Billiards, Markov chains, and statistical physics

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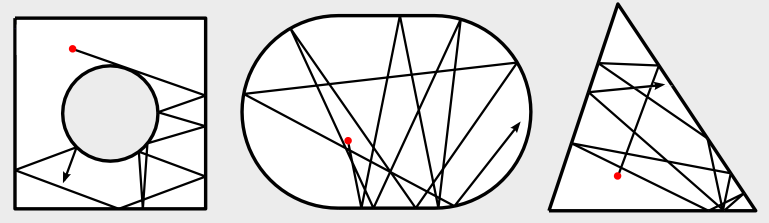
Billiards

Engraving from Charles Cotton's 1674 book, *The Complete Gamester*

Math billiards - different shapes

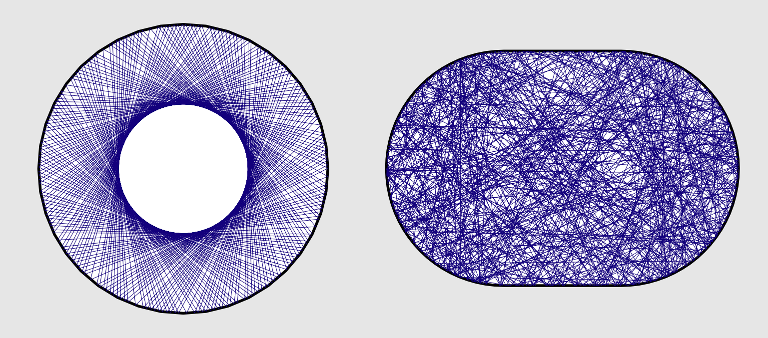


Mathematical billiards: simple models of mechanical systems that

- help to explore the foundations of statistical mechanics,
- used to develop the mathematical theory of dynamical systems
- has deep connections with many areas of mathematics.

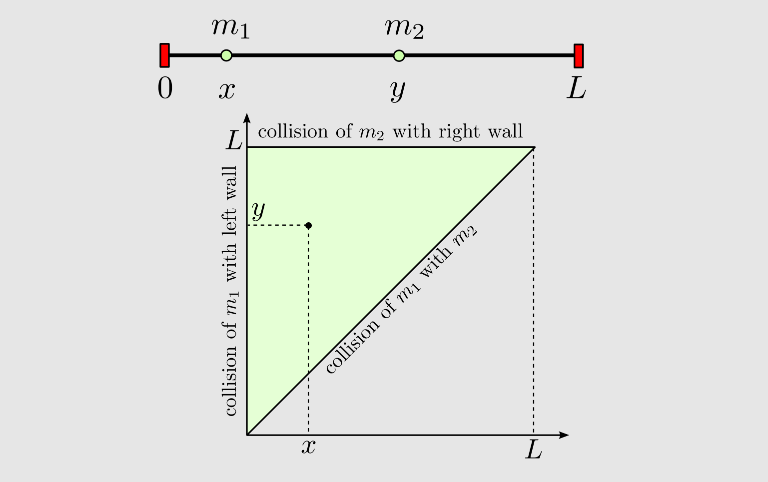
We don't think of it as a game of skill ...

... but a game of observation. We set the ball in motion and try to understand what happens to it over long periods of time and how what it does is affected by the shape of the table.



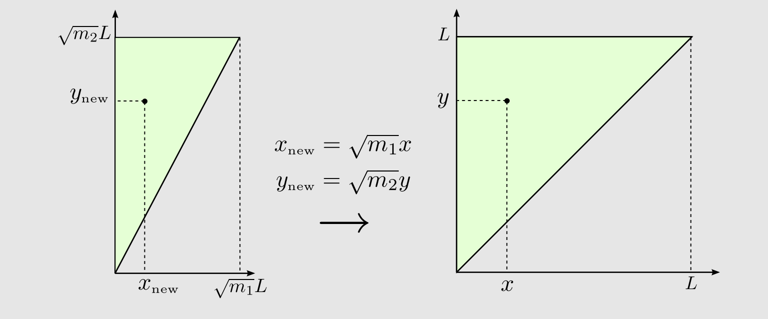
Very different long term behavior of trajectories for different shapes. The example on the left shows fairly regular behavior. The one on the right is very unstable and "chaotic." The stadium billiard is said to be **ergodic**.

What if there are many balls?



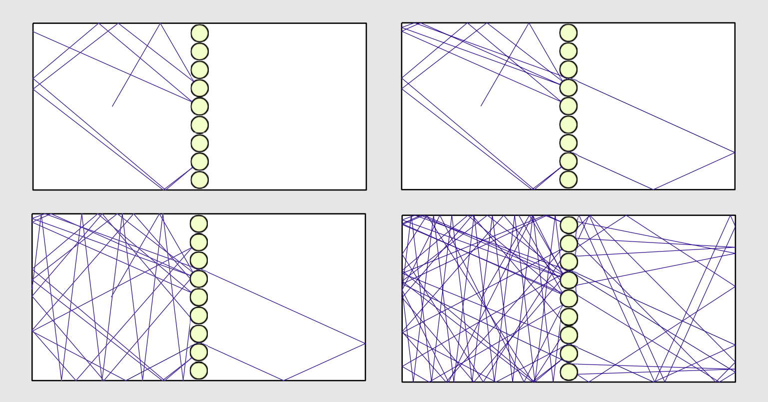
Single particle system in dimension 2 describes two-particle system in dimension 1. This idea applies to any number of particles in two or three dimensions.

How to make reflections mirror-like?



A linear change of coordinates makes the total kinetic energy proportional to the square of the length of a vector. This makes collisions mirror-like. This idea holds in any dimension, for any number of particles.

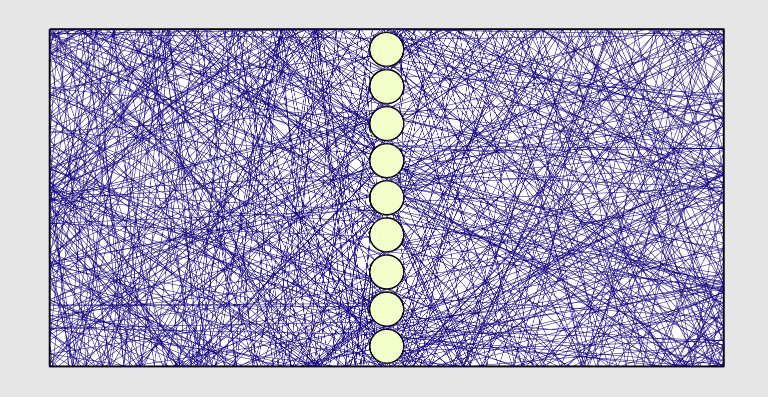
A simple experiment



A chamber divided by a permeable solid “membrane” made of circular scatterers. In the long run, a “billiard gas” will distribute evenly between the two sides.

In the long run ...

In the long run, a trajectory explores the entire chamber evenly.

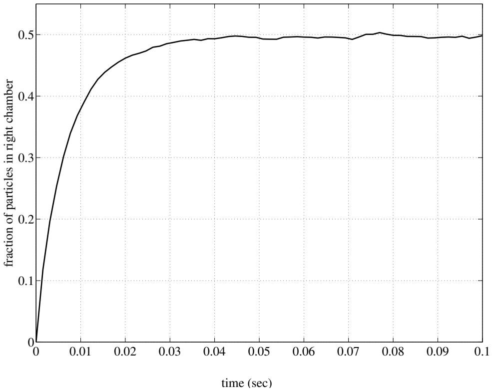


Theorem (Birkhoff, Sinai)

The fraction of time spent in a region equals its normalized area.

We cannot say where exactly the particle will be in the distant future, but we can give very precise probabilities. This system is **ergodic**.

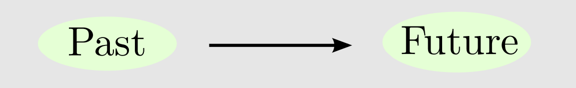
The "long run" is approx. 0.05 seconds ...



50000 (non-interacting) billiard particles are released in the left-hand side of the divided chamber. Chamber is 20 cm long by 9 cm tall, and the spacing between circular scatterers is 1 mm. Assume particles move with speed of approximately 515 m per sec. (This is the mean speed of N_2 mol. at 25 degrees Celsius.)

Some intellectual drama

- The fundamental laws of mechanics do not distinguish Future and Past. There is no **time arrow**.



  But, somehow, the system with many particles prefers to move in a time direction where particles are approximately evenly divided between the two chambers.

- Where does **probability** come from? What justifies applying probabilistic thinking to a deterministic system?

Boltzmann's ergodic hypothesis

The first person to seriously grapple with these questions was Ludwig Boltzmann.

Ludwig Eduard Boltzmann (1844-1906). Properties of the system that are defined by an integral along trajectories can also be obtained by volume integration over the *phase space* of the system. But the system must be **ergodic**, which roughly means "probabilistically connected."

Deterministic and stochastic dynamical systems

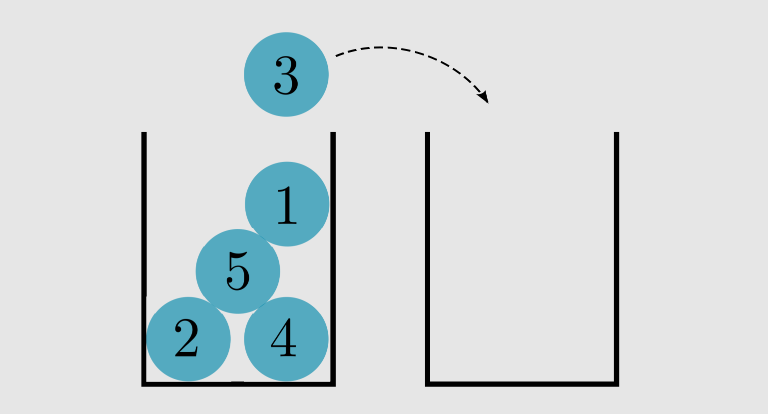
Deterministic dynamical systems:

- Differential equations
- Potentials, forces, Newton's second law
- Iteration of maps

Probabilistic dynamical systems:

- Markov chains
- Random walks
- Stochastic differential equations
- Brownian motion

A Markov chain model of the two-chambers system



The Ehrenfest urn model. Choose a ball at random, then flip a coin. If heads, move that ball to the other urn. If tails, keep the ball where it was. The *state* of the system at a given time is the number of balls in the first urn. The set of *states* is $S = \{0, 1, 2, 3, 4, 5\}$.

The transition probabilities matrix

state at time step $n+1$ →

state at time step n ↓

$$P = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 \\ \frac{1}{10} & \frac{1}{2} & \frac{2}{5} & 0 & 0 & 0 \\ 0 & \frac{1}{5} & \frac{1}{2} & \boxed{\frac{3}{10}} & 0 & 0 \\ 0 & 0 & \frac{3}{10} & \frac{1}{2} & \frac{1}{5} & 0 \\ 0 & 0 & 0 & \frac{2}{5} & \frac{1}{2} & \frac{1}{10} \\ 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

The probability of going from 2 balls in the left urn at time step n to 3 balls at time step $n+1$ is 0.3. To obtain the transition probabilities in k steps, multiply the matrix by itself k times: P^k. The evolution of the system is described by the sequence $P, P^2, P^3, \ldots$.

Long run behavior for the Ehrenfest chain model

$$P^{200} = \begin{pmatrix} 0.0313 & 0.1563 & 0.3125 & 0.3125 & 0.1563 & 0.0313 \\ 0.0313 & 0.1563 & 0.3125 & 0.3125 & 0.1563 & 0.0313 \\ 0.0313 & 0.1563 & 0.3125 & 0.3125 & 0.1563 & 0.0313 \\ 0.0313 & 0.1563 & 0.3125 & 0.3125 & 0.1563 & 0.0313 \\ 0.0313 & 0.1563 & 0.3125 & 0.3125 & 0.1563 & 0.0313 \\ 0.0313 & 0.1563 & 0.3125 & 0.3125 & 0.1563 & 0.0313 \end{pmatrix}$$

The **stationary distribution** of probabilities is

$$\begin{aligned} &\mathrm{Prob}(0) = 0.0313, \quad \mathrm{Prob}(1) = 0.1563, \quad \mathrm{Prob}(2) = 0.3125, \\ &\mathrm{Prob}(5) = 0.0313, \quad \mathrm{Prob}(4) = 0.1563, \quad \mathrm{Prob}(3) = 0.3125. \end{aligned}$$

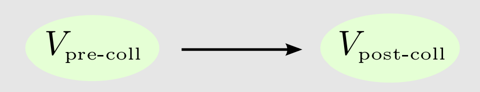
This is interpreted as the **equilibrium state** of the system.

A drastically simple model of thermal interaction

- m_1 moves freely on $0 \le x_1 \le l$, bounces off elastically at $0, l$
- m_2 moves freely along 1-D container, collides elastically with m_1
- As m_2 enters wall zone, choose random initial condition for m_1:
  - position x_1 is uniformly distributed over $0 \le x_1 \le l$
  - velocity $\dot{x}_1$ is normal with mean 0 and variance σ_1^2:

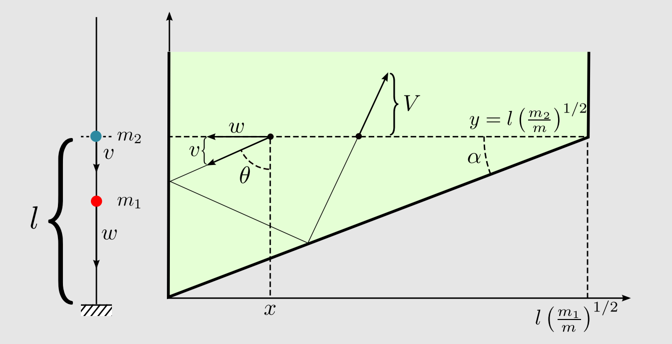
$$\rho_{\text{wall}}(\dot{x}_1) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\dot{x}_1^2/\sigma_1^2\right)$$

How to specify Markov chain transitions for the velocity of m_2?



Markov chain transitions: $V_{\text{pre-coll}} \longrightarrow V_{\text{post-coll}}$

Reparametrize speed of m_2: $v = \dot{y}$, where $y = l\sqrt{m_2/(m_1 + m_2)}$.



From this, one obtains a Markov operator $P : \rho_{\text{pre-coll}} \mapsto \rho_{\text{post-coll}}$

$$\rho_{\text{post-coll}}(V) = \int_0^\infty k(V,v)\rho_{\text{pre-coll}}(v)\,dv$$

where ρ represents probability densities.

Equilibrium distribution (Maxwell-Boltzmann)

The equilibrium distribution $\rho_{\text{equi}}(v)$ for the speed of m_2 is

$$\rho_{\text{equi}} = \lim_{n\to\infty} P^n \rho_{\text{initial}}$$

for an arbitrary ρ_{initial}.

Theorem (The Maxwell-Boltzmann distribution)

The equilibrium distribution for the velocity of m_2 is

$$\rho_{equi}(v) = \frac{\dot{x}_2}{\sigma_2^2} \exp\left(-\frac{1}{2}\dot{x}_2^2/\sigma_2^2\right)$$

where σ_2 satisfies

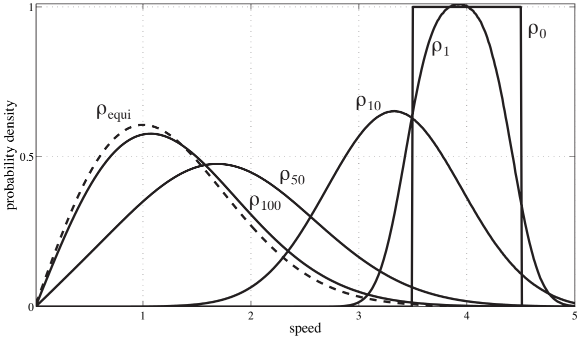
$$m_1\sigma_1^2 = m_2\sigma_2^2.$$

It makes sense to call the quantity $m_i\sigma_i^2$ the common *temperature* of the wall ($i = 1$) and the molecule ($i = 2$). In fact,

$$m_1\sigma_1^2 = kT$$

where k is known as the Boltzmann constant.

Rate of approach to thermal equilibrium



It turns out that the speed of convergence depends on the masses:

$$\underbrace{\|\rho_{\text{equi}} - P^n \rho_{\text{initial}}\|}_{\text{difference between equilibrium state and state at time } n} \leq C \underbrace{(1 - 4m_2/m_1)^n}_{\text{goes to 0 exponentially fast}}$$

when the ratio of masses is small (say, $m_2/m_1 < 0.2$).

One moral (among many) to take away

- Equilibrium properties are general (Maxwell-Boltzmann distribution, equidistribution, etc), but
- the way in which equilibrium is attained depends on details of system (in this example, the ratio of masses).