Physics 210B

Module I - Kinetic Theory

I.) Mechanics Foundations

Boltzmann Eqn./Kinetic Theory Founded on Hamiltonian Mechanics

→ Review of Foundations in Classical Mechanics ⇒ Develop Kinetic Theory!

Statistical Dynamics is simply the marriage of mechanics and statistical treatment of a large number of particles ($N \gg 1$) / DOFs.

→ Key Concepts: (Meaning?)

- Hamiltonian System, Liouville Theorem
- Integrability
- Resonances and Chaos
- Ergodicity and Mixing, Kolmogorov/Dynamical Entropy

N.B.: - Not self-contained
- See standard refs - list.

– Hamiltonian Systems

How Hamiltonian?

$L = L(q, \dot{q}, t)$

or

$\mathcal{L} = \mathcal{L}(\phi, \dot{\phi}, \partial\phi/\partial x)$ $\qquad \phi \equiv$ field

$\Rightarrow p = \partial L/\partial \dot{q}$, [solve $\dot{q}$ in terms p. → Invertibility $A_{ij} = \frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j}$]

$H = H(p, q) = p\underbrace{\dot{q}}_{\text{eliminate}} - L$

$$\boxed{\dot{p} = -\frac{\partial H}{\partial q}, \quad \dot{q} = \frac{\partial H}{\partial p}}$$

– p, q "equal footing"

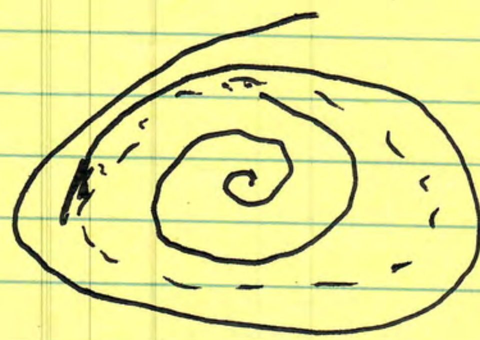
– usual phase space parametrization

i.e. $f(p, q, t) \equiv$ <u>phase</u> <u>space</u> <u>density</u>

→ distribution function

No attractors $\Leftrightarrow$ No sources, sinks, asymptotically stable cycles.

Yes



No

$$\int d^3p \; f(\underline{p}, \underline{q}, t) = n(\underline{q}, t) \quad , \quad \text{etc.}$$

Liouville Thm:

- "Phase volume conserved"
- "Phase space density conserved along particle orbits."

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial \underline{q}} \cdot (\dot{\underline{q}} f) + \frac{\partial}{\partial \underline{p}} \cdot (\dot{\underline{p}} f) = 0$$

$$\frac{\partial \dot{q}}{\partial \underline{q}} + \frac{\partial \dot{p}}{\partial \underline{p}} = \underline{\nabla} \cdot \underline{V}_{\Gamma} = 0$$

Phase space flow incompressible for Hamiltonian system

$$\frac{\partial f}{\partial t} + \underline{V}_{\Gamma} \cdot \underline{\nabla}_{\Gamma} f = 0 = \frac{df}{dt}$$

$$\underline{V}_{\Gamma} = (\dot{\underline{q}}, \dot{\underline{p}})$$

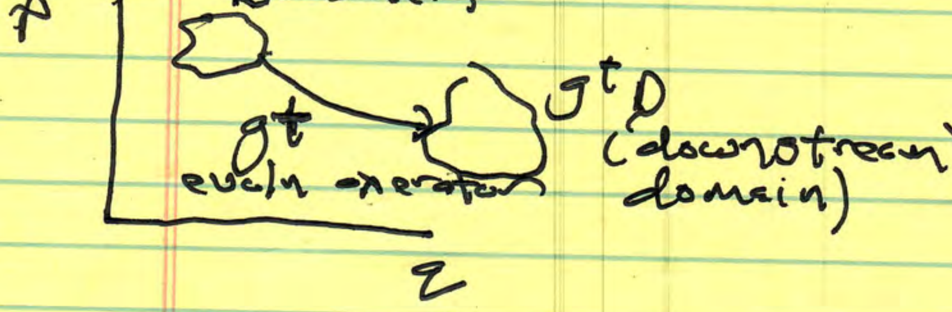
$\Rightarrow \underline{\nabla} \cdot \underline{V}_{\Gamma} = 0$

$\boxed{\text{\underline{no} \underline{attractors} in Hamiltonian Mechanics.}}$

⇒ Related: Poincare Recurrence Theorem

Define: phase space flow
g^t: transformation s/t

$p(0), q(0) \rightarrow p(t), q(t)$, along trajectories



g^t ↳ transformation in time (small increment)

First: Another look at Liouville ...

- Now, Hamiltonian equations constitute autonomous system.

$$\underline{\dot{x}} = \underline{f}(\underline{x})$$

$$\begin{pmatrix} \dot{\underline{q}} \\ \dot{\underline{p}} \end{pmatrix} = \begin{pmatrix} \partial H/\partial \underline{p} \\ -\partial H/\partial \underline{q} \end{pmatrix}$$

↓ defines $\underline{x}$ ↓ defines $\underline{f}$

then for small increment:

$$g^t(\underline{x}) = \underline{x} + \underline{f}(\underline{x})\,t + o(t^2)$$

so phase volume V_{t_0} at t:

$$V_{t_0}(t) = \int_{D(0)} d\underline{x} \left| \frac{\partial \underline{x}'}{\partial \underline{x}} \right|$$

↳ Jacobian of transform

$$= \int_{D(0)} d\underline{x} \, \det \left| \frac{\partial \underline{g}^t(\underline{x})}{\partial \underline{x}} \right|$$

$$\frac{\partial \underline{g}^t(\underline{x})}{\partial \underline{x}} = \underline{\underline{I}} + \frac{\partial \underline{f}}{\partial \underline{x}} t + o(t^2)$$

t small, identity:

$$\det(\underline{\underline{I}} + \underline{\underline{A}}\,t) \cong 1 + t \operatorname{tr} \underline{\underline{A}}$$

so $$V_{t_0}(t) = \int d^2x \left[1 + t \operatorname{tr}\left[\frac{\partial \underline{f}}{\partial \underline{x}}\right] + o(t^2) \right]$$

but $\text{tr}\, \dfrac{\partial \underline{f}}{\partial \underline{x}} = \underline{\nabla} \cdot \underline{f}$

and $\underline{V}_p = \underline{f}$ $\quad \underline{\nabla} \cdot \underline{V}_p = 0$ so

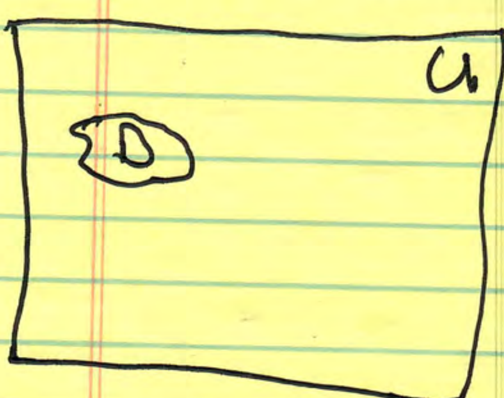
$\underline{\nabla} \cdot \underline{f} = 0.$

so $\boxed{V_\Gamma(t) = V(0)}$ phase volume conservancy

$\Rightarrow$ Recurrence

→ Fundamental to $\boxed{\text{ergodic}}$ theory

⇒ loosely, "what goes around, comes around, arbitrarily closely", for bounded Hamiltonian system

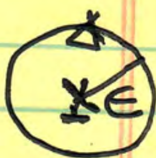


$U \equiv$ system universe, bounded

g^t Hamiltonian – volume preserving

For any $\underline{x}$ in U, can define

$B(\underline{x}, \epsilon)$



ball (neighborhood) in phase space around point $\underline{x} \leftrightarrow (\underline{q}, \underline{p})$ of radius ϵ

then

$$\exists\, \underline{x}' \in B(\underline{x}) \text{ such that}$$

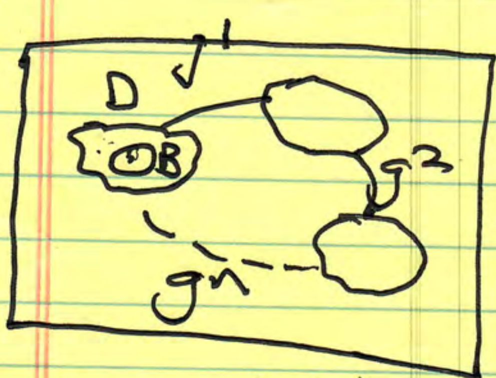
$$g^n(\underline{x}') \in B(\underline{x})$$

$\Rightarrow$ there is a point in the ϵ-ball of $\underline{x}$ such that n-iterations of evolution operator yield a point in ϵ ball

$\rightarrow$ Point/orbit recurs, arbitrarily closely

N.B. Why is this of concern in statistical mechanics?

Proof:



Consider $g^n(B)$,

if each g^i disjoint,

$\lim_{n\to\infty} \bigcup g^n \Rightarrow \infty$, but U bounded

$\Rightarrow$ contradiction!

So, must have:

$$g^k(B) \cap g^l(B) \neq \emptyset$$

intersection of arbitrary iterates not empty

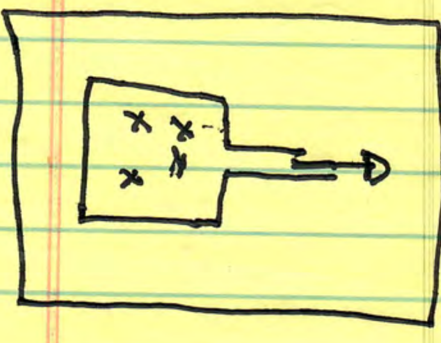
$\Rightarrow$

$$\boxed{g^{k-l}(B) \cap B \neq \emptyset}$$

So, $\exists$ some $\underline{x}'$ arbitrarily close to x.

Q.E.D. / AADFCPS

Implications

- 

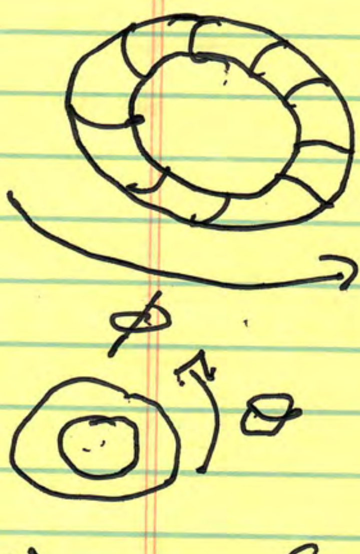
  box with particles

  → particles escape thru hole

  → eventually (?) will re-enter

  Time.

- torus (why?)



$\dot{\varphi}_1 = \alpha_1$
$\dot{\varphi}_2 = \alpha_2$ or $\dot{\theta} = \alpha_1$, $\dot{\phi} = \alpha_2$

$\boxed{\text{Consider } \alpha_1/\alpha_2 \text{ \underline{irrational}}}$

then: if $g^t(\varphi_1, \varphi_2) = (\varphi_1 + \alpha_1 t, \varphi_2 + \alpha_2 t)$

then α_1/α_2 irrational $\Rightarrow$ winding 'fills' the torus

i.e. comes arbitrarily close to i.c.

But stays on torus.

$\Rightarrow$ Classic example of ergodicity. N.B linear in time.

→ Integrability and Torus Destruction

Integrability $\Rightarrow$ can canonically transform

$\underline{p}, \underline{q} \rightarrow \underline{J}, \underline{\theta}$ $\left\{ \begin{array}{l} \text{action angle} \\ \text{variables} \end{array} \right.$

s/t

$$\frac{d\underline{J}}{dt} = 0, \quad \frac{d\underline{\theta}}{dt} = \underline{\omega}(\underline{J})$$

i.e. $\left\{ \begin{array}{l} \text{all variables cyclic.} \\ \underline{J} \text{ constant} \rightarrow \text{IoMs} \end{array} \right.$

motion defines torus
(n-torus)

$$\frac{d\theta}{dt} = \omega_1 (J_1)\, t$$

$$\frac{d\phi}{dt} = \omega_2 (J_2)\, t$$

scanning J_1, J_2 ⇒ define <u>nested tori</u>

i.e. box and particle: <u>2D</u>

$$\begin{cases} \omega_1 = \pi^2 J_1 / m a^2 \\ \omega_2 = \pi^2 J_2 / m b^2 \\ E = J_1 \omega_1 + J_2 \omega_2 \end{cases}$$

- motion on each toroidal surface ergodically, unless ω_1 / ω_2 rational

- set of surfaces ⇒ Volume of phase space.

- motion is <u>conditionally periodic</u>
  ⇒ Poincare Recurrence guarantees 'almost return' to <u>i.c.</u>

Begs two questions:

→ what if unable to integrate?

⇒ integrate approximately

$$H = H_0(\underline{J}) + \epsilon H_1(\underline{J}, \underline{\theta})$$

unperturbed, integrable

symmetry breaking perturbation

integrate to some order in ϵ,

i.e. transform $\underline{J}, \underline{\theta} \to \underline{I}, \underline{\phi}$

$$\text{s/t} \quad \underline{\dot{I}} = 0$$

$$\underline{\dot{\phi}} = \omega(\underline{I})$$

→ How fragile are surfaces? Can nested structure be maintained with $O(\epsilon)$ deformation?

Answer (?) via canonical perturbation theory - i.e. PT which maintains Hamiltonian structure.

Perturbation expansion as canonical transformation.

1 DOF

$$\phi = \theta + \epsilon \frac{\partial S_1}{\partial \underline{I}}(\underline{J},\theta)$$

$$I = \underline{J} - \epsilon \frac{\partial S_1}{\partial \theta}(\underline{J},\theta)$$

$$\omega = \omega_0(\underline{I}) + \epsilon \frac{\partial}{\partial \underline{I}} K_1(\underline{I})$$

$$\boxed{\begin{aligned} S_1 &= -\sum_n \frac{H_{n,1}(\underline{I})}{\boxed{i n \omega_0(\underline{I})}} e^{in\theta} \\ K_1 &= \langle H_1 \rangle \end{aligned}}$$

1 DOF ok. | Beyond: (2+ DOF)

[redacted] $n\omega_0(\underline{I}) \rightarrow \boxed{\underline{n} \cdot \underline{\omega}_0(\underline{I})} \rightarrow 0$! ?

i.e. $n_1 \omega_{0,1} + n_2 \omega_{0,2} = 0$

$n_1 \alpha_1 + n_2 \alpha_2 = 0$

Resonance !

⇒ occurs at rational surfaces, i.e.

$\alpha_1/\alpha_2 = -n_2/n_1$ (sign irrelevant)

winding ratio is rational number

$-\frac{n_2}{n_1} = \frac{\text{pitch}}{\text{winding}} = \frac{\omega_1}{\omega_2}$ pitch of perturbation

Trajectories close ⇒ don't ergodically cover the surface.

⇒ identifies where:

- perturbative integration fails
- surfaces most 'fragile'.

⇒ $\boxed{\text{Welcome to the small denominator problem !}}$

- crucial to Hamiltonian chaos.

See Ott, Chapt. 7

Examples:

e.g. - Wave - particle

$V = \omega/k$

$E_0 e^{i(kx-\omega t)}$

$\left(\frac{\partial S}{\partial t} = H - H'\right)$

time explicit

- field lines / tokamak

$q = m/n$. $\quad q = q(r)$

How forward ?!

$\Rightarrow$ If 1 (isolated) resonance, secular perturbation theory (~ avg. over fast variable)

[see SI notes, Lichtenberg, Lieberman

Can transform into form:

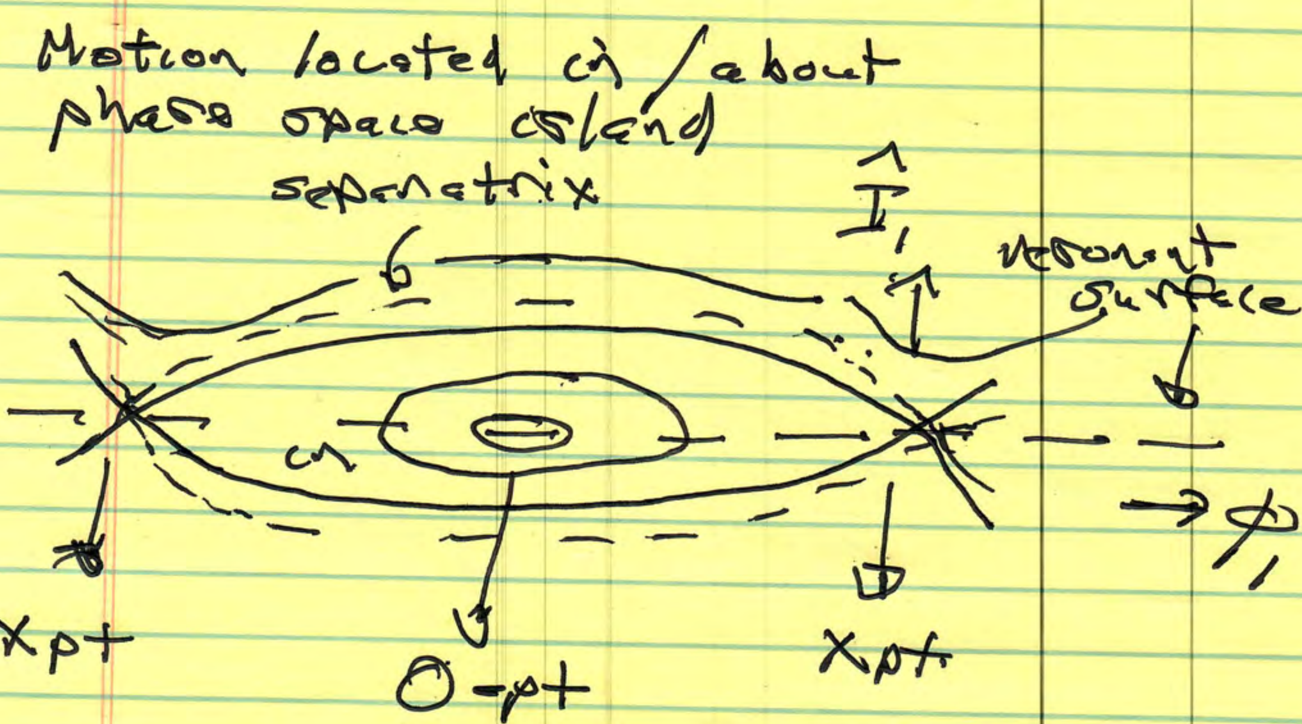
$$\boxed{\begin{aligned}
\langle H(\hat{I}_1, \phi_1)\rangle &= \frac{1}{2}(\hat{I}_1 - \hat{I}_{1,0})^2 \left.\frac{\partial^2 H_0}{\partial \hat{I}_1^2}\right|_{\hat{I}_{1,0}} - F\cos\phi_1 \\
&= \frac{G}{2}(\hat{I}_1 - \hat{I}_{1,0})^2 - F\cos\phi_1 \\
G &= \left.\frac{\partial^2 H_0}{\partial \hat{I}_1^2}\right|_{\hat{I}_{1,0}}, \quad F = -2\epsilon H'_{1,s}
\end{aligned}}$$

~ pendulum

~ $\frac{\partial^2 H}{\partial \hat{I}_1^2} = \frac{\partial \omega}{\partial \hat{I}_1} \neq 0$ "sheer"
→ differential rotation in θ

"accidental resonance"

⇒ Motion located in/about phase space island



- divides phase space into bounded/trapped and circulating orbits

- "island" → island chain

- foliates on distorts resonant surface

– Width of separatrix → "island width"

$$(\Delta I)_{max} \cong 2(F/G)^{1/2}$$

$$\cong 2\left(-2\epsilon H^{(1)}_{n,s} \Big/ \left.\frac{\partial^2 H_0}{\partial I_1^2}\right|_{I_{1,0}}\right)^{1/2}$$

i.e. if particle + wave:

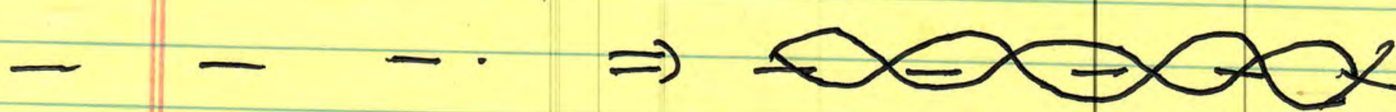
$$H = (p + m\omega/k)^2/2m + q\phi_0 \cos kx$$

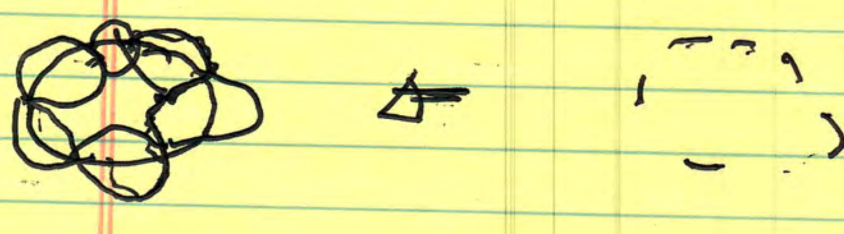
$$\Delta p = (q\phi_0 m)^{1/2}$$

$$\Delta v = (q\phi_0/m)^{1/2}$$ → trapping width

So

→ Resonant surfaces foliated / filamented





- not destroyed

- motion remains on surface, though surface ruffled.