Derivation of the Boltzmann equation: Loschmidt and Zermelo's paradoxes

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In 1900, Hilbert proposed 23 problems in mathematics. Hilbert's sixth problem is concerned with deriving the laws of physics axiomatically. A key part of this is the derivation of Boltzmann's equation from Newton's laws, a problem that has still not been completely resolved. In this project we aim to understand an overview of this derivation and the two main paradoxes that arise given by Loschmidt and Zermelo.

The Boltzmann equation

The Boltzmann equation is a partial differential equation (PDE). If we let $f(t, x, v)$ denote the density of particles at time t with position x moving with velocity v, then it reads

$$\frac{\partial f}{\partial t} + v \cdot \nabla f = Q(f, f)$$

Here Q is a quadratic operator that models the collisions between particles.

Derivation

We start by considering N hard spheres of radius $r > 0$ moving via Newton's laws of classical mechanics. When they collide, energy and momentum must be conserved. We assume that collisions between particles can be modelled by specular reflection (see Figure 1). This gives a flow on our state space.

Then given the probability densities $f^N(t, x, v)$, the flow on the state space induces a flow on the densities, $(f_t^N)_{t\geq 0}$.

We then introduce the marginals $f_t^{(k)}$ for $k = 1 \dots N$ with

$$f_t^{(k)} = \int f_t^N dx_{k+1} dv_{k+1} \dots dx_N dv_N.$$

Focusing on $k = 1$ which describes a single particle, we can look at the gain and loss of particles in a small region of space, in terms of the movement of single particles, as the system evolves. But in order to interpret a collision we then require the data encoded in the second marginal $f_t^{(2)}$. In order to relate the marginals, we assume molecular chaos which means

$$f_t^{(2)} = f_t^{(1)} \otimes f_t^{(1)}.$$

Proceeding in this way up to $k = N$ we derive a system of equations that govern the interaction of N particles in terms of the marginals, known as the BBGYK hierarchy.

Then taking the Boltzmann-Grad limit, $N \to \infty$ and $r \to 0$ such that $Nr^2 \to 1$, yields the Boltzmann equation.

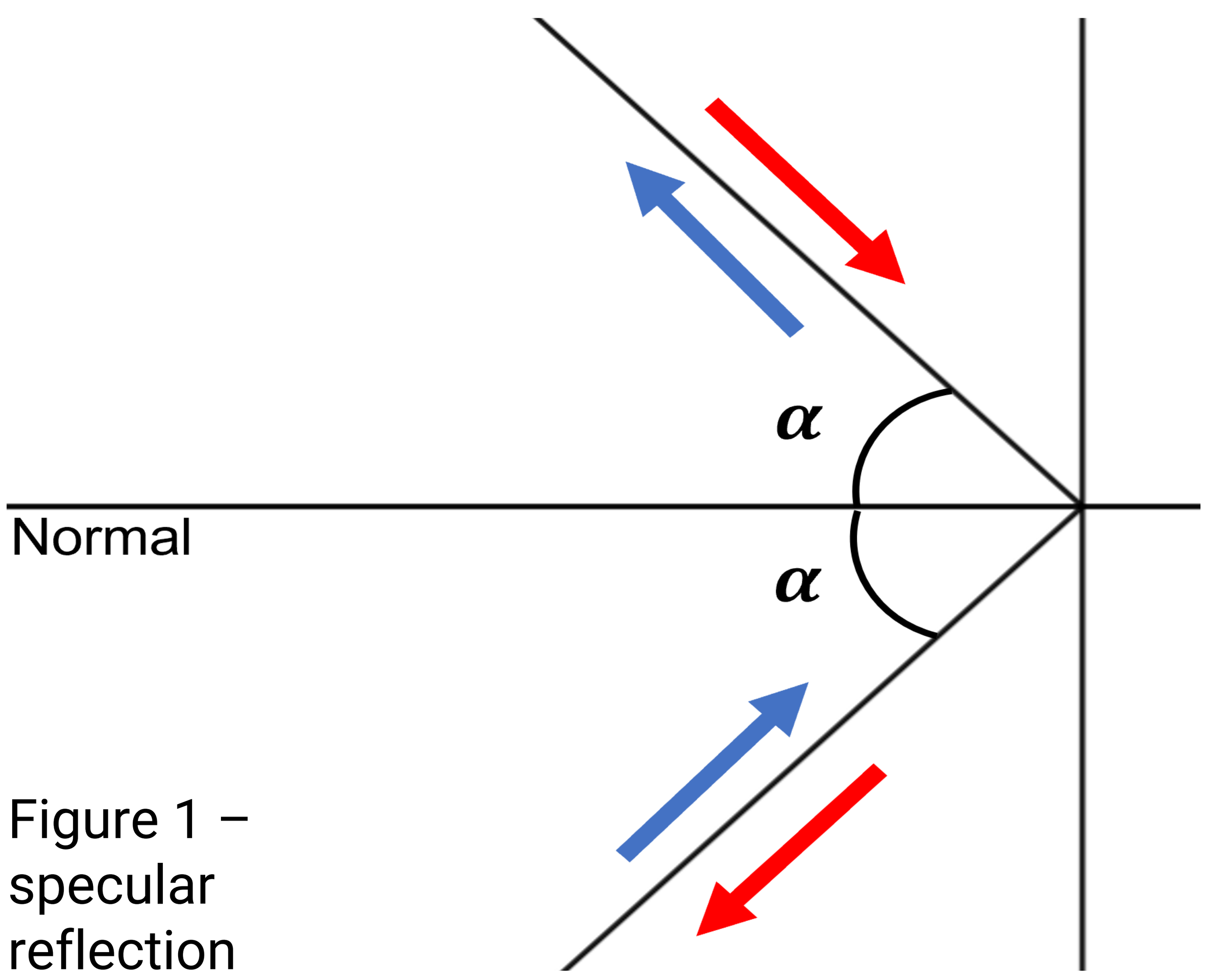

Figure 1 – specular reflection

Loschmidt's paradox

Define the entropy functional $H = \int f \log f$. Then Boltzmann's H-theorem states that

$$\frac{dH}{dt} \leq 0.$$

The H-theorem is a statement of irreversibility however Newton's laws state that classical mechanics is reversible in time. This appearance of irreversibility is Loschmidt's paradox. In particular, Loschmidt says that we can take a system with given initial state and let it evolve until time $t_1 > 0$. Then reverse all velocities and let it evolve until time $2t_1$. Classical mechanics tells us that the system should return to its initial state. But this would imply that

$$\frac{dH}{dt} > 0.$$

This is in direct contradiction with Boltzmann's H-theorem. The answer lies in the seemingly reasonable assumption of molecular chaos.

Zermelo's paradox

The Poincare recurrence theorem states that (under suitable assumptions), a set of points evolving via a flow will return to its initial state (and in fact return infinitely often). The first iteration for which it returns is called the recurrence time.We can apply this to the system given in our derivation - after the recurrence time our system will have returned to its initial state.

However, this is in direct contradiction with the H-theorem. H is initially decreasing but for the system to return to its initial state it must increase again at some point!

Boltzmann himself argued that the recurrence time of a typical gas is so large that we can ignore the paradox since we observe the gas on much smaller timescales – but this is a physical argument. There is still no satisfactory mathematical resolution to this paradox.

Molecular chaos

Intuitively, this assumption says that the velocities of colliding particles are uncorrelated. The key point is that this holds only for pre-collisional particles – after colliding the positions and velocities of the particles are now dependent on the collision. This is the idea of "one-sided chaos". This assumption implicitly introduces a "forward direction" of time into our system. By having a defined direction of time, irreversibility is then introduced into the system. In some sense, this is the answer to Loschmidt's paradox. It is an explanation of how irreversibility enters our fully time-reversible system. But currently we have no precise mathematical formulation for the chaos assumption. This is summed up nicely by Cedric Villani:

"The physical derivation of the Boltzmann equation is based on the propagation of one-sided chaos, but no-one knows how this property should be expressed mathematically – if meaningful at all" – Cedric Villani

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