Lecture 13 (Nov. 16)

- ## Hamiltonian mechanics

Recall that $H(q,p,t) = \sum_{\sigma=1}^{n} p_\sigma \dot{q}_\sigma - L(q,\dot{q},t)$ is a Legendre transform:

$$dH = \sum_\sigma \left(\cancel{p_\sigma d\dot{q}_\sigma} + \dot{q}_\sigma dp_\sigma - \frac{\partial L}{\partial q_\sigma} dq_\sigma - \cancel{\frac{\partial L}{\partial \dot{q}_\sigma} d\dot{q}_\sigma} \right) - \frac{\partial L}{\partial t} dt$$

$$= \sum_\sigma \left(- \frac{\partial L}{\partial q_\sigma} dq_\sigma + \dot{q}_\sigma dp_\sigma \right) - \frac{\partial L}{\partial t} dt$$

We conclude

$$\frac{\partial H}{\partial q_\sigma} = - \frac{\partial L}{\partial q_\sigma} = - \dot{p}_\sigma \quad , \quad \frac{\partial H}{\partial p_\sigma} = \dot{q}_\sigma$$

as well as

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} = - \frac{\partial L}{\partial t}$$

Note:

(i) If $\partial L/\partial t = 0$, then $dH/dt = 0$, i.e. H is a constant of the motion.

(ii) To express $H = H(q,p,t)$, we must invert the relation $p_\sigma = \frac{\partial L}{\partial \dot{q}_\sigma} = p_\sigma(q,\dot{q})$ to obtain $\dot{q}_\sigma(q,p)$. This requires that the Hessian,

$$\frac{\partial p_\sigma}{\partial \dot{q}_{\sigma'}} = \frac{\partial^2 L}{\partial \dot{q}_\sigma \partial \dot{q}_{\sigma'}}$$

be nonsingular. (cf. inverse function theorem)

(iii) Define the rank $2n$ vector $\vec{\xi}$ by

$$\vec{\xi} \equiv \begin{pmatrix} q_1 \\ \vdots \\ q_n \\ p_1 \\ \vdots \\ p_n \end{pmatrix} \Rightarrow \quad \xi_i \equiv \begin{cases} q_i & \text{if } 1 \le i \le n \\ p_{i-n} & \text{if } n < i \le 2n \end{cases}$$

Then we may write Hamilton's equations of motion as

$$\left.\begin{aligned} \dot{q}_\sigma &= \frac{\partial H}{\partial p_\sigma} \\ \dot{p}_\sigma &= -\frac{\partial H}{\partial q_\sigma} \end{aligned}\right\} \Rightarrow \quad \dot{\xi}_i = J_{ij} \frac{\partial H}{\partial \xi_j} \quad ; \quad J = \begin{pmatrix} 0 & \mathbb{1}_{n\times n} \\ -\mathbb{1}_{n\times n} & 0 \end{pmatrix}$$

Note that J is an antisymmetric rank $2n$ matrix. The coordinates $\{\xi_1, \dots, \xi_{2n}\} = \{q_1, \dots, q_n, p_1, \dots, p_n\}$ define a $2n$-dimensional **phase space**. If $\partial H/\partial t = 0$, then the equations of motion specify a rank $2n$ **dynamical system**, $\dot{\xi}_i = V_i(\vec{\xi})$, where

$$V_i(\xi) = J_{ij} \frac{\partial H(\vec{\xi})}{\partial \xi_j} = \text{velocity vector in phase space}$$

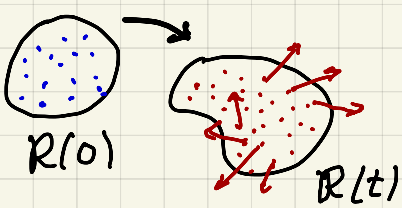
[If $\partial H/\partial t \ne 0$, define $\xi_0 = t$ and we have a rank $(2n+1)$ DS with $\dot{\xi}_0 = 1$ and $\dot{\xi}_i = V_i(\xi_0, \xi_1, \dots, \xi_{2n})$.]

– Incompressible flow in phase space

Consider the (autonomous) dynamical system

$$\frac{d\vec{\xi}}{dt} = \vec{V}(\vec{\xi})$$

where $\vec{\xi}(t) \in \mathbb{R}^N$. Consider now the evolution of a compact region $\mathcal{R}(t)$, each point in which evolves according to our DS. We have



$$\mathcal{R}(t) = \left\{ \vec{\xi}(t) \,\middle|\, \vec{\xi}(0) \in \mathcal{R}(0) \right\}$$

Now define $\Omega(t) = \mathrm{vol}\, \mathcal{R}(t) = \int_{\mathcal{R}(t)} d\mu$, where

$$d\mu = d\xi_1 \cdots d\xi_N$$

Then

$$\Omega(t+dt) = \int_{\mathcal{R}(t+dt)} d\mu' = \int_{\mathcal{R}(t)} d\mu \; \underbrace{\left\| \frac{\partial \xi_i(t+dt)}{\partial \xi_j(t)} \right\|}_{\text{Jacobian}}$$

where

$$\left\| \frac{\partial \xi_i(t+dt)}{\partial \xi_j(t)} \right\| = \frac{\partial(\xi_1', \ldots, \xi_N')}{\partial(\xi_1, \ldots, \xi_N)} = \det \frac{\partial \xi_i(t+dt)}{\partial \xi_j(t)}$$

i.e. the determinant of the Jacobian. Now

$$\xi_i(t+dt) = \xi_i(t) + V_i(\vec{\xi}(t))\, dt + \mathcal{O}(dt^2)$$

and therefore

$$\frac{\partial \xi_i(t+dt)}{\partial \xi_j(t)} = \delta_{ij} + \left. \frac{\partial V_i}{\partial \xi_j} \right|_{\vec{\xi}(t)} dt + \mathcal{O}(dt^2)$$

We now invoke the identity $\ln\det A = \mathrm{Tr}\ln A$ for any matrix A, which is easily demonstrated when A is put in diagonal form. Thus, with $A \equiv \mathbb{1} + \epsilon M$

$$\begin{aligned}\det(\mathbb{1}+\epsilon M) &= \exp \mathrm{Tr}\ln(\mathbb{1}+\epsilon M)\\ &= \exp \mathrm{Tr}\left(\epsilon M - \tfrac{1}{2}\epsilon^2 M^2 + \ldots\right)\\ &= 1 + \epsilon\,\mathrm{Tr}\,M + \tfrac{1}{2}\epsilon^2\left[(\mathrm{Tr}M)^2 - \mathrm{Tr}\,M^2\right] + \ldots\end{aligned}$$

and with $\epsilon = dt$ and $M_{ij}(\vec{\xi}) = \left.\dfrac{\partial V_i}{\partial \xi_j}\right|_{\vec{\xi}}$, we have

$$\Omega(t+dt) = \Omega(t) + \int\limits_{\mathcal{R}(t)} d\mu\, \vec{\nabla}\cdot\vec{V}\,dt + \mathcal{O}(dt^2)$$

i.e. the rate of change of $\Omega(t) = \mathrm{vol}\,\mathcal{R}(t)$ is given by

$$\frac{d\Omega}{dt} = \int\limits_{\mathcal{R}(t)} d\mu\, \vec{\nabla}\cdot\vec{V}$$

where $\vec{\nabla}\cdot\vec{V} = \sum\limits_{i=1}^{N} \dfrac{\partial V_i}{\partial \xi_i}$ = divergence of phase space velocity.

Alternate derivation: Let $\rho(\xi,t)$ be the density of some collection of points in phase space. This must satisfy the continuity equation,

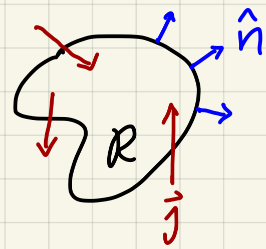
$$\frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot(\rho\vec{V}) = 0$$

Integrate over a region $\mathcal{R}$:

$$\frac{d}{dt}\int\limits_{\mathcal{R}} d\mu\,\rho = -\int\limits_{\mathcal{R}} d\mu\,\vec{\nabla}\cdot(\rho\vec{V}) = -\int\limits_{\partial\mathcal{R}} dS\,\hat{n}\cdot\rho\vec{V}$$

where $\partial\mathcal{R}$ is the boundary of $\mathcal{R}$. It is perhaps useful to think of ρ as a number or charge density and $\vec{j} \equiv \rho\vec{V}$ as the corresponding current density. Then if $Q_{\mathcal{R}} = \int_{\mathcal{R}} d\mu\,\rho$, then

$$\frac{dQ_{\mathcal{R}}}{dt} = -\int_{\partial\mathcal{R}} dS\, \underbrace{\hat{n}\cdot\vec{j}}_{(-\text{flux})}$$



Note that the Leibniz rule says

$$\frac{\partial\rho}{\partial t} + \vec{V}\cdot\vec{\nabla}\rho + \rho\vec{\nabla}\cdot\vec{V} = 0$$

and if $\vec{\nabla}\cdot\vec{V} = 0$, then

$$\frac{D\rho}{Dt} = \left(\frac{\partial}{\partial t} + \vec{V}\cdot\vec{\nabla}\right)\rho = 0$$

We call $\frac{D\rho}{Dt}$ the **convective derivative**, as it tells us the rate of change of ρ in a frame comoving with the local velocity $\vec{V}$. Thus,

$\dot{\vec{\xi}} = \vec{V}$

$$\frac{d}{dt}\rho(\vec{\xi}(t),t) = \frac{\partial\rho}{\partial t} + \dot{\vec{\xi}}\cdot\vec{\nabla}\rho = \frac{D\rho}{Dt}$$

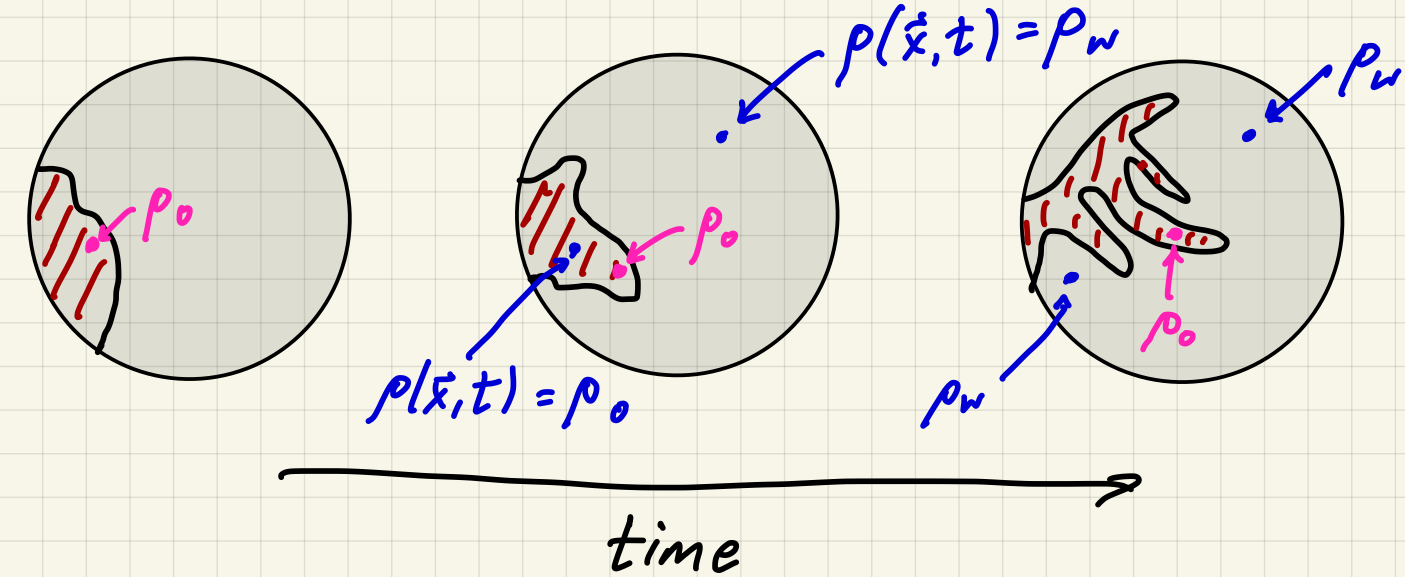
If we define

$$\rho(\vec{\xi}, t=0) = \begin{cases} 1 & \text{if } \vec{\xi}\in\mathcal{R}_0 \\ 0 & \text{if } \vec{\xi}\notin\mathcal{R}_0 \end{cases}$$

i.e. the "characteristic function" of $\mathcal{R}_0$, then the

Scratch

Immiscible fluids (e.g. oil and water):



Two possible values of $\rho(\vec{x},t)$: ρ_w and ρ_o

Volume of red region is preserved by dynamics.

vanishing of the convective derivative says that $\rho(\vec{\xi}(t), t)$ is a constant, hence the image $\mathcal{R}(t)$ of the set $\mathcal{R}(0) \equiv \mathcal{R}_0$ always has the same volume. In other words, the phase space flow is **incompressible.** Hamiltonian evolution is always incompressible:

$$\vec{\nabla} \cdot \vec{V} = \frac{\partial V_i}{\partial \xi_i} = \frac{\partial}{\partial \xi_i}\left(J_{ij} \frac{\partial H}{\partial \xi_j}\right) = J_{ij} \frac{\partial^2 H}{\partial \xi_i \partial \xi_j} = 0$$

- Poisson brackets

Consider the time evolution of any function $F(\vec{\xi}(t), t)$. We have

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \sum_{\sigma=1}^{n} \left\{ \frac{\partial F}{\partial q_\sigma} \dot{q}_\sigma + \frac{\partial F}{\partial p_\sigma} \dot{p}_\sigma \right\}$$

$$\equiv \frac{\partial F}{\partial t} + \{F, H\}$$

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

where

$$\{A, B\} \equiv \sum_{\sigma=1}^{n} \left(\frac{\partial A}{\partial q_\sigma} \frac{\partial B}{\partial p_\sigma} - \frac{\partial A}{\partial p_\sigma} \frac{\partial B}{\partial q_\sigma} \right) = \sum_{i,j=1}^{2n} J_{ij} \frac{\partial A}{\partial \xi_i} \frac{\partial B}{\partial \xi_j}$$

is the **Poisson bracket** of A and B. Properties of the PB:

- Antisymmetry : $\{A, B\} = -\{B, A\}$
- Bilinearity : for constant λ,

$$\{A + \lambda B, C\} = \{A, C\} + \lambda \{B, C\}$$

- Associativity:

$$\{AB, C\} = A\{B,C\} + B\{A,C\}$$

- Jacobi identity:

$$\{A,\{B,C\}\} + \{B,\{C,A\}\} + \{C,\{A,B\}\} = 0$$

We also have

- If $\{A,H\} = 0$ and $\partial A/\partial t = 0$, then $dA/dt = 0$, i.e. $A(q,p)$ is a constant of the motion.

- If $\{A,H\} = 0$ and $\{B,H\} = 0$, then by the Jacobi identity we have $\{\{A,B\},H\} = 0$, and if $\partial A/\partial t = 0$ and $\partial B/\partial t = 0$ (or, more weakly, if $\partial\{A,B\}/\partial t = 0$), then $\{A,B\}(q,p)$ is a constant of the motion.

- It is easily established that

$$\{q_\sigma, q_{\sigma'}\} = \{p_\sigma, p_{\sigma'}\} = 0 \quad , \quad \{q_\sigma, p_{\sigma'}\} = \delta_{\sigma\sigma'}$$

– Any density function $\rho(q,p,t)$ must satisfy continuity, hence

$$\frac{D\rho}{Dt} = \frac{\partial\rho}{\partial t} + \{\rho, H\} = 0 \Rightarrow \frac{\partial\rho}{\partial t} = -\{\rho,H\} = +\{H,\rho\}$$

Liouville eqn.

Consider a distribution $\rho(q,p,t) = \rho(\Lambda_1,\dots,\Lambda_k)$ where each Λ_a is conserved, i.e. $\Lambda_a = \Lambda_a(q,p)$ with

$$\frac{d\Lambda_a}{dt} = \sum_\sigma \left(\frac{\partial \Lambda_a}{\partial q_\sigma} \dot{q}_\sigma + \frac{\partial \Lambda_a}{\partial p_\sigma} \dot{p}_\sigma \right) = \{\Lambda_a, H\} = 0 .$$

Then $\rho(\Lambda_1, \dots, \Lambda_k)$ is a stationary sol^n to Liouville's equation, i.e.

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

Examples:

- microcanonical distribution:

$$\rho(q,p) = \delta(E - H(q,p))/D(E)$$

where the density of states $D(E)$ fixes the normalization

$$\int_{\mathbb{R}^{2n}} d\mu \, \rho(q,p) = 1 \Rightarrow D(E) = \int_{\mathbb{R}^{2n}} d\mu \, \delta(E - H(q,p))$$

- ordinary canonical distribution:

$$\rho(q,p) = \frac{1}{Z(\beta)} e^{-\beta H(q,p)}$$

with

$$Z(\beta) = \int_{\mathbb{R}^{2n}} d\mu \, e^{-\beta H(q,p)}$$

for normalization. You may know $\beta = 1/k_B T$. temperature

– Aside: It is conventional to define the **Liouvillean operator** $\hat{L}$ by $\hat{L}\,\bullet = i\{H,\bullet\}$, where $\bullet$ = anything. Thus,

$$\frac{\partial \rho}{\partial t} = \{H,\rho\} = -i\hat{L}\rho$$

which bears a resemblance to the Schrödinger equation.

- **Poincaré recurrence theorem** $\quad g_\tau \vec{\xi}(t) = \vec{\xi}(t+\tau)$

Let g_τ be the "τ-advance mapping" which evolves time by τ, i.e. integrate the dynamical system $\dot{\xi}_i = V_i(\vec{\xi})$ forward by a time $\Delta t = \tau$. We assume three conditions:

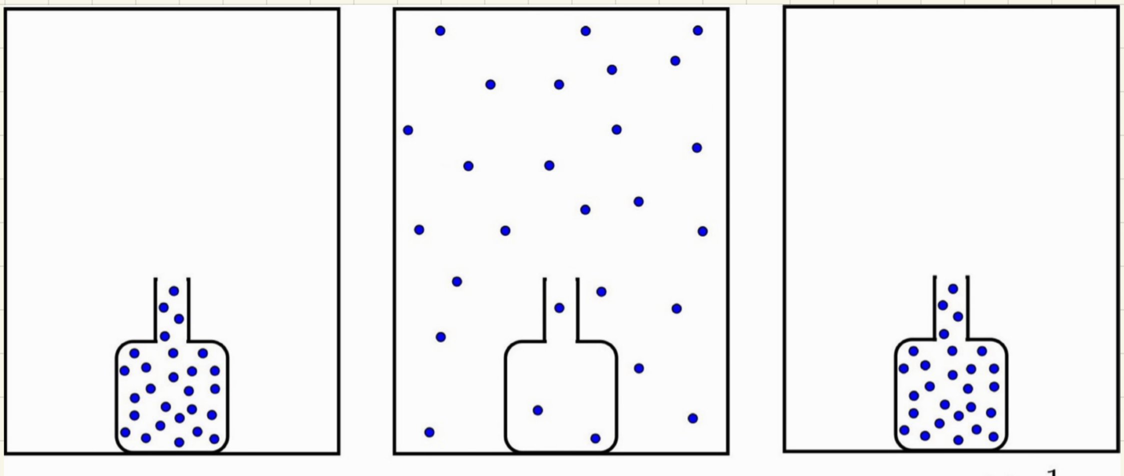
(i) g_τ is invertible (integrate DS backward by $-\tau$)
(ii) g_τ is volume-preserving (evolution is Hamiltonian)
(iii) accessible phase space volume is finite, e.g.

$$\int_{\mathbb{R}^{2n}} d\mu\, \Theta\big(E+\Delta E - H(q,p)\big)\,\Theta\big(H(q,p)-E\big) = \int_E^{E+\Delta E} dE'\, D(E') < \infty$$
$$\approx D(E)\,\Delta E$$

We will henceforth refer to the $(2n-1)$-dimensional hypersurface Γ defined by $H(q,p)=E$ as the "phase space" for Hamiltonian evolution.

Theorem: In any finite neighborhood $R_0 \subset \Gamma$ there exists a point $\vec{\xi}_0$ which returns to R_0 after finitely many applications of g_τ.

Before proving the theorem, let's consider first its remarkable consequences. Suppose we had a bottle of perfume which we open at time $t=0$ in an evacuated room. Initially all the perfume molecules are inside the bottle, with CM positions $\vec{R}_a(0)$ and orientations (for diatomic or polyatomic molecules) $\{\phi_a(0), \theta_a(0), \psi_a(0)\}$. The initial conditions also specify the corresponding velocities $\{\dot{X}_a(0), \dot{Y}_a(0), \dot{Z}_a(0), \dot{\phi}_a(0), \dot{\theta}_a(0), \dot{\psi}_a(0)\}$. With N polyatomic molecules, there are $6N$ coordinates and $6N$ velocities $\Rightarrow$ $12N$-dim$^{\ell}$ phase space. We choose $\mathcal{R}_0$ to be a ball in this space of arbitrarily small but finite size. The theorem says that there is an initial condition within the ball $\mathcal{R}_0$ which will repeat after a finite time $m\tau$, where $m \in \mathbb{Z}$. Thus, all the molecules return to the bottle, and to within $\mathcal{R}_0$ of their initial configuration! (However, this **recurrence time** may be much, much



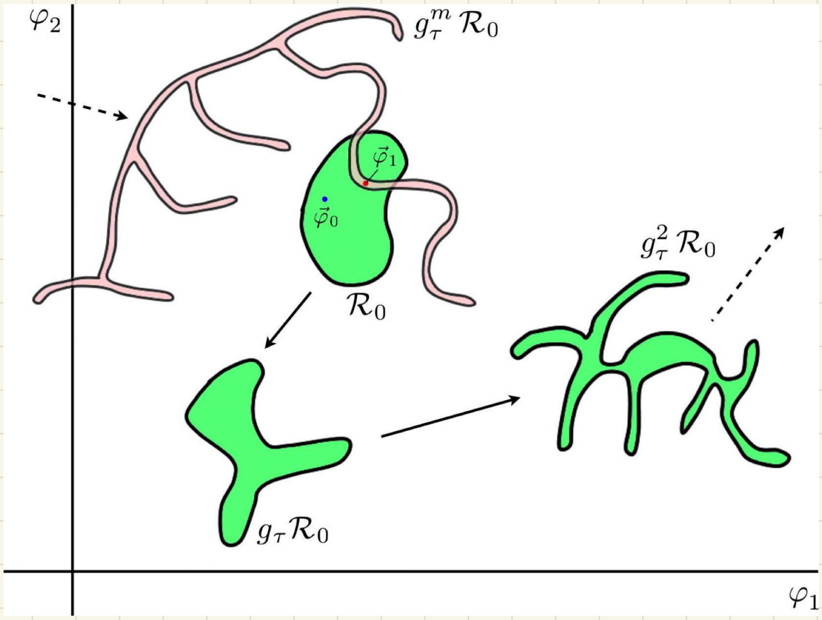
$t=0$ $\quad$ $t=1\,\mathrm{s}$ $\quad$ $t>>\mathsf{H}^{-1}$

greater than the age of the universe!)

Proof: Assume the theorem fails and there is no recurrence. We will prove this results in a contradiction. Consider the union $\Delta = \bigcup_{k=0}^{\infty} g_\tau^k R_0$ of all the images of $g_\tau^k R_0$, where $k \in \{0, 1, \ldots, \infty\}$. Suppose all these images are disjoint. Then

$$\mathrm{vol}(\Delta) = \sum_{k=0}^{\infty} \mathrm{vol}(g_\tau^k R_0) = \sum_{k=0}^{\infty} \mathrm{vol}(R_0) = \infty$$

where we have used that g_τ is **volume-preserving**. Since $\mathrm{vol}(\Gamma) < \infty$, we contradict **finite volume**. Therefore the sets $\{g_\tau^k R_0 \mid k \in \mathbb{Z}_{\geq 0}\}$ cannot be disjoint, i.e. there must exist two finite integers k and l with $k \neq l$ such that $g_\tau^k R_0 \cap g_\tau^l R_0 \neq \emptyset$. Due to **invertibility**, the inverse map g_τ^{-1} exists. Assume wolog that $k > l$ and apply



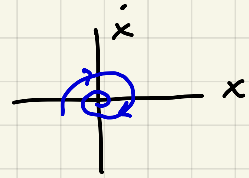
the map $(g_\tau^{-1})^\ell$ to this relation, obtaining

$$R_0 \cap g_\tau^m R_0 \neq \phi$$

where $m = k - \ell > 0$. Now choose any point $\vec{\xi}_1 \in R_0 \cap g_\tau^m R_0$.
Then $\vec{\xi}_0 \equiv (g_\tau^{-1})^m \vec{\xi}_1 \in R_0$ lies within R_0 and we have proven the theorem!

Each of the three conditions – volume preservation, invertibility, and finite phase space volume – are essential here, and if any one doesn't hold the proof fails, viz.

- g_τ not volume-preserving: E.g. damped oscillator with $\ddot{x} + 2\beta\dot{x} + \omega_0^2 x = 0$. Then with $\vec{\xi} = (x, \dot{x})$ we have $\vec{V} = (\dot{x}, -2\beta\dot{x} - \omega_0^2 x)$ and



$$\vec{\nabla}\cdot\vec{V} = \frac{\partial \dot{x}}{\partial x} + \frac{\partial(-2\beta\dot{x} - \omega_0^2 x)}{\partial \dot{x}} = -2\beta$$

Thus phase space volumes collapse: $\Omega(t) = e^{-2\beta t}\,\Omega(0)$.
The set Δ can be of finite volume even if all the $g_\tau^k R_0$ are distinct, because

$$\sum_{k=0}^{\infty} \Omega(k\tau) = \sum_{k=0}^{\infty} e^{-2k\beta\tau}\,\Omega_0 = \frac{\Omega_0}{1 - e^{-2\beta\tau}} < \infty$$

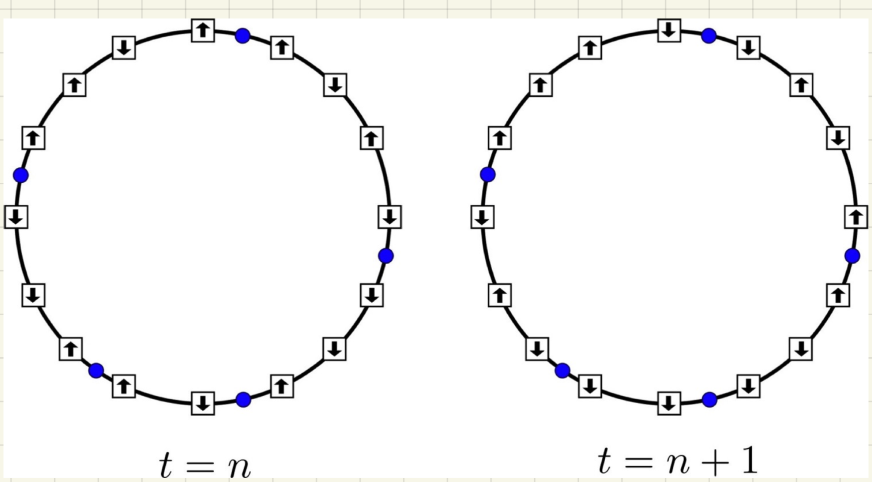
The phase space orbits all spiral into the origin and will not be recurrent. Note g_τ is invertible and phase space is of finite total volume.

- g_τ not invertible: Let $g : \mathbb{R} \to [0,1)$ with $g(x) = \mathrm{frac}(x)$, the fractional part of x. Acting on sets of volume (length) less than one, this map is volume preserving, but obviously g is not invertible, so the proof fails.

- Γ not finite: Let $g : \mathbb{R} \to \mathbb{R}$ with $g(x) = x + a$. Clearly this is invertible and volume-preserving, but not recurrent.

- Kac ring model   Lecture 14 (Nov. 18)

Can a system exhibit both equilibration and recurrence? Formally no, but practically yes. We noted how for the case of the open perfume bottle, the recurrence time could be vastly longer than age of the universe. A nice example due to Mark Kac shows how both equilibration and recurrence can be present, on different but accessible time scales. Consider N spins $\uparrow$ or $\downarrow$ on



a ring which evolve by rotating clockwise. There are thus N sites and N links. Along F of these links are