Statistical physics

Statistical physics is a branch of physics that uses methods of probability theory and statistics, and particularly the mathematical tools for dealing with large populations and approximations, in solving physical problems. It can describe a wide variety of fields with an inherently stochastic nature. Its applications include many problems in the fields of physics, biology, chemistry, neurology, and even some social sciences, such as sociology. Its main purpose is to clarify the properties of matter in aggregate, in terms of physical laws governing atomic motion.
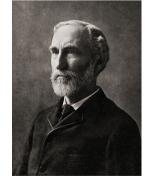
https://en.wikipedia.org/wiki/Statistical_physics

James Clerk Maxwell
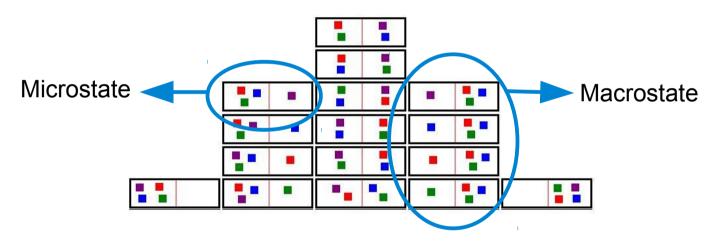
Ludwig Boltzmann

Josiah Willard Gibbs

Albert Einstein

Enrico Fermi

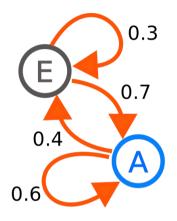Lev D. Landau

Statistical physics

Ensemble: an idealization consisting of a large number of virtual copies (sometimes infinitely many) of a system, considered all at once, each of which represents a possible state that the real system might be in. In other words, an ensemble is a probability distribution for the state of the system.

Microstate   Macrostate

- Microcanonical ensemble (or NVE): The total energy of the system and the number of particles in the system are each fixed.
- Canonical ensemble (or NVT): The energy is not known exactly but the number of particles and the temperature are fixed.
- Grand canonical ensemble (or μVT): neither the energy nor particle number are fixed, but the temperature and chemical potential are specified.

Statistical physics

0.3

0.7

0.4

0.6

$$\frac{d\omega_\mu}{dt} = \sum_\nu [\omega_\nu(t) R(\nu \to \mu) - \omega_\mu(t) R(\mu \to \nu)$$

$$\sum_\mu \omega_\mu(t) = 1$$

Probability of being in state
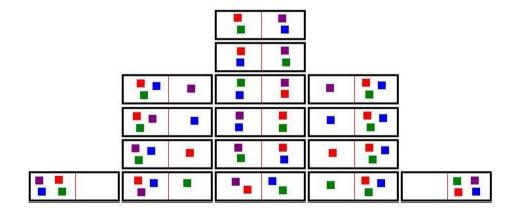
Transition probability between states

$$\langle Q \rangle = \sum_\mu Q_\mu \omega_\mu(t) \qquad \text{Expectation of Q}$$
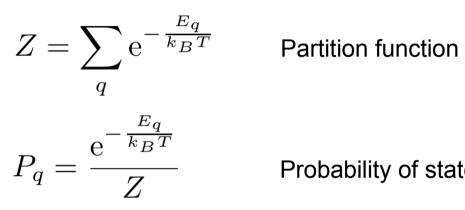
$$p_\mu = \lim_{t \to \infty} \omega_\mu(t) \longrightarrow p_\mu = \frac{1}{Z} e^{-E_\mu / k_B T} \qquad \text{Boltzmann distribution (Gibbs, 1902)}$$

$$Z = \sum_q e^{-\frac{E_q}{k_B T}} \qquad \text{Partition function}$$

Statistical physics

Equal a priori probability postulate: For an isolated system with an exactly known energy and exactly known composition, the system can be found with equal probability in any microstate consistent with that knowledge.

Ergodic hypothesis: An ergodic state is one that evolves over time to explore "all accessible" states: all those with the same energy and composition.

Statistical physics

$$Z = \sum_q e^{-\frac{E_q}{k_B T}}$$ Partition function

$$P_q = \frac{e^{-\frac{E_q}{k_B T}}}{Z}$$ Probability of state *q*

$$\langle E \rangle = \sum_q E_q P_q = \frac{1}{Z} \sum_q E_q e^{-\frac{E_q}{k_B T}} = k_B T^2 \frac{\partial \ln Z}{\partial T}$$ Energy
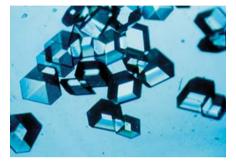
$$S = -k_B \sum_q P_q \ln P_q = \frac{\partial}{\partial T}(k_B T \ln Z)$$ Entropy
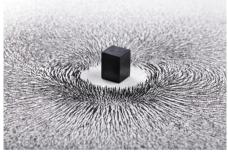
Statistical physics

Gas, smoke;

Liquids;

Solids, semiconductors;

Phase transitions;

Ferromagnetism;
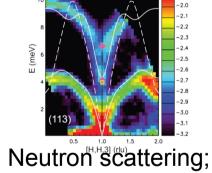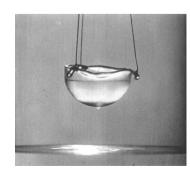
Universality, criticality;

Plasma;
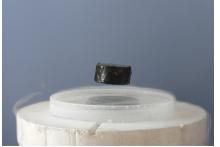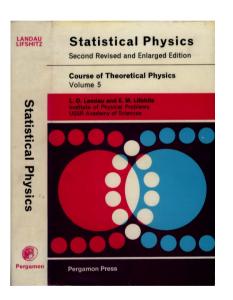
Neutron scattering;

Cosmology;

Superfluidity;

Superconductivity;

Complexity.

Statistical physics
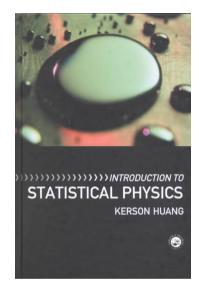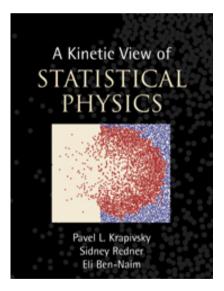

K Huang
Introduction to Statistical Physics

L D Landau & E M Lifshitz
Statistical Physics

P L Krapivsky, S Redner & E Ben-Naim
A Kinetic View of Statistical Physics

Monte Carlo methods

- **Monte Carlo methods** are a broad class of computational algorithms that rely on repeated random sampling to obtain numerical results.

horstein the Learned says that there was a settlement on the Island of Hísing which had alternately belonged to Norway and to Gautland. So the kings agreed between them to draw lots and throw dice for this possession. And he was to have it who threw the highest. Then the Swedish king threw two sixes and said that it was no use for King Olaf to throw. He replied, while shaking the dice in his hand, "There are two sixes still on the dice, and it is a trifling matter for God, my Lord, to have them turn up." He threw them, and two sixes turned up. Thereupon Olaf, the king of Norway, cast the dice, and one six showed on one of them, but the other split in two, so that six and one turned up; and so he took possession of the settlement.[1]

Ivar Ekeland, "The Broken Dice, and Other Mathematical Tales of Chance".

Monte Carlo methods

Brother Edvin ca. 1240

675248
seed

4559598861504

seed²

959861
output

output becomes next seed

Middle-square method

$$r = (a + b) \bmod 6$$

$$X_{n+1} = (aX_n + b) \bmod m$$

John von Neumann   Stanisław Ulam

Monte Carlo methods

"The first thoughts and attempts I made to practice [the Monte Carlo Method] were suggested by a question which occurred to me in 1946 as I was convalescing from an illness and playing solitaires. The question was what are the chances that a Canfield solitaire laid out with 52 cards will come out successfully? After spending a lot of time trying to estimate them by pure combinatorial calculations, I wondered whether a more practical method than "abstract thinking" might not be to lay it out say one hundred times and simply observe and count the number of successful plays. This was already possible to envisage with the beginning of the new era of fast computers, and I immediately thought of problems of neutron diffusion and other questions of mathematical physics, and more generally how to change processes described by certain differential equations into an equivalent form interpretable as a succession of random operations. Later [in 1946], I described the idea to John von Neumann, and we began to plan actual calculations."
–Stanislaw Ulam

Nicholas Metropolis suggested the code name Monte Carlo, after the Monaco casino.

Monte Carlo methods

General pattern:
- Define a domain of possible inputs.
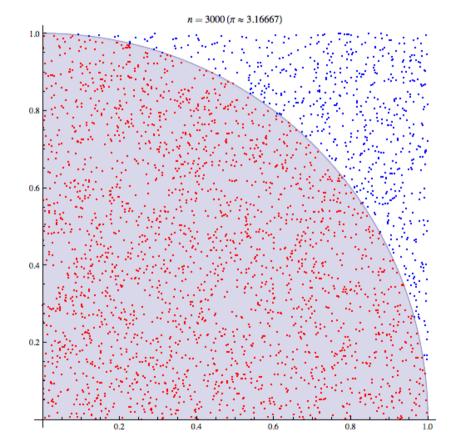- Generate inputs randomly from a probability distribution over the domain.
- Perform a deterministic computation on the inputs.
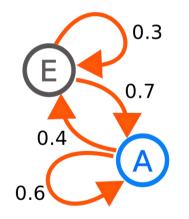- Aggregate the results.

Example:
- Draw a square on the ground, then inscribe a circle within it.
- Uniformly scatter some objects of uniform size (grains of rice or sand) over the square.
- Count the number of objects inside the circle and the total number of objects.
- The ratio of the two counts is an estimate of the ratio of the two areas, which is π/4. Multiply the result by 4 to estimate π.
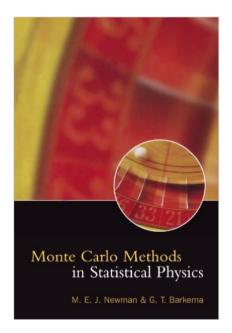
$n = 3000 \, (\pi \approx 3.16667)$

How to gauge accuracy?

Monte Carlo methods

- A **Markov chain**, named after Andrey Markov, is a random process that undergoes transitions from one state to another on a state space. It must possess a property that is usually characterized as "memorylessness": the probability distribution of the next state depends only on the current state and not on the sequence of events that preceded it.

- Markov Chain Monte Carlo (MCMC) sampler: Design a judicious Markov chain model with a prescribed stationary probability distribution. By the ergodic theorem, the stationary probability distribution is approximated by the empirical measures of the random states of the MCMC sampler.

Monte Carlo methods

M E J Newman & G T Barkema
Monte Carlo Methods in Statistical Physics