Liouville's theorem

Liouville's theorem is of fundamental importance to statistical mechanics. This theorem is based on the fact that the volume in the phase space is invariant under a canonical transformation.

To see this, lets consider the phase space of a system with one degree of freedom with the coordinate q and momentum p. The volume element in the phase space is

$$dV = dq\, dp$$

Under a canonical transformation $(q,p) \longrightarrow (Q,P)$ and the volume element is given by

$$dV' = dQ\, dP$$

We can write the volume element dV' in terms of the original coordinates. However, we must include the Jacobian as well

$$dV' = |J|\, dq\, dp$$

where the Jacobian is
$$J = \begin{vmatrix} \frac{\partial Q}{\partial q} & \frac{\partial Q}{\partial p} \\ \frac{\partial P}{\partial q} & \frac{\partial P}{\partial p} \end{vmatrix}$$

But the Jacobian is nothing but the (absolute value) of the Poisson bracket of the <u>new</u> phase-space coordinates in terms of the <u>old</u> ones. Hence

$$J = \{Q, P\}^{q,p} = 1$$

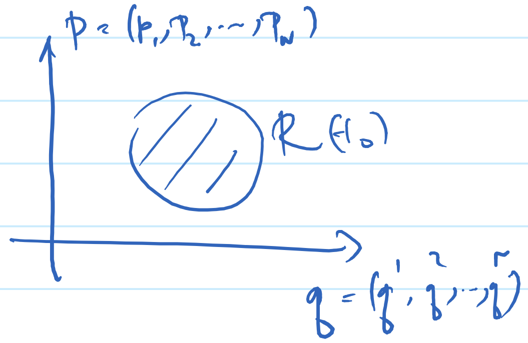
Therefore, the volume of the phase space is invariant under any canonical transformation.

However, why should we even care about the volume of the phase space?

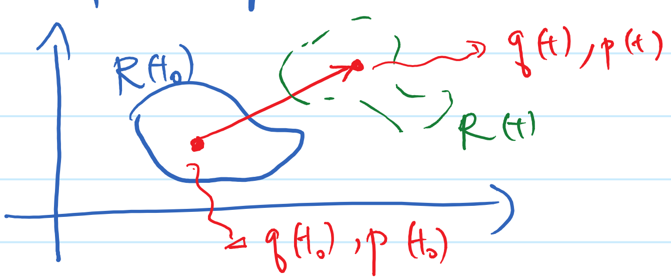
The answer, as advertised before, lies in the relation to statistical mechanics. In this context, we typically want to talk about the state of many particles $(q_1, q_2, \dots, q_N, p_1, \dots, p_N)$ where $N \sim 10^{23}$ for a macroscopic system.
It is hopeless to even attempt to specify and keep track of the state of all particles. In addition, initial conditions, are only incompletely known. We may be able to state that the energy at a given time has a certain value, however, we cannot determine the initial coordinates and velocities of all particles.

→ Statistical physics gets around this complicated task by making predictions about certain average properties. This average is done over an ensemble of systems. The appropriate quantity is then the number of systems in the neighborhood of a given point in phase space.

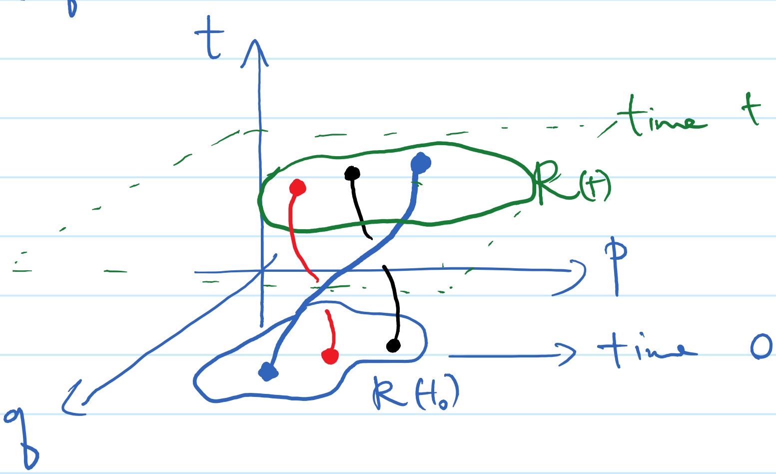
Let's consider a region in phase space representing different states of the system at time $t = 0$.



As time goes on, the system points defining the volume move around the phase space and takes different shapes



It is clear that the number of systems inside the volume does not change: If some system were to leave the volume, it has to cross the border. But then the phase-space orbits never collide because given any point in phase space, its future evolution should be unique.



Hence, the system can never leave the volume.

On the other hand, the volume also doesn't change either. This is because the Hamiltonian itself provides a canonical transformation

$$(q, p) \longrightarrow (q(t), p(t))$$

This can be seen by first inspecting infinitesimal changes under Hamiltonian dynamic. For infinitesimal Δt

$$q(t+\Delta t) \approx q(t) + \{q(t), H\}\,\Delta t$$

$$p(t+\Delta t) \approx p(t) - \{p(t), H\}\,\Delta t$$

Next we compute the Poisson bracket of $q(t+\Delta t)$ & $p(t+\Delta t)$

$$\{q(t+\Delta t),\ p(t+\Delta t)\}$$

$$\approx 1 + \Delta t\Big[\{\{q, H\}, p\} + \{q, \{p, H\}\}\Big]_{\text{at time } t}$$

$$= 1 + \Delta t \ \{\{q, p\}, H\}$$

$$= 1 \qquad \text{if} \quad \{q(t), p(t)\} = 1$$

This means that if $q(t)$ and $p(t)$ are canonical coordinates, they will remain so under the evolution by the Hamiltonian.

In general, the flow $q = q(\epsilon)$ and $p = p(\epsilon)$ defined by

$$\frac{d}{d\epsilon} q = \{q, f\} \quad \& \quad \frac{d}{d\epsilon} p = \{p, f\}$$

for any function f defines a one-parameter transformation (depending on ϵ). In this sense, f is the generator of the transformation. Hamiltonian is special as the generator of dynamical transformation. Under any such generator, phase-space coordinates flow to a new set of canonical coordinates $(q(\epsilon), p(\epsilon))$

Therefore, the volume of the phase space is invariant as time evolves.

It then follows that the same number of states occupy the same phase-space volume at all times.

A similar statement can be made in terms of the density of states near a point in the phase space

$$D = \frac{\Delta N}{\Delta V}$$

where ΔN is the number of systems occupying a volume ΔV in phase space. Liouville's theorem states

$$\int_{R_0} D(p,q,t_0)\, dV = \int_{R} D\left(p(t), q(t), t\right) dV'$$

Equivalently, we have

$$\rightsquigarrow \quad \frac{dD}{dt} = \left\{D, H\right\} + \frac{\partial D}{\partial t} = 0$$

When the system is in statistical equilibrium, the number of systems in a given state must be constant in time $\longrightarrow$ The density of states at a given point is constant in time

$$\frac{\partial D}{\partial t} = 0$$

which, together with Liouville's theorem, dictates

$$\left\{D, H\right\} = 0 \quad \text{in equilibrium.}$$

For example, a density of states that is a function of H automatically satisfies this equation. As an example, in microcanonical ensemble, D is constant for one value of H and zero otherwise $\left(D(H) = \delta(H - E) \right)$.