion of $\rho \dot{q}_k$ and $\rho \dot{p}_k$.

From the flux components in q_k and p_k directions the number of points that get accumulated in the volume element is

$$\rho \dot{q}_k \, dp_k \, du_k - \left(\rho \dot{q}_k + \frac{\partial}{\partial q_k} (\rho \dot{q}_k) \, dq_k \right) dp_k \, du_k$$

$$+ \rho \, \dot{p}_k \, dq_k \, du_k - \left(\rho \dot{p}_k + \frac{\partial}{\partial p_k} (\rho \dot{q}_k) \, dp_k \right) dq_k \, du_k$$

$$= - \left(\frac{\partial}{\partial q_k} (\rho \dot{q}_k) + \frac{\partial}{\partial p_k} (\rho \dot{p}_k) \right) du$$

By summing over all $k = 1 \ldots n$ we obtain the total number of points accumulated due to particle flux from all sides of the hyper-rectangle. This quantity must correspond to the change with time of the density multiplied by du:

$$\frac{\partial \rho}{\partial t} du = - \sum_{k=1}^{n} \left(\frac{\partial}{\partial q_k} (\rho \dot{q}_k) + \frac{\partial}{\partial p_k} (\rho \dot{p}_k) \right) du$$

or, if we drop du:

$$\frac{\partial \rho}{\partial t} = - \sum_{k=1}^{n} \left(\frac{\partial}{\partial q_k} (\rho \dot{q}_k) + \frac{\partial}{\partial p_k} (\rho \dot{p}_k) \right) \qquad (*)$$

This is essentially a continuity equation in the form

$$\frac{\partial \rho}{\partial t} + \mathrm{div}(\rho \dot{\vec{u}}) \qquad \text{with} \qquad \dot{\vec{u}} = \begin{pmatrix} \dot{q}_1 \\ \dot{q}_2 \\ \vdots \\ \dot{q}_n \\ \dot{p}_1 \\ \vdots \\ \dot{p}_n \end{pmatrix}$$

where the divergence is taken in the $2n$-dimensional phase space

When we take the derivatives of products in (*) we obtain

$$\sum_{k=1}^{n}\left(\frac{\partial \rho}{\partial q_k}\dot{q}_k + \rho\frac{\partial \dot{q}_k}{\partial q_k} + \frac{\partial \rho}{\partial p_k}\dot{p}_k + \rho\frac{\partial \dot{p}_k}{\partial p_k}\right) + \frac{\partial \rho}{\partial t} = 0$$

Now from the Hamilton equations we have

$$\frac{\partial \dot{q}_k}{\partial q_k} = \frac{\partial}{\partial q_k}\frac{\partial H}{\partial p_k} \quad \text{and} \quad \frac{\partial \dot{p}_k}{\partial p_k} = \frac{\partial}{\partial p_k}\left(-\frac{\partial H}{\partial q_k}\right)$$

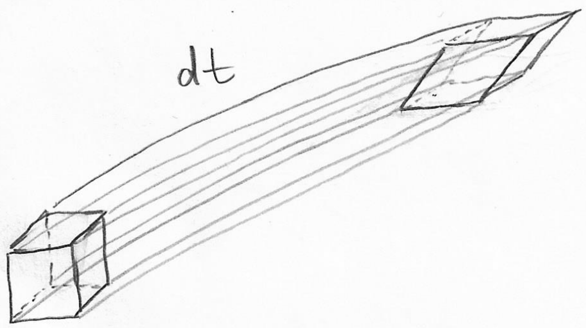
If the second partial derivatives are continuous those two terms will cancel each other and we will get

$$\sum_{k=1}^{n}\left(\frac{\partial \rho}{\partial q_k}\dot{q}_k + \frac{\partial \rho}{\partial p_k}\dot{p}_k\right) + \frac{\partial \rho}{\partial t} = 0 \qquad (**)$$

which is equal to the total time derivative of ρ:

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

Therefore ρ must be constant. If we watch a set of points in element of volume $d\mu$ and how the move in phase space we will see that the hyper-rectangle may change its shape but its volume will be unchanged.



Also note that equation (**) can be written using the Poisson bracket:

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \{\rho, H\}$$

This latter equation has the same algebraic structure as the equation that describes the time evolution of the density operator in quantum mechanics:

$$\frac{d\rho}{dt} = \frac{\partial \rho}{dt} + [\rho, H]$$

where [,] is the commutator