PHYS 614 Spring 2022

Note: This version of 614 builds on 613 as taught by Jayson Paulose in Winter 2022. The 613 table of contents was as follows:

Chapter 1 | Principles of Statistical Mechanics (with applications in QM)

§1 Statistical description of large systems

1.1 Phase flow of Hamiltonian systems

Consider a conservative classical mechanical system with f degrees of freedom. Let the generalized coordinates and momenta be

$$q(t) = (q_1(t), \dots, q_f(t))$$
$$p(t) = (p_1(t), \dots, p_f(t))$$

def. 1: The phase space Γ of the system is the set of points

$$z(t) = (q(t), p(t))$$

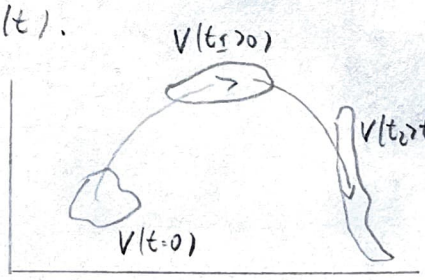
i.e. $2f$-dimensional space

remark: (1) Given an initial condition $z(t_0)$, Hamilton's eqs uniquely determine $z(t)$ $\forall\, t > t_0$ and $\forall\, t < t_0$.

lemma: Liouville's theorem

Let $D \subset \Gamma$ be a bounded region, and consider its time evolution $D(t)$ according to Hamilton's eqs. Let $V(t)$ be a volume of $D(t)$.

Then $\boxed{V(t) = V(t=0) = \text{const}}$



remark: (2) Phase flow is a volume-preserving mapping in Γ

proof: PHY 5 61]

def. 2: Let $G = \{f_\alpha, \alpha \in \mathbb{R}\}$ be a set of mappings. G is called a <u>one-parameter group of transformations</u> if

(1) G is a group under successive mapping operations, and

(2) $f_{\alpha=0} = 1$ and $f_{\alpha+\beta} = f_\alpha f_\beta$

remark: (3) All such groups are isomorphic to $\mathbb{R}(+)$.

def. 3: The operator U that describes phase flow via

$$\boxed{z(t) = U(t-t_0)\,z(t_0)}$$

is called <u>time evolution operator</u>

lemma 2: The set of time evolutions $\{U(t), t \in \mathbb{R}\}$ forms a one-parameter group under successive time evolutions.

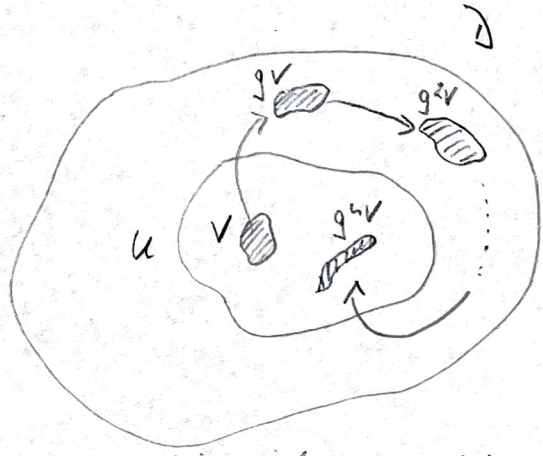
proof: PHYS 613

remark: (4) Time evolution is continuous and invertible.

1.2 Poincaré's theorem

theorem: <u>Poincaré's recurrence theorem</u>

Let G be a group of volume-preserving, continuously invertible mappings of $\mathbb{R}_n$ onto itself. Let D be a bounded region in $\mathbb{R}_n$ with $GD \subset D$. Then for every region $U \subset D$ and for every $g \in G$ there exists a $n \geq 1$ ($n \in \mathbb{N}$) and a region $V \subset U$ such that $\boxed{g^n V \subset U}$



remark: (1) V returns to U after a finite number of mapping ⇝ recurrence theorem

(2) $n < \infty$ ⇝ theorem occurs arbitrarily many times

U can be arbitrarily small ⇝ theorem is arbitrarily accurate!

proof: Assume the elements of $\{g^n U; 0 \le n \le N\}$ are pairwise disjoint,

i.e., $g^n U \cap g^m U = \emptyset \quad \forall n, m \le N \quad \forall N \in \mathbb{N}$

⇝ $\mathrm{Vol}\left(\bigcup_{n=0}^{N} g^n U\right) = (N+1)\,\mathrm{Vol}(U) \le \mathrm{Vol}(D)$

⇝ $N+1 \le \mathrm{Vol}(D)/\mathrm{Vol}(U) \quad (*)$

Choose $N = \mathrm{int}\left(\mathrm{Vol}(D)/\mathrm{Vol}(U)\right)$

⇝ $N+1 > \mathrm{Vol}(D)/\mathrm{Vol}(U)$, which contradicts $(*)$

⇝ $\exists N \in \mathbb{N}$: the elements of $\{g^n U; 0 \le n \le N\}$ are not pairwise disjoint

⇝ $\exists k_1, k_2,\ 0 \le k_1 < k_2 \le N: g^{k_1} U \cap g^{k_2} U \ne \emptyset$

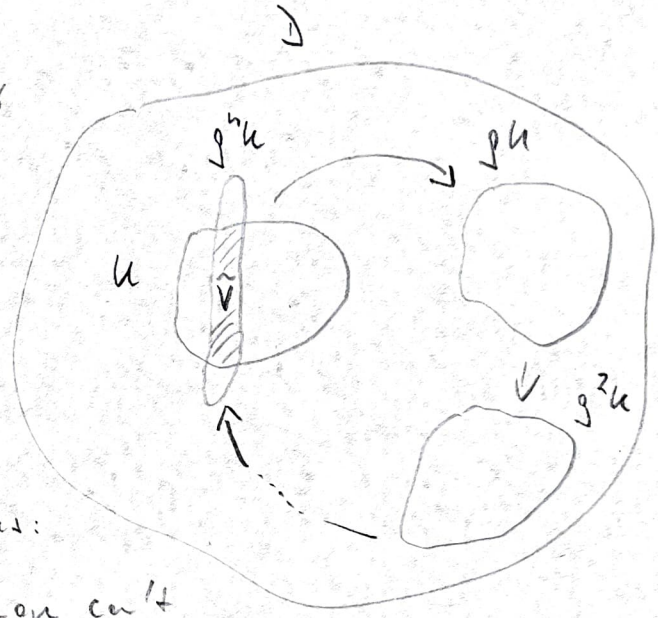
⇝ $\exists x, y \in U: g^{k_1} x = g^{k_2} y$ ⇝ $\underset{\substack{\cap \\ g^{k_2-k_1} U}}{g^{k_2-k_1}} = y \in U$

Choose $n = k_2 - k_1$ (⇝ $1 \le n \le N$) ⇝ $g^n U \cap U \ne \emptyset$

define $\tilde{V} := g^n U \cap U \neq \emptyset$

define $V := g^{-n} \tilde{V}$

$\rightsquigarrow$ $\underline{\underline{g^n V = \tilde{V} \in U}}$ $\square$



remark: (1) important premises:

$GD \subset D$ $\rightsquigarrow$ image can't get out of D

g is volume preserving $\rightsquigarrow$ mapping runs out of space to put the image $\sim$

Problem 1 (plane flow)
Problem 2 (Circle translations)
Problem 3 (Torus translations)
Problem 4 (Powers of 2)

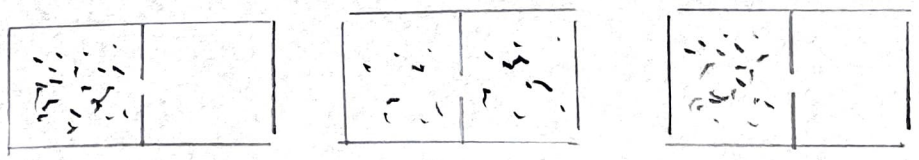
(4) This is a purely geometrical theorem. For physical applications, let

D = hypersurface in Γ allowed by energy conservation

U = ε-neighborhood of some point $z \in D$.

corollary: Let a mechanical system at time t_0 be in a state given by $z_0 \in \Gamma$. Then within a finite amount of time it comes arbitrarily close again to z_0.

example: gas in a partitioned container



t_0 $\qquad$ $t_1 > t_0$ $\qquad$ $\infty > t_2 > t_1$

(cf. Kerigan's book p 20ff)

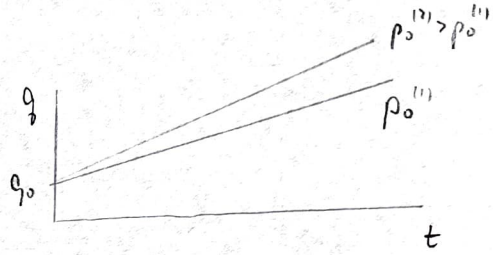
1.5 Necessity of a statistical description of many-particle systems

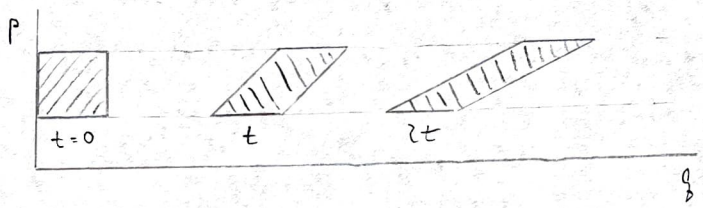
Consider time evolution of single systems in phase space according to Liouville's and Poincaré's theorems.

examples: (1) Free particle in $d=1$

$p(t) = p_0$

$q(t) = q_0 + (p_0/m)\,t$



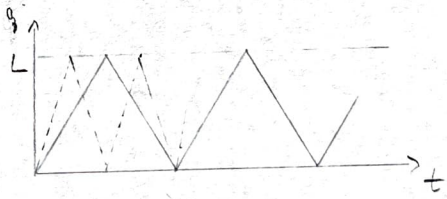


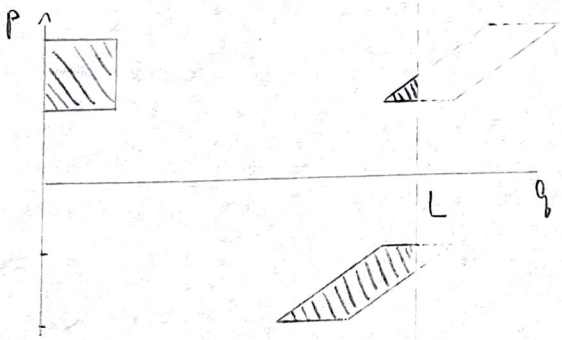
(2) Particle in a 1-d potential well

$p(t) = \pm p_0$

$q(t) = q_0 + (p_0/m)\,t$

+ inverted motion





p not continuous ⇒ system becomes disconnected

$t \to \infty$: disconnected parts become thinner and thinner, but must not overlap
⇒ folded structure

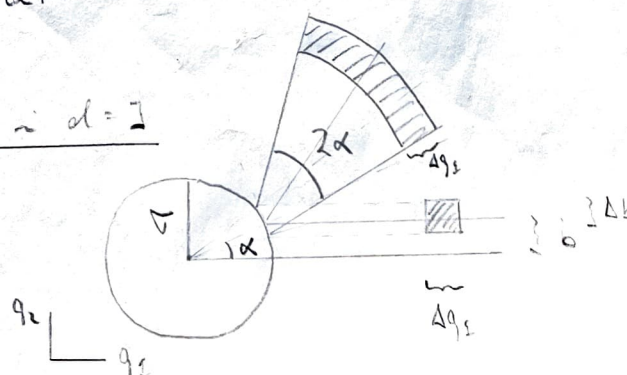
demonstration: Poincaré portrait

(3) Particle scattered by hard spheres in $d=2$

$b/\sigma = \sin\alpha$

$\Delta q_1' = \Delta q_1$

⇒ q-contribution to phase space

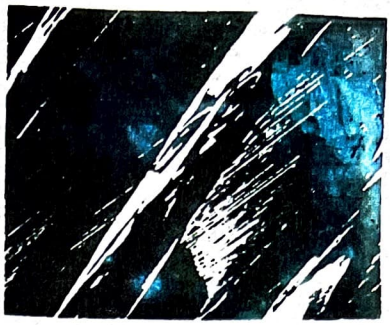


$\sqrt{a}$

0

1

2



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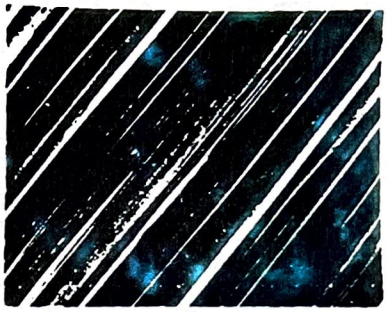

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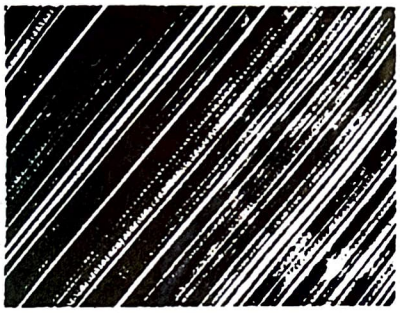

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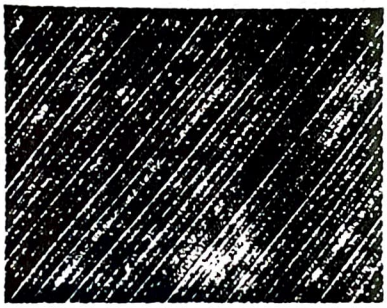

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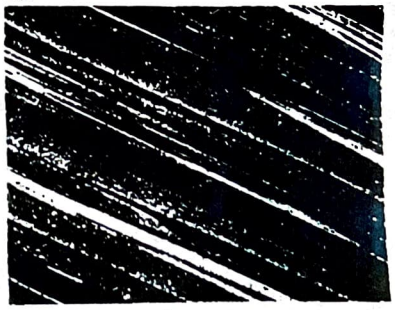

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let $\alpha \ll 1 \rightarrow \Delta\alpha = \Delta b/\sigma = \Delta q_2/\sigma$

then - for path $l \gg \sigma \rightarrow$ new spatial volume after 1 collision:

$$\underline{V'} = \Delta q_1' \cdot l \cdot 2\Delta\alpha = \Delta q_1 \cdot l \cdot 2\Delta q_2/\sigma$$
$$= \underline{V(2l/\sigma)}$$

$\rightarrow$ in d dimensions, $V' \sim V(2l/\sigma)^{d-1}$

Liouville $\rightarrow$ $\boxed{\text{momentum contribution to phase space volume has decreased by a factor of } (\sigma/2l)^{(d-1)N} \text{ after } N \text{ collisions.}}$

problem: <u>"Butterfly effect" (Bond)</u>

After N collisions, a single volume in Γ has been transformed into a foliated structure with typical dimensions

$$\boxed{(\Delta p)_N / \Delta p \sim (\sigma/2l)^{(d-1)N}}$$

example: classical gas of hard spheres with radius σ, density $n \rightarrow l = 1/n\sigma^2$

$\rightarrow \sigma/l \sim n\sigma^3 =: n^* \sim 10^{-3}$ in a typical gas

<u>$d=3, N=3$</u>: $(\Delta p)_N/\Delta p \sim (10^{-3})^{2\cdot 3} = 10^{-18}$ (!)

$\rightarrow$ After a few collisions, ridiculous accuracy is required to maintain the foliated structure!

remark: (1) <u>real experiment</u>: weakest force: gravity $F/m = \frac{Gm}{r^2} = 7\times10^{-8}\,\frac{m}{s^2}$

momentum uncertainty due to uncontrollable forces:

$$\Delta p \sim F/\tau \rightarrow \Delta p/p \sim \frac{F}{m}\frac{\tau}{v}$$

classical gas: $v \sim 10^5$ m/s, $\tau \sim 10^{-9}$ s typical

$\rightarrow$ $\boxed{\Delta p/p \sim 10^{-21}\, m/r^2 \; [\text{cgs}]}$

(i) $M = 1g$ at distance $r = 100m$ (butterfly outside lab)

$\rightsquigarrow \Delta p/p \sim 10^{-29}$

$\rightsquigarrow$ folded structure destroyed after $N \sim \frac{29}{3.2} \sim 5$ collisions

(ii) $M = 1g$ at distance $r = 1\,pc = 3 \times 10^{16}\,m$ (butterfly on Sirius)

$\rightsquigarrow \Delta p/p \sim 10^{-54}$

$\rightsquigarrow$ folded structure destroyed after $N \sim \frac{54}{3.2} = 9$ collisions

(2) computer experiment: rounding error introduces uncontrollable perturbation.

conclusion: (1) microscopically deterministic description of N-particle systems (with time reversibility, Poincaré's theorem, etc.) is impossible, since we have no control over butterflies on Sirius.

(2) Experiment $\rightsquigarrow$ time averages of macroscopic quantities are independent of these instabilities.

(3) Develop statistical (rather than deterministic) description of many-particle systems.

Week 1

Problem 1 (#1, 2, 3, 4)