Billiards, Markov chains, and statistical physics

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Billiards

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

Math billiards - different shapes

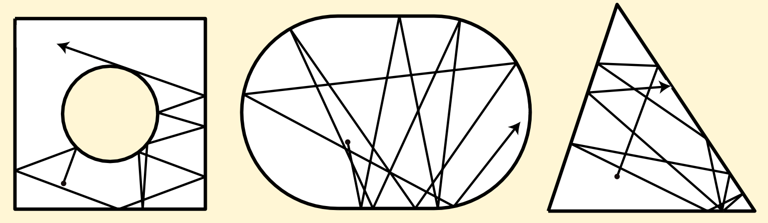

Figure: Mathematical billiards are simple models of mechanical systems. They are used to study the foundations of statistical mechanics, chaotic dynamical systems, etc. (We can assume that the billiard ball is a point particle by "thickening" the table boundary by the radius of the ball.)

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.

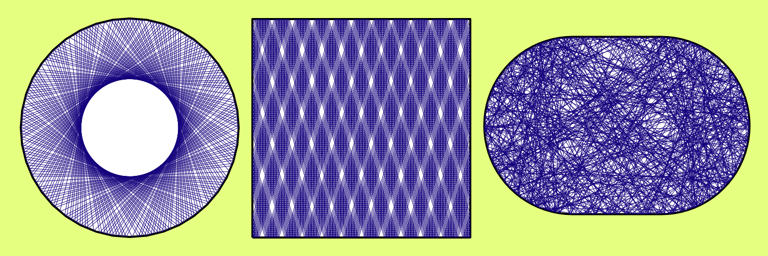

Figure: Very different long term behavior of billiard trajectories for different shapes. The first two examples show fairly regular behavior. The third is very unstable and "chaotic." The stadium billiard is said to be **ergodic**.

What if there are many balls?

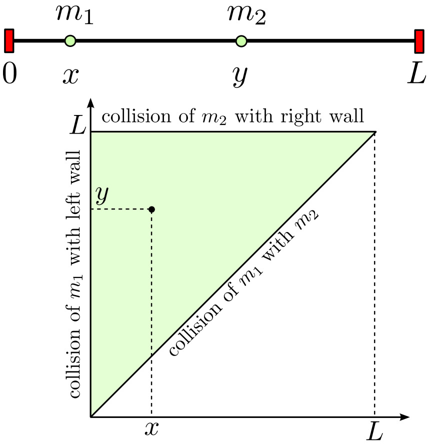

Figure: Single particle system in dimension 2 describes two-particle system in dimension 1. This idea applies to any number of particles in two or three dimensions.

How to make reflections mirror-like?

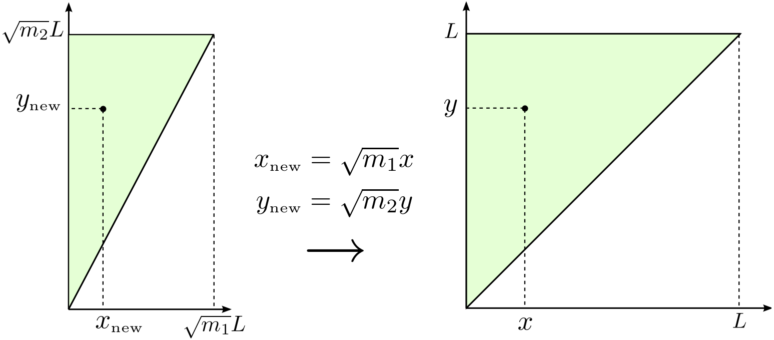

Figure: Make a change of coordinates so that the total kinetic energy is proportional to the square of the length of a vector. In this way, collisions are described, on the left-hand side, by mirror-like reflections. This idea holds in any dimension, for any number of particles.

A simple experiment (experiment I)

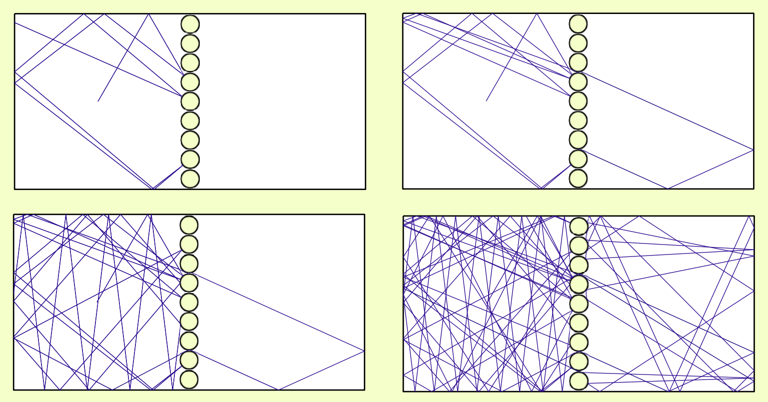

Figure: A chamber divided by a permeable solid "membrane" made of circular scatterers. In the long run, a "billiard gas" will distribute evenly between the two sides.

In the long run ...

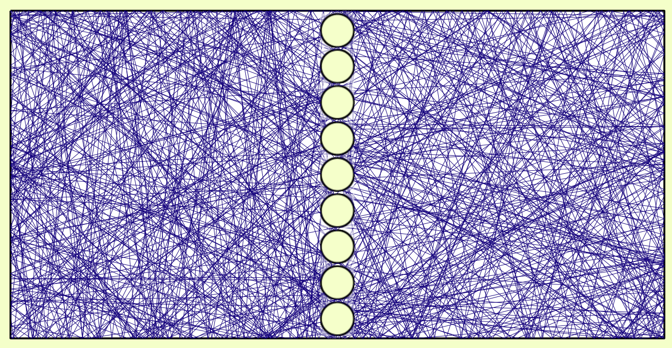

Figure: In the long run, the trajectory explores the entire chamber evenly. Theorem: the fraction of time spent in a region of the chamber is equal to the normalized area of that region. We cannot say where exactly the particle will be in the distant future, but we can give very precise probabilities. Like the stadium billiard, this one is also **ergodic**.

The “long run” is approx. 0.05 seconds ...

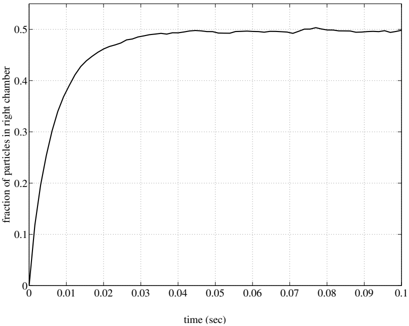

Figure: 50000 (non-interacting) billiard particles are released in the left-hand side of the divided chamber. Chamber is 20 cm long by 9 cm tall, and the spacing between circular scatterers is 1 mm. Assume particles move with speed of approximately 515 m per sec. (This is the mean speed of N_2 mol. at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

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

Boltzmann's ergodic hypothesis

Figure: 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

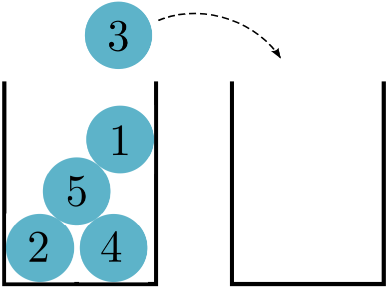

Figure: The Ehrenfest urn model. Choose a ball at random, then flip a coin. If heads, move that ball to the other urn. If tails, keep the ball where it was. The *state* of the system at a given time is the number of balls in the first urn. The set of *states* is $S = \{0, 1, 2, 3, 4, 5\}$.

The transition probabilities matrix

$$\begin{array}{cc} & \xrightarrow{\text{state at time step } n+1} \\ P = & \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 \\ \frac{1}{10} & \frac{1}{2} & \frac{2}{5} & 0 & 0 & 0 \\ 0 & \frac{1}{5} & \frac{1}{2} & \boxed{\frac{3}{10}} & 0 & 0 \\ 0 & 0 & \frac{3}{10} & \frac{1}{2} & \frac{1}{5} & 0 \\ 0 & 0 & 0 & \frac{2}{5} & \frac{1}{2} & \frac{1}{10} \\ 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix} \Bigg\downarrow \text{state at time step } n \end{array}$$

Figure: 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

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

Markov chains and billiard scattering (experiment II)

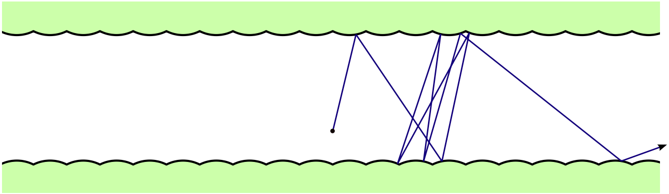

Figure: An experiment to investigate the **distribution of angles** as the number of collisions increases. What is the **stationary** distribution of angles? How does approach to stationarity provide information about the microscopic contour of the channel surface? Here, this contour is specified by a parameter K (the **curvature** of the bumps) equal to the ratio of the distance between corners divided by the radius of the bumps.

Defining transition probabilities for the angle scattering

Transition probabilities are now specified by a **linear operator**, which is a kind of infinite dimensional matrix. We define the transition probabilities operator by the effect it has on functions:

$$(Pf)(\theta) = \int_0^1 f(\Psi_\theta(r))\,dr.$$

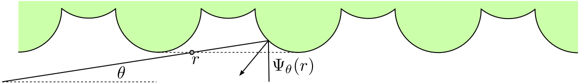

Figure: The surface of the channel has a "molecular microstructure" defined by a billiard table contour. We assume that the coordinate r is random (uniform between 0 and 1).

What happens to angles after many collisions?

Stationary distribution of angles is given by the **Knudsen law**:

$$\text{Probability}(a < \theta < b) = \int_a^b \frac{1}{2}\sin\theta \, d\theta.$$

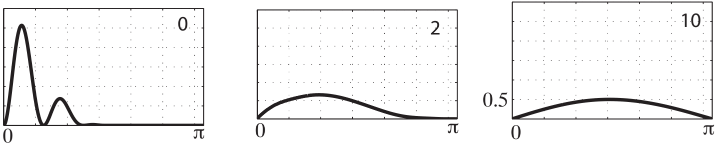

Figure: After many collisions, the system approaches a stationary distribution of angles that does not depend on the microgeometry.

Approaching equilibrium–now details matter!

The **speed** at which equilibrium distribution of angles is achieved **depends on the geometric details** of the billiard boundary surface, so we can learn something about those details by measuring this speed. This sort of information is contained in the **spectrum of eigenvalues** of P. An **eigenvalue** of P is a number c so that

$$P\Psi = c\Psi$$

for some function Ψ not equal to 0 (an eigenfunction.)
The top eigenvalue of P is always 1; the eigenvalues form a sequence of numbers between -1 and 1:

$$c_1, c_2, c_3, \ldots$$

that are like a **numerical signature** of the microgeometry. The rate of tending to equilibrium is controlled by the **spectral gap**

$$\gamma = c_1 - c_2.$$

Spectral gap and curvature (for the bumps surface)

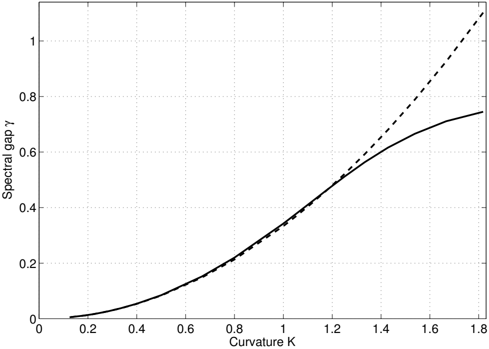

Figure: The spectral gap of P for the microstructure of the channel with circular bumps. The dashed line is the graph of the function $K^2/3$, where K measures how much the surface bumps are curved.

One moral of this story:

Equilibrium properties are often simple and universal, that is, they don't depend very much on a detailed description of interactions at a microscopic level. So to learn about some of those details, begin by looking at the way the system approaches equilibrium.