State of a system

Classical	Quantum
$\underline{p}_i, \underline{r}_i \quad i = 1, N$ Spin $\uparrow\downarrow$ (not really classical)	$\lvert\psi\rangle \in$ Hilbert space

We are not interested in these states only in a few intrinsic / extrinsic variables.

? Connection ?

Classical

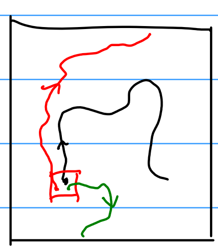
entropy

$$\boxed{S = k_B \ln \Omega}$$

Phase space

$\Gamma = \{ q^{3N}, p^{3N} \}$ 6N-dimensional

Phase space (cartoon)



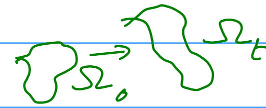
$$\dot{q}_{j\alpha} = \frac{\partial H}{\partial p_{j\alpha}} \qquad \alpha = x, y, z$$

$$j = 1, \ldots, N$$

$$\dot{p}_{j\alpha} = -\frac{\partial H}{\partial q_{j\alpha}}$$

Volume in phase space: (Lecture notes 2.3)

$$V(t) = \int_{\Omega_t} d^{3N}p \, d^{3N}q$$



Consider two times, $t=0$ and $t>0$ which is small

So we go from $\underline{p}_j(t=0)$ $\underline{q}_j(t=0)$ to $\underline{p}_j(t)$, $\underline{q}_j(t)$

The end values for $\underline{p}_j$ and $\underline{q}_j$ depend on the starting values:

$$\underline{q}_j(t) = \underline{q}_j(\underline{p}_j(0), \underline{q}_j(0)) \text{ and } \underline{p}_j(t) = \underline{p}_j(\underline{p}_j(0), \underline{q}_j(0))$$

We can view this as a 'mapping':

$$\underbrace{\underline{p}_j(0) \quad \underline{q}_j(0)}_{x} \xrightarrow{t} \underbrace{\underline{p}_j(t), \underline{q}_j(t)}_{y}$$

The integral changes according to the Jacobian J of the mapping:

$$J_{ij} = \frac{\partial y_i}{\partial x_j} \qquad x_i \to y_i$$

$$\to \quad V(0) = \int_{\Omega} d^{6N}x \qquad q^{3N} \, p^{3N}$$

$$\text{and } V(t) = \int_{\Omega} \det(J) \, d^{6N}x$$

Now use the fact that t is small:

$$q_{j\alpha}(t) = q_{j\alpha}(0) + t\,\frac{\partial H(\underline{p}_j(0), \underline{q}_j(0))}{\partial p_{j\alpha}} \qquad \alpha = x, y, z$$

$$p_{j\alpha}(t) = p_{j\alpha}(0) - t\,\frac{\partial H(\underline{p}_j(0), \underline{q}_j(0))}{\partial q_{j\alpha}}$$

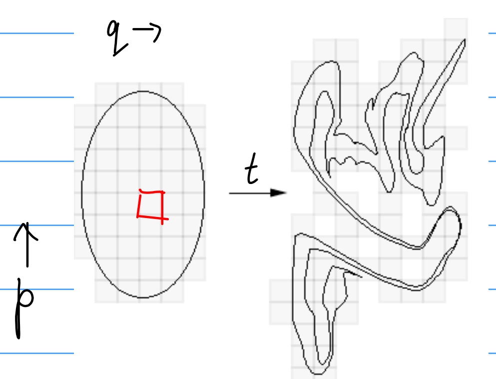
$$\rightarrow \quad J = \begin{array}{c c} & \begin{array}{cc} p & q \end{array} \\ \begin{array}{c} p \\ q \end{array} & \left(\begin{array}{c|c} \mathbb{1} - t\,\dfrac{\partial^2 H}{\partial q_{j\alpha}\,\partial p_{k\beta}} & t\,\dfrac{\partial^2 H}{\partial p_{j\alpha}\,\partial p_{k\beta}} \\ \hline -t\,\dfrac{\partial^2 H}{\partial q_{j\alpha}\,\partial q_{k\beta}} & \mathbb{1} + t\,\dfrac{\partial^2 H}{\partial p_{j\alpha}\,\partial q_{k\beta}} \end{array}\right) \end{array} =$$

$$\det(J) = 1 + \mathcal{O}(t^2)$$

So $V(t) = V(t=0) + \mathcal{O}(t^2)$

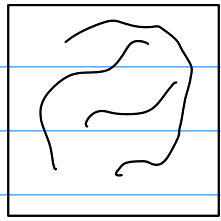
hence $\dfrac{dV}{dt} = 0 \Rightarrow$ volume remains constant

Note: $$\underset{\uparrow \atop \text{large}}{V(t)} = \int_0^t \underbrace{\frac{dV(t')}{dt'}}_{=0} dt' + V(0) = V(0).$$



$$\Delta p\, \Delta q \geq h = 2\pi\hbar$$

Phase space



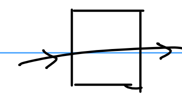
We study the flow in phase space . . (Lect notes 2.3)

$\rho(p^{3N}, q^{3N}; t)$: density of points in phase space.

$$\rho(p^{3N}, q^{3N}, t)\, d^{3N}p\, d^{3N}q = \text{nr of points within } d^{3N}p\, d^{3N}q$$

No sources and sinks of trajectories:

Change in density $\rightarrow$ $\dfrac{\partial \rho}{\partial t} = -\underline{\nabla}\cdot \underline{j}$ $\rightarrow$ difference between flow through opposing faces.



$$\underline{j} = \rho\, \underline{v}$$

$$\underline{v} = (\dot{p}^{3N}, \dot{q}^{3N})$$

$$\nabla = \Big(\overbrace{\frac{\partial}{\partial p_{j\alpha}}}^{3N}, \overbrace{\frac{\partial}{\partial q_{j\alpha}}}^{3N} \Big)$$

$$\frac{\partial}{\partial p_{1x}}, \frac{\partial}{\partial p_{1y}}, \ldots \quad \frac{\partial}{\partial p_{Ny}}, \frac{\partial}{\partial p_{Nz}}, \frac{\partial}{\partial q_{1x}}, \frac{\partial}{\partial q_{1y}}, \ldots$$

$$\frac{\partial \rho}{\partial t} = -\sum_{j\alpha}\left(\frac{\partial}{\partial p_{j\alpha}}(\rho\, \dot{p}_{j\alpha}) + \frac{\partial}{\partial q_{j\alpha}}(\rho\, \dot{q}_{j\alpha}) \right)$$

Use $\dot{p}_{j\alpha} = -\dfrac{\partial H}{\partial q_{j\alpha}}$; $\dot{q}_{j\alpha} = \dfrac{\partial H}{\partial p_{j\alpha}}$

$$= \sum_{j\alpha}\left(\frac{\partial \rho}{\partial p_{j\alpha}}\frac{\partial H}{\partial q_{j\alpha}} + \cancel{\rho\frac{\partial^2 H}{\partial p_{j\alpha}\partial q_{j\alpha}}} - \frac{\partial \rho}{\partial q_{j\alpha}}\frac{\partial H}{\partial p_{j\alpha}} - \cancel{\rho\frac{\partial^2 H}{\partial q_{j\alpha}\partial p_{j\alpha}}} \right).$$

$$= \sum_{j\alpha}\left(\frac{\partial \rho}{\partial p_{j\alpha}}\frac{\partial H}{\partial q_{j\alpha}} - \frac{\partial \rho}{\partial q_{j\alpha}}\frac{\partial H}{\partial p_{j\alpha}} \right) = -\{\rho, H\}$$

$$\{f, g\} = \sum_{j\alpha}\left(\frac{\partial f}{\partial q_{j\alpha}}\frac{\partial g}{\partial p_{j\alpha}} - \frac{\partial f}{\partial p_{j\alpha}}\frac{\partial g}{\partial q_{j\alpha}} \right)$$

$\{\ ,\ \}$ is called Poisson bracket

Some properties:

$$\{\rho, H\} = -\{H, \rho\}$$

$$\{H, H\} = 0$$

$$\{f(H), H\} = 0$$

Equilibrium: $\frac{\partial \rho}{\partial t} = 0$; $\{\rho, H\} = 0$

$\rho = \delta(H(p,q) - E)$. microcanonical ensemble

$$\rho = \frac{e^{-H(p,q)/k_B T}}{Z}$$ canonical ensemble.