# Chapter 1: Introduction

## 1.1) What is statistical mechanics?

20th century, 3 scientific revolutions

→ quantum mechanics for the infinitely small (2022 Nobel prize on Bell inequalities)

→ relativity for the infinitely large (2017 Nobel Prize on gravitational wave)

→ statistical mechanics with the infinitely complex (2024 Nobel prize for neural networks)

In a Nutshell

$$\boxed{\text{Microscopic constituents}} \xrightarrow[\text{mechanics}]{\text{statistical}} \boxed{\text{Complex emerging behaviors}}$$

Rather small number of atoms $\xrightarrow{\text{emergence}}$ Very complex macroscopic world

Question: How do we account for this?

① "More is different" Phil Anderson, 1972

A large number of particles can self-organize into states of matter with properties unmatched at the single-particle level

ex: Solid state can resist external forces

→ Does this mean that accounting for this diversity is hopeless? No, because

## (II) Different is often the same

Many emerging phenomena look alike.

ex: Hexagonal packing in honeycomb, pineapple, Giant causeway, cell tissue (eye of flies), etc.

→ The recurrence of these patterns suggests the existence of underlying organizing principles. Deciphering them is the goal of statistical mechanics.

## (III) More can also be simpler

* Poincaré: 3-body problem is not solvable & classical mechanics with few degrees of freedom is very hard
* $1\,m^3$ of air $\sim 10^{23}$ molecules ⇒ horribly complicated!

But $T = 22°C$, $P = 1$ bar, Humidity $= 50\%$ are 3 numbers that suffice to characterize pretty well these $\sim 10^{23}$ degrees of freedom.

→ emerging simplicity

Goal of statistical mechanics: Identify the microscopic details that are useless, eliminate them & construct selfcontained theory that accounts for the emerging properties of a system.

Comments: This is generic and may apply outside physics: economy, epidemiology, computer science, sociology have research fields at the interface with statistical physics. Here: focus on particles.

# 1.2) Equilibrium statistical mechanics: the ensemble approach

Most laws of physics are dynamical: Maxwell's equations, Einstein's equation, Schrödinger's equation, etc.

$\Rightarrow$ Very complicated PDEs that predict the state of a system given the perfect knowledge of its state at an earlier time

## Two limitations

(i) Measuring the state of a system is very hard $(N \sim 10^{23})$

(ii) Solving these equations is very hard

## Ensemble approach

Do not even try, this is useless.

Instead, characterize the probability to find the system in a given state.

## Classical system

$N$ degrees of freedom $(q_1, \dots, q_N, p_1, \dots, p_N) \equiv (\vec{q}, \vec{p})$

* Prepare the system with some initial condition & let it evolve. Repeat $\mathcal{N}$ times

$$\vec{q}_i(0), \vec{p}_i(0) \xrightarrow{\text{evolution}} \vec{q}_i(t), \vec{p}_i(t) \quad ; \quad i \in \{1, \dots, \mathcal{N}\}$$

* Initial conditions not always the same

$\rho(\vec{q}^{\,0}, \vec{p}^{\,0}, t=0) \underbrace{\prod_j dq_j\, dp_j}_{\equiv\, d\Gamma}$ is the proba that initial condition is such that

$q_i(t=0) \in [q_i^0, q_i^0 + dq_i]$ & $p_i(t=0) \in [p_i^0, p_i^0 + dp_i]$

evolution of trajectories

the proba that, at time $t$,

$\rho(\vec{q}^{\,0}, \vec{p}^{\,0}, t)\, d\Gamma$

$q_i(t) \in [q_i^0, q_i^0 + dq_i]$ & $p_i(t) \in [p_i^0, p_i^0 + dp_i]$

$\rho(\vec{q}^{\,0},\vec{p}^{\,0},t)$ is the probability density to find $\vec{q}(t)$, $\vec{p}(t)$ within a volume $d\Gamma$ of $\vec{q}^{\,0}$, $\vec{p}^{\,0}$ at time $t$.

For simplicity, we drop the "$0$" superscript & write $\rho(\vec{q},\vec{p},t)$. ⚠ Here $\vec{q}$ & $\vec{p}$ are fixed position & momenta, while $\vec{q}(t)$ & $\vec{p}(t)$ are solutions of Hamilton's equation...

Averages Consider some quantity $O(\vec{q},\vec{p})$, that we refer to as an observable. We define the average of $O$ at time $t$ as

$$\langle O(t)\rangle = \lim_{\mathcal{N}\to\infty} \frac{1}{\mathcal{N}} \sum_{i=1}^{\mathcal{N}} O(\vec{q}_i(t),\vec{p}_i(t)) \qquad (1)$$

$$= \int d\vec{q}\,d\vec{p} \quad O(\vec{q},\vec{p})\,\rho(\vec{q},\vec{p},t) \qquad (2)$$

Again, in (1), $\vec{q}_i(t)$ & $\vec{p}_i(t)$ are trajectories while in (2) they are fixed vectors.

If we have $\rho(\vec{q},\vec{p},t)$, then we can predict the values of $\langle O(t)\rangle$ for any observable.

Statistical mechanics As $t\to\infty$, the probability density $\rho(\vec{q},\vec{p},t)$ converges towards its steady-state value $\rho_{ss}(\vec{q},\vec{p}) = \lim_{t\to\infty} \rho(\vec{q},\vec{p},t)$.

Equilibrium statistical mechanics Boltzmann, Gibbs & others guessed what $\rho_{ss}$ is for a wide class of systems.

## 1.2.1) The microcanonical ensemble

Consider an isolated classical system characterized by a time independent Hamiltonian $H(\vec{q}, \vec{p})$.

Dynamics $\vec{q}(t)$ & $\vec{p}(t)$ solutions of $\dot{\vec{q}}(t) = \frac{\partial H}{\partial \vec{p}}$ & $\dot{\vec{p}}(t) = -\frac{\partial H}{\partial \vec{q}}$, where $\frac{\partial}{\partial \vec{q}} = \left(\frac{\partial}{\partial q_1}, \dots, \frac{\partial}{\partial q_N}\right)$ & $\frac{\partial}{\partial \vec{p}} = \left(\frac{\partial}{\partial p_1}, \dots, \frac{\partial}{\partial p_N}\right)$.

The energy $E(t) = H(\vec{q}(t), \vec{p}(t))$ is a constant of motion

$$\frac{d}{dt} E(t) = \frac{\partial H}{\partial \vec{q}} \cdot \dot{\vec{q}}(t) + \frac{\partial H}{\partial \vec{p}} \cdot \dot{\vec{p}}(t) = 0 \qquad \text{(Chain rule)}$$

$\Rightarrow$ the dynamics takes place along the energy surface $\{\vec{q}, \vec{p} \text{ s.t. } H(\vec{q}, \vec{p}) = E(0)\}$

Microcanonical hypothesis For a sufficiently complex system, the energy surface is visited uniformly & ergodically $\Rightarrow$ All configurations with the same energy are visited with equal probability.

Microcanonical measure for discrete systems

Classical isolated system described by a set of configurations $\{\varphi\}$. Then, if the system is at energy $E$, its microcanonical distribution is

$$\boxed{P_E(\varphi) = \frac{1}{\Omega(E)} \quad \delta_{H(\varphi), E}} \qquad (1)$$

where: * $\Omega(E)$ is the number of configurations of energy $E$

* $\delta_{a,b}$ is the KROENECKER delta, such that $\delta_{a,b} = 1$ if $a = b$ & $\delta_{a,b} = 0$ otherwise