Advanced Stat. Mech.

Stat Mech is the study of systems with very many particles: solid, liquid, EM radiation → physical & biological.
Presently, systems with very many particles are probably the most active field of research, maybe outside high-energy physics.

In HE-physics: we study interactions →
→ challenge.

In many-body systems: interactions are known. But are these systems understood in principle? No! This is misleading.

For example, Laplace: give me a full description of the system(s) at t_0, and I will predict its future → hopeless!
In practice: complexity of equations of motion makes this statement nearly meaningless.
⟹ butterfly effect: read Ray Bradbury's "Sound of Thunder": sensitive dependence on ICs! ⟹ in extreme case → chaos!

Stat. Mech: Intro + History

First **core** physical theory in which probabilistic concepts & explanations played a fundamental role.

Start: 17th century: mostly empirical

material (physical) systems can be described by a small number of parameters that are related in simple law-like ways.

These parameters – geometric, dynamical & thermal properties of matter.

Examples: * ideal gas law ($P, V \to T$)

* concept of equilibrium

$\Downarrow$

Stat Mech to handle systems with many degrees of freedom

Usual fundamental laws of phys. are **deterministic** (i.e. explainable)

$\Longleftrightarrow$ predictability, causality

Some History.

17th century – mostly empirical approach

* Torricelli – mercury barometer
* Boyle – introduced P
* Boyle – Mariotte law: PV = const for T = const.

* concept of equilibrium vs non-equil.

18 century – modest developments

* Bernoulli (1738) – billiard model of gas flow → kinetic gas theory
  gas laws rederived (kinetic vs caloric theory)

19 century – wow!

* Herapath (1821), Joule (1851) } kinetic theory of gases ($P \leftrightarrow$ molecular motion)
* Krönig (1856) – equal probability to fly $\pm x, \pm y, \pm z$
* Clausius (1857) (father of stat mech) – mean square v, m.f.p. → transport
* Maxwell (1860), Boltzmann (1868-71) } $e^{-\beta\epsilon}$ factor
  ⇒ equipartition theorem
  ⇒ MB – distribution ← collisions
  ⇒ H-theorem (1872) → approach to equilibrium

{h or η}

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H-theorem ⇒ tendency of a physical system to approach equilib.

⇓

attacked by Loschmidt (76/77)
Zermelo (1896)

⇓

main issue : reversibility vs irreversibility of physical laws (eqs. of motion)

⇒ from kinetic theory ⇒ ensembles (∞ no. of identical systems)

20th century — !!!

Gibbs (1902) - contact between theory & experiment
- generalized mech. systems

⇓

* they are mechanical
* obey Lagrange & Hamilton eqs of motion

Planck (1900) - quantum hypothesis

Fermi-Dirac (1926)
Bose-Einstein (1924/5)

Pauli (1925) - exclusion principle

Belinfante (1939) } relation of FD/BE to
Pauli (1940) } particle spin

Ensembles

In classical mech: a system can be specified by a set of canonically conjugate generalized coordinates and momenta:

$$(q_a, p_a)$$

$a = 1 \ldots N_f$

N_f – # of degrees of freedom

Example: N particles in a box

$$q_a = (\vec{x}_i, \; i = 1 \ldots N)$$

where $\vec{x}$ is d-dimensional vector representing the position

$$p_a = (\vec{p}_i, \; i = 1 \ldots N)$$

where $\vec{p}$ is d-dimensional momentum

Here $\quad N_f = Nd$

Example: radiation in a box

q_a – $\vec{A}(\vec{x}) \leftarrow$ vector potential at point $\vec{x}$

p_a – $\vec{E}(\vec{x}) \leftarrow$ electric field at point $\vec{x}$

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Observable quantities

$F(q_a, p_a)$ some function

Phase Space

$(q_a; p_a)$ coordinates on a $2N_f$-dimensional space

point on this space $\equiv$ state of the system

Hamiltonian systems

As time evolves, the state also evolves

$\Longrightarrow q_a(t), p_a(t)$

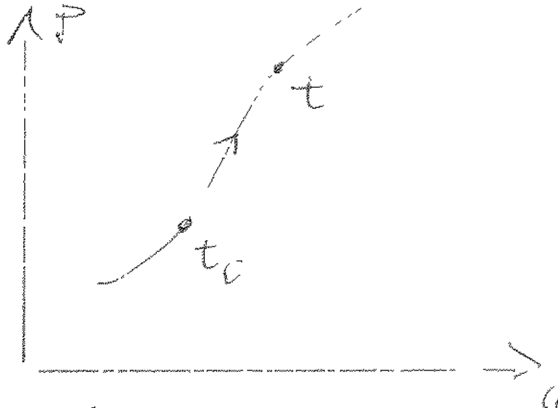
For Hamiltonian systems

$$\begin{cases} \dot{p}_a(t) = -\dfrac{\partial H}{\partial q_a(t)} \\ \dot{q}_a(t) = \dfrac{\partial H}{\partial p_a(t)} \end{cases}$$ Hamiltonian eqs. of motion

$H(p_a, q_a, t)$ is a function on phase space

Since these are 1st order eqs. in time, p_a, q_a at a given time $t = t_i$ specifies $q_a(t), p_a(t)$ at all times.

$\Rightarrow$ May represent time evolution by a trajectory in phase space



For any observable $F(q_a, p_a, t)$

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \sum_a \left(\frac{\partial F}{\partial q_a} \frac{\partial q_a}{\partial t} + \frac{\partial F}{\partial p_a} \frac{\partial p_a}{\partial t} \right) =$$

$$= \frac{\partial F}{\partial t} + \sum_a \left(\frac{\partial F}{\partial q_a} \frac{\partial H}{\partial p_a} - \frac{\partial F}{\partial p_a} \frac{\partial H}{\partial q_a} \right) =$$

$$= \frac{\partial F}{\partial t} + \underbrace{\{F, H\}_{PB}}_{\text{Poisson brackets}}$$

where

$$\{A, B\} = \sum_a \left(\frac{\partial A}{\partial q_a} \frac{\partial B}{\partial p_a} - \frac{\partial A}{\partial p_a} \frac{\partial B}{\partial q_a} \right)$$

<u>Here</u>, we use Einstein summation convention

Example: $H = \frac{P^2}{2m} + \frac{1}{2} m\omega^2 x^2$

$N_f = 1$

$$\Rightarrow \frac{dx}{dt} = \frac{P}{m} \; ; \quad \frac{dP}{dt} = -m\omega^2 x$$

A general solution:

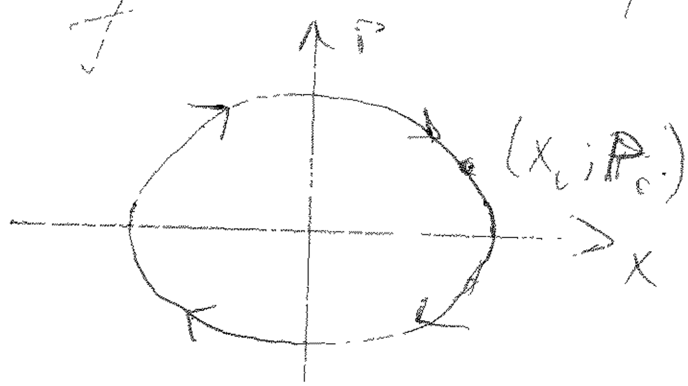
$$\begin{cases} x(t) = x_0 \cos\omega t + \frac{P_0}{m\omega} \sin\omega t \\ P(t) = P_0 \cos\omega t - m\omega x_0 \sin\omega t \end{cases}$$

$$\begin{cases} x_0 = x(0) \\ P_0 = P(0) \end{cases}$$

H is time-independent.

$$\frac{dH}{dt} = 0 \Rightarrow H = E \text{ for all times}$$

Trajectory is an ellipse:



All points on the ellipse have the same value of $H = E_0$

Different ellipses $\Rightarrow$ harmonic oscillator with different energies

Here the ellipse is a constant energy surface.

A simple H is a trivial example of a system where during the course of time evolution, the system visits every possible state with a given energy.

anti-Example: $H = \frac{1}{2m}\left(P_1^2 + P_2^2\right) + \frac{1}{2}m\omega^2\left(X_1^2 + X_2^2\right)$

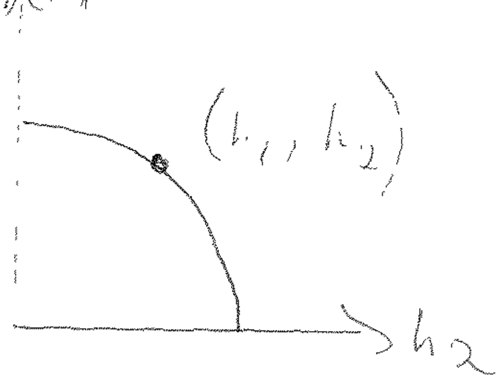
This is an example of a system which has additional conserved quantity

$$\begin{cases} h_1 = \frac{1}{2m}P_1^2 + \frac{1}{2}m\omega^2 X_1^2 \\ h_2 = \frac{1}{2m}P_2^2 + \frac{1}{2}m\omega^2 X_2^2 \end{cases}$$

where h_1, h_2 are individually conserved

$$E = h_1 + h_2$$

This system does **not** visit all possible states with same total energy — but visits all possible states with same (h_1, h_2) — two decoupled oscillators



system does **not** visit all $E \rightarrow$ set $\Gamma(E)$

All we need is a "weather" condition
$\Rightarrow$ mixing

Mixing: consider an initial compact distribution of points in $\Gamma(E)$. As it evolves, region fills entire $\Gamma(E)$

$\Longrightarrow$ a hypothesis that leads to Stat. Mech.

$\Downarrow$

initial distribution of points in $\Gamma(E)$ very quickly distorts into a convoluted object which permeates the entire surface while occupying the same volume $\Rightarrow$ Liouville theorem