PHYS20040: Statistical Mechanics

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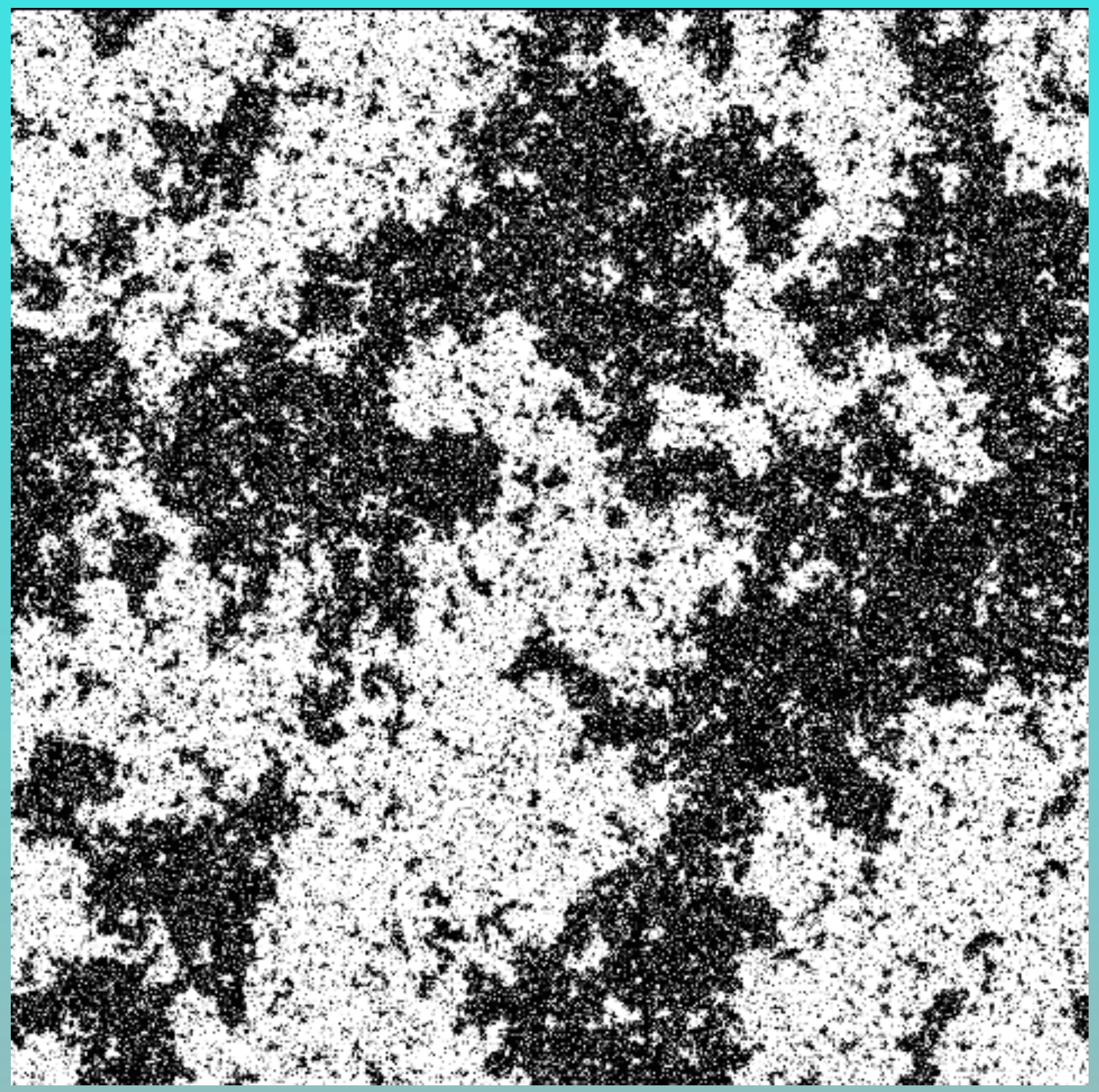


Welcome!

1. Introduction

What is Statistical Mechanics?

Statistical mechanics, together with **classical thermodynamics**, form two branches of **thermal physics**

Each branch represents a distinct approach to thermal physics:

Macroscopic Approach (Classical Thermodynamics)

- deals with **macroscopic** variables i.e. variables that do not refer to any microscopic details
- input is phenomenological laws e.g. equation of state
- output is general relations between macroscopic variables
- advantage is the generality of the approach

Microscopic Approach (Statistical Mechanics)

- starts from a **microscopic** description and seeks to explain macroscopic properties
- input is a microscopic model of a given system
- output is predictions for macroscopic properties and behaviour
- predictions can be compared to experiment thus allowing refinement of the microscopic model

What is Statistical Mechanics?

	Thermodynamics	**Statistical Mechanics**
Quantity of interest	Macroscopic properties (eg. P, V, T, C_P, C_V)	Microscopic properties (eg: molecular speeds)
Strategy	Avoid microscopic model	Build on microscopic model
Strengths	Generality of results	Provides way of refining microscopic understanding
Weaknesses	No understanding of system-specific features. Conceptually opaque.	Requires additional input (the model). Requires additional techniques (probability theory; classical and quantum mechanics)

What is Statistical Mechanics?

- Provides powerful concepts and tools that help us understand the properties of complex systems with very many constituents.

- Used in research of systems as diverse as earthquakes, traffic jams, superconductivity, economics, and many more.

- **Aim of this course:** Show how key concepts that you have met in thermodynamics, such as the Boltzmann factor, entropy, and the second law, can be formulated and find expression in statistical terms.

- Develop and illustrate fundamental concepts and methods use two prototype systems:

  - Gases (classical and quantum)

  - Classical magnets

- For more advanced Soft Matter systems (eg. polymers, liquid crystals, glasses, surfactants, active matter) see M-level unit: **Complex and Disordered Matter**

The microscopic approach

- In principle, can imagine solving Newton's equation for the atomic and molecular motions in a system of interest to determine its behaviour.

- But typical systems contain of order a mol, ie. 10^{23} particles - more than all the grains of sand on all the beaches in the world, or stars in the visible universe!

- So exact approach is impractical and therefore we instead appeal to ideas from statistics and seek to make probabilistic statements about a systems behaviour.

- This works well because as the number of particles becomes very large, things get simpler…

Exercise: Revise your probability notes from first year laboratory, particularly on probability distributions and summary statistics; read the section on probability in the lecture notes (end of sec 1.3)

Simplicity at large N

Statistical Mechanics

Toss a fair coin N times.

What is the probability p_n of getting n heads?

Denote by p the probability that a head results from a single toss; then $q = 1 - p$ is probability for a tail.

This is binomial statistics. Recall:

$$\begin{aligned} p_n &\equiv \text{number of distinct ways of obtaining } n \text{ heads} \\ &\times \text{probability of any specific way of getting } n \text{ heads} \\ &= \binom{N}{n} p^n q^{N-m} \end{aligned}$$

The distribution p_n has mean $\bar{n} \equiv \sum_{n=0}^{N} n p_n = Np$

and variance $\overline{\Delta n^2} \equiv \sum_{n=0}^{N} (n - \bar{n})^2 p_n = Npq$

Simplicity at large N

For a fair coin $p = q = \dfrac{1}{2}$

Define $f = n/N$, the fraction of tosses resulting in a head:

$$\bar{f} = \frac{\bar{n}}{N} = p = \frac{1}{2}$$

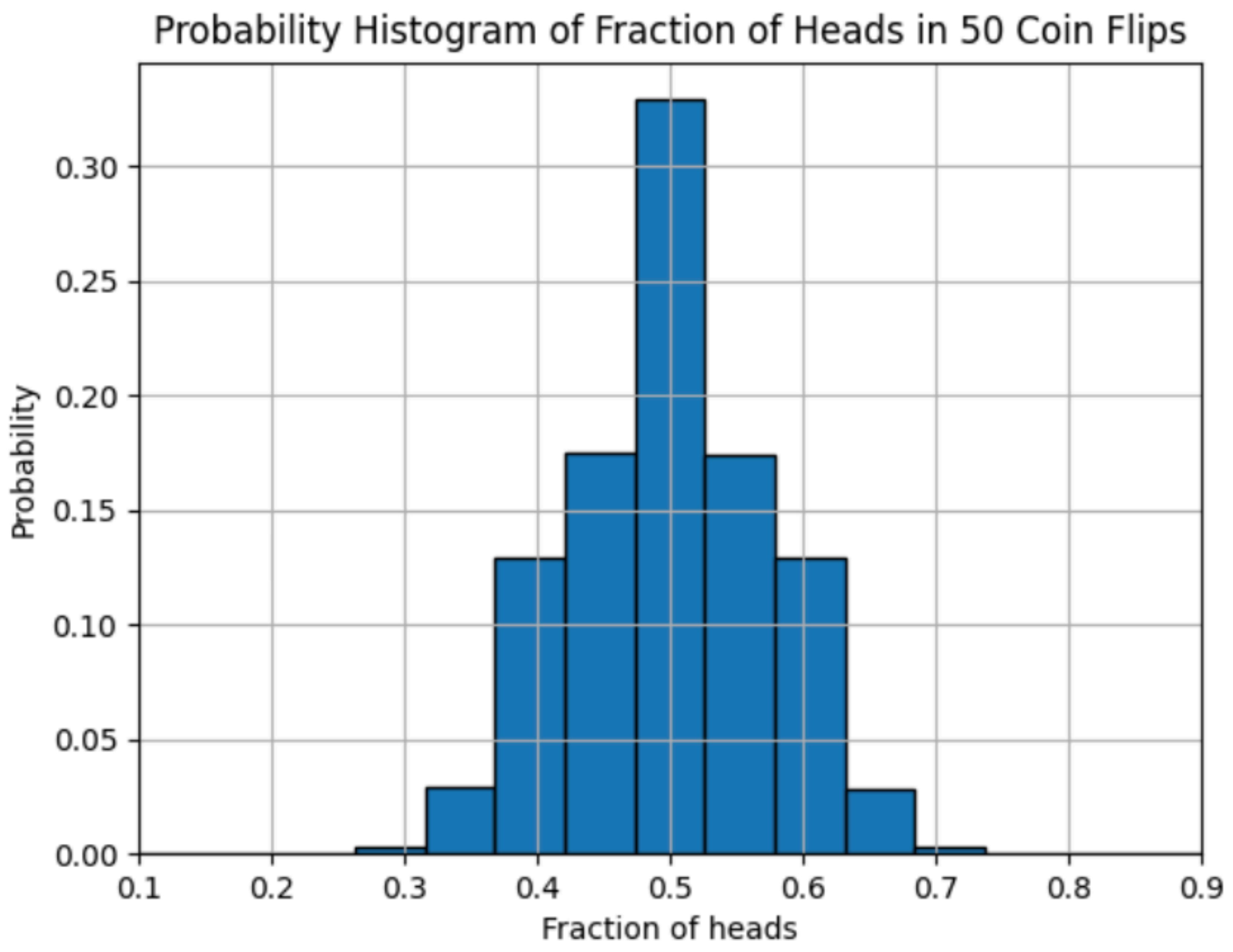
The standard deviation of f is

$$(\overline{\Delta f^2})^{1/2} \equiv \frac{(\overline{\Delta n^2})^{1/2}}{N} = \left(\frac{pq}{N}\right)^{1/2} = \frac{1}{2N^{1/2}}$$

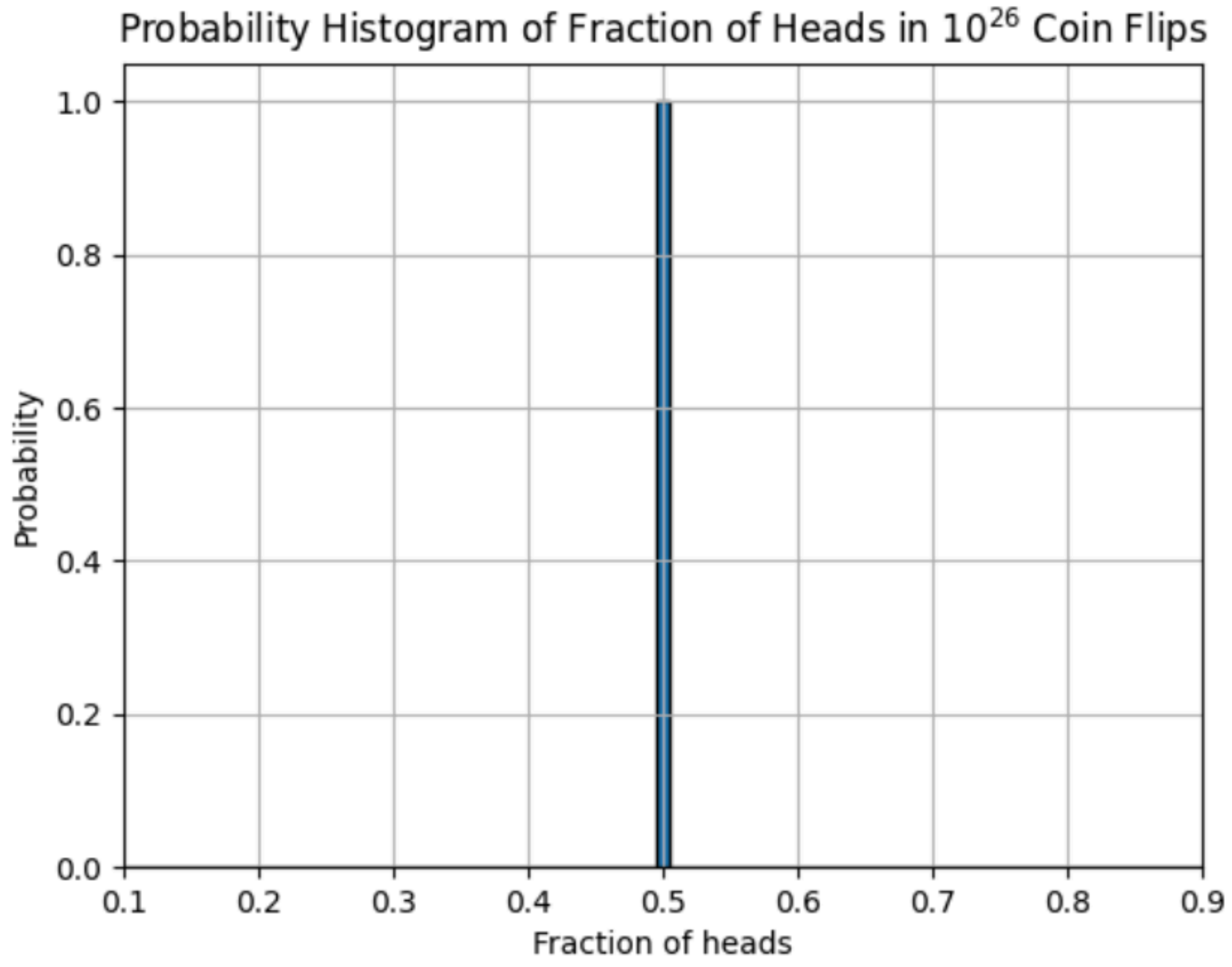
The typical deviation of f from its mean value is thus vanishingly small for large N

Simplicity at large N

Statistical Mechanics



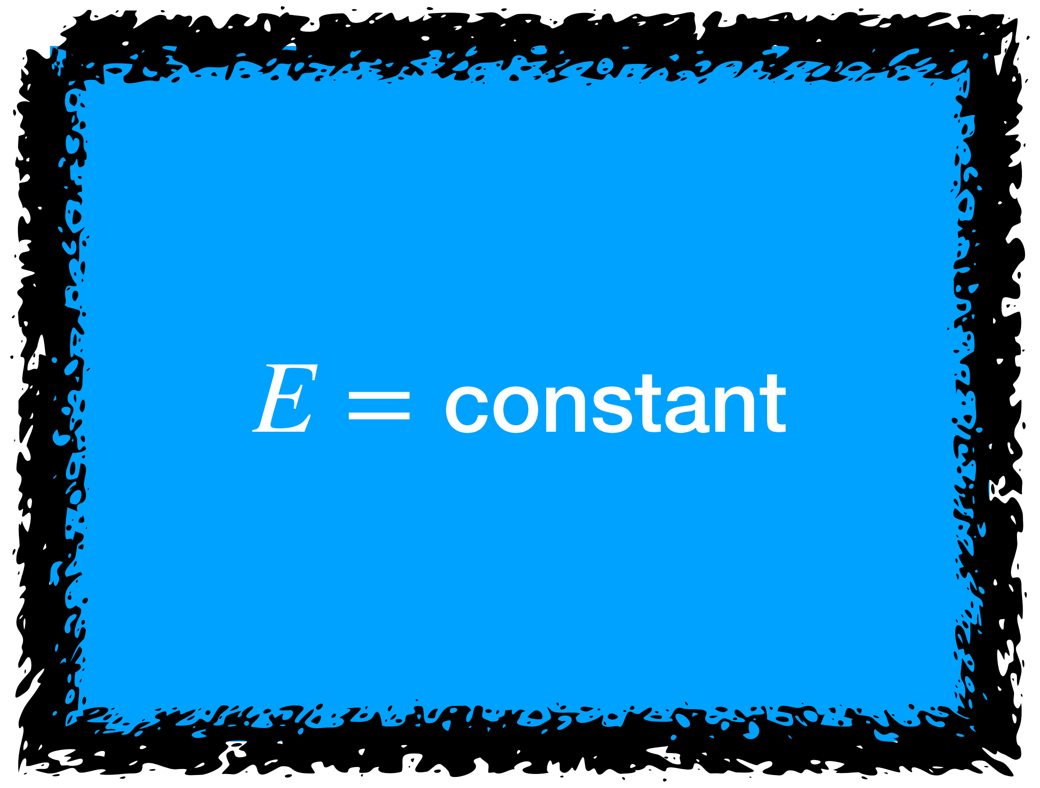
(a) For $N = 50$ *tosses, we can be reasonably sure that* f *will be close to* 0.5



(b) For $N = 10^{26}$ *tosses We can be absolutely sure that* f *will be indistinguishable from* 0.5

2. Foundations: equilibrium of an isolated system

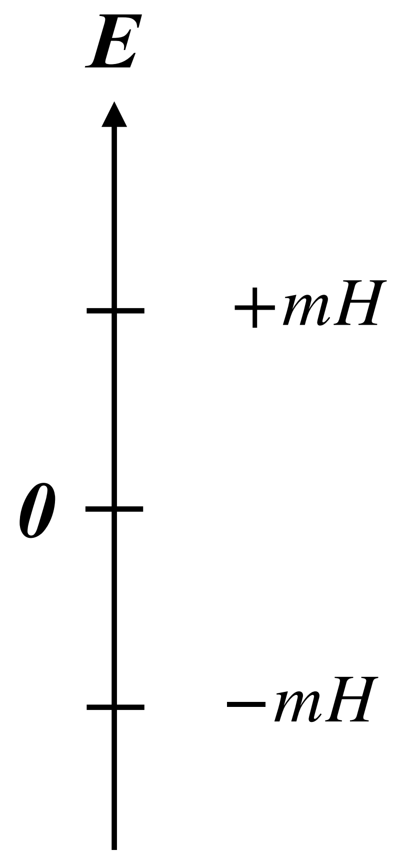
- Isolated ‘system': no transfer of energy to the surroundings, so it’s total energy is constant



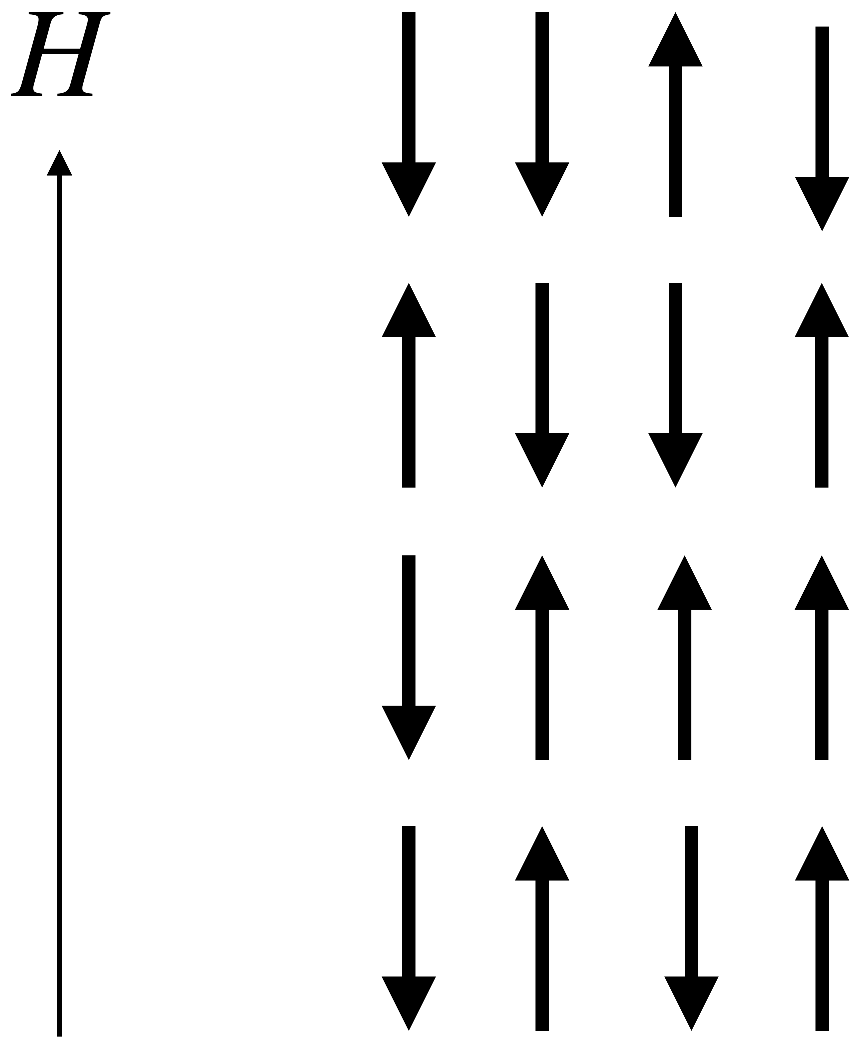
- We shall consider case where the system is either an ideal gas or a simple magnet
- Magnet can be thought of as a crystalline lattice of magnetic dipoles each with a magnetic dipole moment m which are assumed to be in a magnetic field H.

2. Foundations: equilibrium of an isolated system

- Each dipole is assumed to be able to align parallel or antiparallel to H

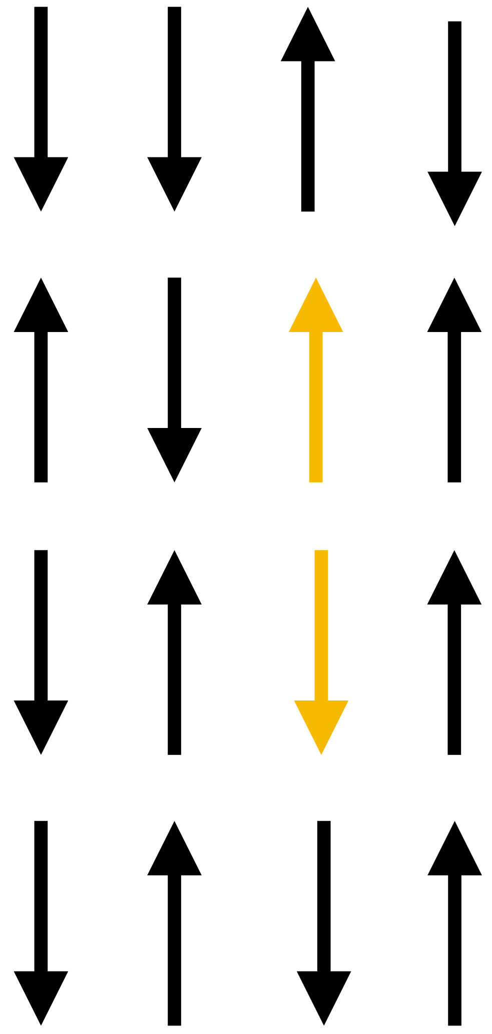


  - Parallel to H with energy $\epsilon = -mH$ (ground state)
  - Antiparallel to H with energy $\epsilon = +mH$ (excited state)



Dipole configuration

- Transitions of individual dipoles (or 'spins') can change if they interact with three neighbours, subject to conserving total E



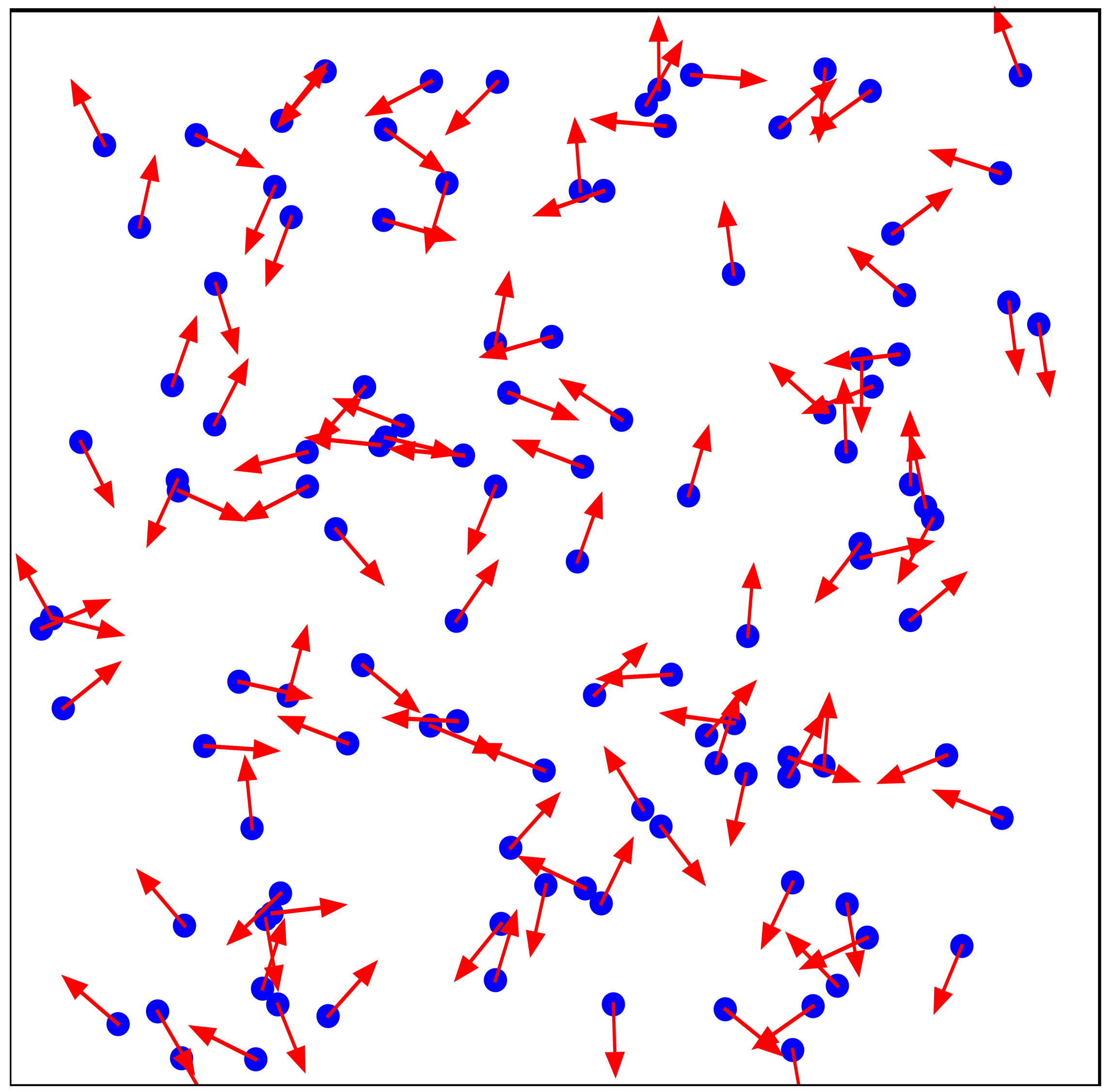
Microstates and macrostates

Two different levels of description of a system: **microstates** and **macrostates**

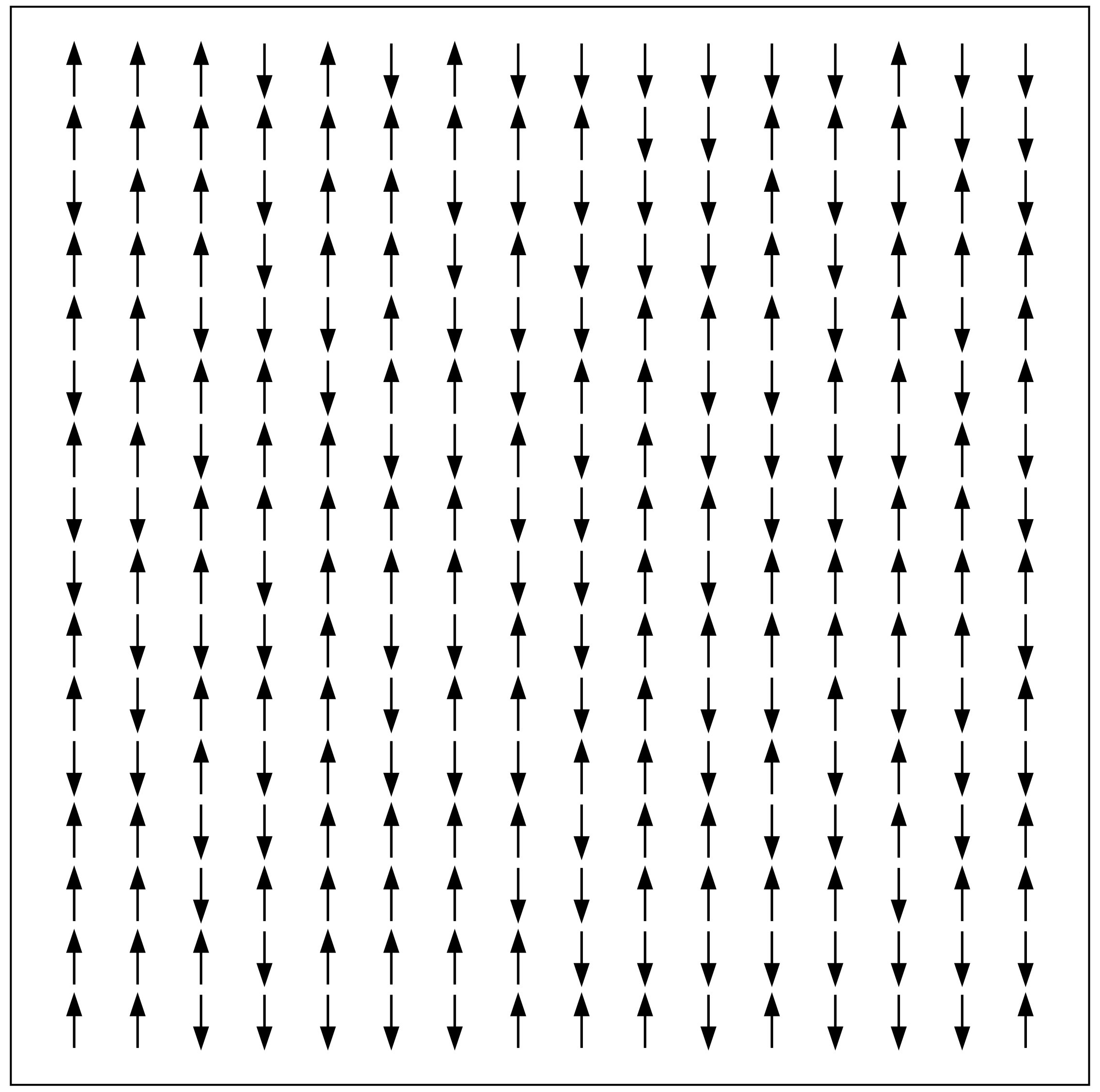
- Key point 1: *A microstate is a complete specification of the state of the system according to the microscopic model.*

Ideal gas

Requires knowledge of the position and velocity vectors of each molecule



Model magnet



Requires knowledge of the orientation of each dipole on the lattice

The microstate will change continually as the particles exchange energy

Microstates and macrostates