Classical Systems: Liouville

- classical systems evolve according to Hamilton's equations of motion

$$\Rightarrow H(\vec{q}_1, \dots, \vec{q}_\nu; \vec{p}_1, \dots, \vec{p}_\nu)$$

$$\dot{\vec{q}}_i = \frac{\partial H}{\partial \vec{p}_i} \qquad \dot{\vec{p}}_i = -\frac{\partial H}{\partial \vec{q}_i}$$

- phase space: space spanned by all coordinates $\vec{q}_1, \dots \vec{q}_\nu$ and all momenta $\vec{p}_1, \dots, \vec{p}_\nu$

a microstate in classical mechanics corresponds to one point in phase space (i.e. one particular set of values ~~for~~ all of $\vec{q}_1, \dots, \vec{q}_\nu$ and $\vec{p}_1, \dots, \vec{p}_\nu$)

- time-development is given by Hamilton's equations of motion: each point in phase space will trace out a trajectory in phase space

* Hamiltonian dynamics is reversible:

  - suppose that we start a trajectory at time $t=0$ $\vec{q}_1(0), .. \vec{q}_\nu(0); \vec{p}_1(0), \dots, \vec{p}_\nu(0)$

and let it evolve to $t=\tau$

$$\vec{q}_1(\tau), \dots, \vec{q}_\nu(\tau); \vec{p}_1(\tau), \dots, \vec{p}_\nu(\tau)$$

there will be a trajectory between $t=0$ and $t=\tau$

suppose that at time τ we reverse all momenta

$$\vec{p}_1(\tau), \dots, \vec{p}_N(\tau) \longrightarrow -\vec{p}_1(\tau), \dots, -\vec{p}_N(\tau)$$

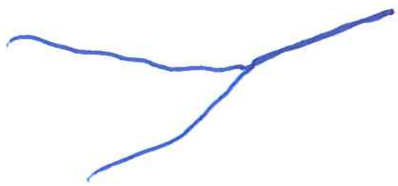
$$\vec{q}_1(\tau), \dots, \vec{q}_N(\tau) \longrightarrow \vec{q}_1(\tau), \dots, \vec{q}_N(\tau)$$

the trajectory traced out by the time evolution after time $t = \tau$ will trace out the same trajectory as the initial one from $t = 0$ to $t = \tau$

<u>phase space trajectories are unique!</u>

- to show this assume that they are not unique, and they can cross paths

example



at some point they meet and become one

but! this can not happen since Hamilton's equations of motion ~~are~~ determine a unique trajectory and they are reversible, which is not the case for the above example

⇓ ⇓

if I start with N phase space points and let them evolve in time ⇒ I will always have 1000 phase space points

- in the limit of a very large number of trajectories we can introduce a density associated with phase space (13)

$$\Rightarrow \quad \rho(\vec{q}_1, \dots \vec{q}_N; \vec{p}_1, \dots \vec{p}_N)$$

if the phase space points evolve in time, so does $\rho(\vec{q}_1, \dots \vec{q}_N; \vec{p}_1, \dots \vec{p}_N)$

since no phase space points can be created or destroyed $\Rightarrow$ $\int d\vec{q}_1 \dots d\vec{q}_N \, \rho(\vec{q}_1, \dots \vec{q}_N; \vec{p}_1 \dots \vec{p}_N)$ is fixed for any time

$\Rightarrow$ can define normalization

$$\int d\vec{q}_1 \dots d\vec{q}_N \, d\vec{p}_1 \dots d\vec{p}_N \, \rho(\vec{q}_1, \dots \vec{q}_N; \vec{p}_1 \dots \vec{p}_N) = 1$$

$\rho(\vec{q}_1, \dots \vec{q}_N; \vec{p}_1, \dots \vec{p}_N) \geq 0 \Rightarrow \rho$ is a probability density

~~pr.~~

- time evolution of the volume element

$$d\vec{q}_1(0) \dots d\vec{q}_N(0) \, d\vec{p}_1(0) \dots d\vec{p}_N$$

let us consider it for a 1D / 1-particle system to save notation

$\underline{dq(0)\,dp(0)}$ as time evolves we will have $dq(t)\,dp(t)$

for short time $dp(0)\,dq(0) \to dp(\Delta t)\,dq(\Delta t)$ (14)

the two are related by the Jacobian determinant

$$\begin{vmatrix} \frac{\partial p(\Delta t)}{\partial p(0)} & \frac{\partial p(\Delta t)}{\partial q(0)} \\ \frac{\partial q(\Delta t)}{\partial p(0)} & \frac{\partial q(\Delta t)}{\partial q(0)} \end{vmatrix}$$

$$p(\Delta t) = p(0) + \frac{\partial p(0)}{\partial t}\Delta t = p(0) - \frac{\partial H}{\partial q}\Delta t$$

$$q(\Delta t) = q(0) + \frac{\partial q(0)}{\partial t}\Delta t = q(0) + \frac{\partial H}{\partial p}\Delta t$$

$\Downarrow$

Jacobian: $$\begin{vmatrix} 1 - \frac{\partial H}{\partial p\,\partial q}(0)\,\Delta t & -\frac{\partial^2 H}{\partial q^2}(0)\,\Delta t \\ \frac{\partial^2 H}{\partial p^2}\Delta t & 1 + \frac{\partial^2 H}{\partial p\,\partial q}(0)\,\Delta t \end{vmatrix}$$

$$= 1 + O(\Delta t^2)$$

$\Rightarrow$ the phase space volume element

$d\vec{p}_1(0) \dots d\vec{p}_N(0)\, d\vec{q}_1(0) \dots d\vec{q}_N(0) \to$ does not vary with time

$\to$ consider the time derivative of $\rho(\vec{p}, \vec{q})$

$$\frac{d\rho(\vec{p}_1(0), \dots \vec{p}_N(0); \vec{q}_1(0), \dots \vec{q}_N(0))}{dt}$$

$$= \frac{\partial \rho}{\partial t} + \sum_i \frac{\partial \rho}{\partial \vec{p}_i}\frac{\partial \vec{p}_i}{\partial t} + \sum_i \frac{\partial \rho}{\partial \vec{q}_i}\frac{\partial \vec{q}_i}{\partial t} = 0$$

the total derivative $\frac{d\rho}{dt} = 0$ due to the fact (15)
that trajectories in phase space are neither created nor destroyed

$$\Rightarrow \frac{\partial \rho}{\partial t} = \underbrace{\sum_i \frac{\partial \rho}{\partial \vec{p}_i} \frac{\partial H}{\partial \vec{q}_i} - \sum_i \frac{\partial \rho}{\partial \vec{q}_i} \frac{\partial H}{\partial \vec{p}_i}}_{\text{Liouvillian time evolution}}$$

$$\frac{\partial \rho}{\partial t} = \{ \rho, H \} \Rightarrow \text{Poisson brackets}$$

- can also define operator $i\hat{L}$

$$i\hat{L}\rho = \{\rho, H\}$$

$$\frac{\partial \rho}{\partial t} = i\hat{L}\rho \Rightarrow \boxed{\rho(t) = e^{\overbrace{i\hat{L}t}^{\text{time-propagator}}} \rho(0)}$$

solution

- consider an average of some quantity

$$\bar{A}(0) = \int dp_0 dq_0 \; \rho(p_0, q_0) \, A(p_0, q_0)$$

as a function of time we would have

$$\bar{A}(t) = \int dp_0 dq_0 \; \rho(p_0, q_0) \, A(p_t, q_t)$$

can also be written as

$$\int dp_t dq_t \; \rho(p_0, q_0) \, A(p_t, q_t)$$

in first case:

$$\int dp_0 dq_0 \, \rho(p_0, q_0) A(p_t, q_t)$$

start with a set of phase space points at $t=0$ distributed according to

$$\rho(p_0, q_0)$$

propagate each one to time t

$$p_0, q_0 \longrightarrow p_t, q_t$$

average ~~over~~ $A(p_t, q_t)$ over propagated phase space points

second case:

$$\bar{A}(t) = \int dp_t dq_t \, \rho(p_0, q_0) A(p_t, q_t)$$

start with points at p_t, q_t

propagate them back to p_0, q_0

$$p_t \; q_t \longrightarrow p_0, q_0$$

$$\bar{A}(t) = \int dp_t dq_t \, \rho(p_0(p_t, q_t), q_0(p_t, q_t)) \, A(p_t, q_t)$$

weigh trajectories according to

$$\rho(p_0(p_t, q_t), q_0(p_t, q_t))$$

consider: $\int dp_t\, dq_t\, \rho(p_t, q_t)\, A(p_t, q_t)$

$$= \int dp_t\, dq_t\, \rho(p_t, q_t) \left[e^{i\hat{\mathcal{L}}t} A(p_0, q_0) \right]$$

Liouville acts on $A(p_0, q_0)$ not $\rho(p_t, q_t)$

expand $e^{i\hat{\mathcal{L}}t}$ as $1 + i\hat{\mathcal{L}}t$

consider 1^{st} order term in t

$$\int dp_0\, dq_0\, \rho(p_t, q_t) \left[i\hat{\mathcal{L}} t \right] A(p_0, q_0)$$

$$= t \int dp_0\, dq_0\, \rho(p_t, q_t) \left[\frac{\partial A}{\partial p_0} \frac{\partial p_0}{\partial t} + \frac{\partial A}{\partial q_0} \frac{\partial q_0}{\partial t} \right]$$

$$= -t \int dp_0\, dq_0 \left[\frac{\partial \rho(p_t, q_t)}{\partial p_t} A(p_0, q_0) \frac{\partial p_0}{\partial t} + \frac{\partial \rho(p_t, q_t)}{\partial q_t} A(p_0, q_0) \frac{\partial q_0}{\partial t} \right]$$

$$= \int dp_0\, dq_0 \left[-i\mathcal{L}t\, \rho(p_t, q_t) \right] A(p_0, q_0)$$

One can prove using this reasoning, applying it to higher order terms that

$$\int dp_t\, dq_t\, \rho(p_t, q_t) \left[e^{i\hat{\mathcal{L}}t} A(p_0, q_0) \right]$$

$$= \int dp_t\, dq_t \left[e^{-i\mathcal{L}t} \rho(p_t, q_t) \right] A(p_0, q_0)$$

$$= \int dp_0\, dq_0\, \rho(p_0, q_0)\, A(p_0, q_0)$$

Ergodicity

there are two kinds of averages:

* ensemble average:

$$\bar{A} = \int \rho(p,q)\, A(p,q)\, dp\, dq$$

* time average

$$\tilde{A} = \frac{1}{T} \int_0^T dt\, A(t)$$

- ensemble average: at a given point in time average over all ensemble members
- time average: choose one member of the ensemble and follow its dynamics over a large time $(T \to \infty)$ and perform average

⇒ ergodic hypothesis: according to the ergodic hypothesis, the ensemble average and the time average of the same quantity are equal

$$\Rightarrow \quad \bar{A} = \tilde{A}$$

it is a hypothesis

its content is that the system accesses all states which are available to it

it is necessitated by the fact that experimental time scales are long compared to microscopic time scales, and we want to use ensemble averaging to calculate experimentally accessible quantities