Lanford's theorem and the arrow of time

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Contents

1. The arrow of time in statistical physics

- Main aim of statistical physics is to understand the thermal behaviour of macrosopic systems (e.g. gases) in terms of their molecular constitution and dynamics and probabilistic considerations.
- Main problem: Thermal behaviour is often irreversible (i.e. asymmetric under time-reversal). E.g.: The Second Law of thermodynamics implies that the entropy of a closed system can only increase.
  But molecular dynamics and probability theory are invariant with respect to an interchange of past and future directions of time.
- So how can one obtain time-asymmetric results from (apparently) only time-symmetric assumptions?

2. Assumptions in the Boltzmann equation

Boltzmann considered hard-spheres gas model, initially not in equilibrium. Will it necessarily evolve towards equilibrium?

A gas simulation

Assumptions:

1. A gas is idealized as composed by N molecules (of equal mass $=1$) with diameter a in a finite volume region Λ, moving freely according to classical dynamics so dilute that only binary collisions occur.
2. The state of the gas at time t is described by a distribution function f_t such that:

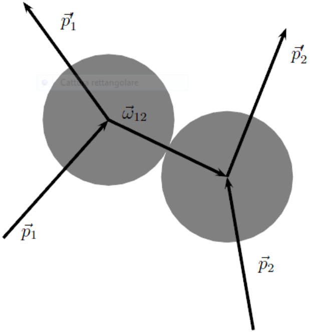
$$f_t(\vec{q},\vec{p})\delta\vec{q}\delta\vec{p} \;\approx\; \frac{1}{N} \times \text{number of particles with positions between } \vec{q} \text{ and } \vec{q}+\delta\vec{q} \text{ and velocities between } \vec{p} \text{ and } \vec{p}+\delta\vec{p}.$$

Collisions in the hard spheres model

Under collisions, momenta change instantaneously:

$$\begin{aligned}\vec{p}_1{}' &= \vec{p}_1 - (\vec{\omega}_{12} \cdot (\vec{p}_1 - \vec{p}_2))\,\vec{\omega}_{12} \\ \vec{p}_2{}' &= \vec{p}_2 + (\vec{\omega}_{12} \cdot (\vec{p}_1 - \vec{p}_2))\,\vec{\omega}_{12},\end{aligned}$$

where $\vec{\omega}_{12}$ is the unit vector pointing from particle 1 to particle 2.



The particles are about to collide iff they touch and $\vec{\omega}_{12} \cdot (\vec{p}_1 - \vec{p}_2) \geq 0$.

Assumptions in the Boltzmann equation (contd.)

The most crucial assumption was

3. the Stosszahlansatz: (i) The relative number of pairs of particles about to collide, with variables $(\vec{q}_1, \vec{p}_1)$, and $(\vec{q}_2, \vec{p}_2)$, is proportional to the product $f_t(\vec{q}_1, \vec{p}_1) f_t(\vec{q}_2, \vec{p}_2)$. I.e:

$$f_t^{(2)}(\vec{q}_1, \vec{p}_1; \vec{q}_2, \vec{p}_2) = f_t(\vec{q}_1, \vec{p}_1) f_t(\vec{q}_2, \vec{p}_2).$$

From these assumptions, Boltzmann gave a heuristic argument for the so-called Boltzmann equation

$$\frac{\partial}{\partial t} f_t + \vec{p}_1 \cdot \frac{\partial}{\partial \vec{q}} f_t \quad = \quad \mathcal{C}(f_t, f_t)$$

where

$$\mathcal{C}(f_t, f_t) = Na^2 \int_{\mathbb{R}^3} d\vec{p}_2 \int_{\vec{\omega}_{12}\cdot(\vec{p}_1-\vec{p}_2)\geq 0} d\vec{\omega}_{12}\,(\vec{p}_1 - \vec{p}_2)\cdot\vec{\omega}_{12} \Big[f_t(\vec{q},\vec{p}_1{}')f_t(\vec{q},\vec{p}_2{}') - f_t(\vec{q},\vec{p}_1)f_t(\vec{q},\vec{p}_2)\Big]$$

Or equivalently:

$$\mathcal{C}f_t^{(2)} = Na^2 \int_{\mathbb{R}^3} d\vec{p}_2 \int_{\vec{\omega}_{12}\cdot(\vec{p}_1-\vec{p}_2)\geq 0} d\vec{\omega}_{12}\,(\vec{p}_1 - \vec{p}_2)\cdot\vec{\omega}_{12} \Big[f_t^{(2)}(\vec{q},\vec{p}_1{}',\vec{q},\vec{p}_2{}') - f_t^{(2)}(\vec{q},\vec{p}_1,\vec{q},\vec{p}_2)\Big]$$

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From the Boltzmann equation, he derived the H-theorem, i.e. the expression:

$$H[f_t] := \int f_t(\vec{q},\vec{p}) \ln f_t(\vec{q},\vec{p})\, d\vec{q}\, d\vec{p}$$

is monotonically decreasing in time:

$$\frac{dH[f_t]}{dt} \leq 0.$$

Comments:

- Boltzmann identified $-H[f]$ with entropy, and claimed he had thus given a strict dynamical proof of the Second Law.
- By focusing on the number of particles that will collide in δt, and not demanding the same thing about particles that just have collided, a time-asymmetrical —and thus non-dynamical— ingredient is introduced.
- But Boltzmann did not draw attention to the crucial role of the Stoszahlansatz:

  "The determination [of the number of collisions] can only be obtained in a truly tedious manner, [...] But since this determination has, apart from its tediousness, not the slightest difficulty, nor any special interest, and because the result is so simple that one might almost say it is self-evident I will only state this result. (1872, p. 323)

Lanford's theorem

- Lanford's theorem is formulated in the BBGKY approach to Hamiltonian mechanics.
- Consider a phase space of N hard spheres,

$$\Gamma_N^{(a)} = \{x = (\vec{q}_1, \vec{p}_1; , \dots \vec{q}_n, \vec{p}_N) \ : \ \ \vec{q}_i \in \Lambda, \|\vec{q}_i - \vec{q}_j\| \geq a\}$$

- A statistical state is represented by a probability density function $\mu(x)$ over $\Gamma_N^{(a)}$.
- Its time evolution is determined by the Hamiltonian flow.
- If both μ and the Hamiltonian are permutation invariant, it is convenient to represent the statistical state μ and its time evolution is by a sequence of (time-dependent) multi-particle correlation functions $\rho_{k,t}^{(a)}$ with $k = 1, ..., N$.

In particular . . .

The BBGKY hierarchy for hard spheres

- For a given probability density $\mu(x)$ on $\Gamma_N^{(a)}$, define a hierarchy of correlation functions $k = 1, \ldots, N$, writing $x = (x_1, \ldots, x_N)$,

$$\rho_k^{(a)}(x_1, \ldots, x_k) \quad := \quad \frac{N!}{(N-k)!} \frac{1}{N^k} \int \mu(x) dx_{k+1} \cdots dx_N$$

The evolution of μ is equivalent to the BBGKY hierarchy:

$$\frac{\partial \rho_{k,t}^{(a)}}{\partial t} = \mathcal{H}_k^{(a)} \rho_{k,t}^{(a)} + \mathcal{C}_{k,k+1}^{(a)} \rho_{k+1,t}^{(a)} \quad k = 1, \ldots N$$

Actually, it suffices to look at $k = 1$. Then the *Liouville operator* is

$$\mathcal{H}_1^{(a)} \rho_{1,t}^{(a)} = -\vec{p}_1 \cdot \frac{\partial}{\partial \vec{q}_1} \rho_{1,t}^{(a)}$$

And the *collision operator* is

$$\mathcal{C}_{1,2}^{(a)} \rho_{2,t}^{(a)} = N a^2 \int d\vec{p}_2 \int_{S^2} d\vec{\omega}_{12} \, \vec{\omega}_{12} \cdot (\vec{p}_2 - \vec{p}_1) \, \rho_{2,t}^{(a)}(\vec{q}_1, \vec{p}_1, \vec{q}_1 + a\vec{\omega}_{12}, \vec{p}_2)$$

The left hand side looks like the Boltzmann equation, but the collision operator is different:

$$\mathcal{C}^{(a)}_{1,2}\rho^{(a)}_{2,t} = Na^2 \int d\vec{p}_2 \int_{S^2} d\vec{\omega}_{12}\,\vec{\omega}_{12}\cdot(\vec{p}_2 - \vec{p}_1)\,\rho^{(a)}_{2,t}(\vec{q}_1, \vec{p}_1, \vec{q}_1 + a\vec{\omega}_{12}, \vec{p}_2)$$

The Boltzmann collision term, on the other hand, is

$$Na^2 \int d\vec{p}_2 \int_{\vec{\omega}_{12}\cdot(\vec{p}_1 - \vec{p}_2)\geq 0} d\vec{\omega}_{12}\,\vec{\omega}_{12}\cdot(\vec{p}_1 - \vec{p}_2) \left[f^{(2)}_t(\vec{q}, \vec{p}_1{}', \vec{q}, \vec{p}_2{}') - f^{(2)}_t(\vec{q}, \vec{p}_1, \vec{q}, \vec{p}_2)\right]$$

Incoming vs Outgoing configuration

The dynamics is discontinuous at a point where a collision occurs $(\|\vec{q}_1 - \vec{q})_{\|} = a)$:

the pre-collision coordinates $x_{pre} = (\vec{q}_1, \vec{p}_1, \vec{q}_2, \vec{p}_2)$ is different from the post-collision coordinates $x_{post} = (\vec{q}_i, \vec{p}_1{}', \vec{q}_2, \vec{p}_2{}')$

Yet, by choosing a topology on $\partial\Gamma^{(a)})_N$ in which x_{pre} and x_{post} are connected without discontinuity, the dynamics becomes smooth.

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CRUCIAL POINT:

Lanford argues to *identify* these two points as being different representations of the same phase point:

Incoming representation

Obtained by replacing all outgoing momenta with incoming momenta.

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BBGKY collision operator in incoming representation

Lanford adopted the **incoming representation** in the BBGKY collision operator,

$$\mathcal{C}^{(a)}_{1,2}\rho^{(a)}_{2,t} = Na^2 \int d\vec{p}_2 \int_{S^2} d\vec{\omega}_{12}\; \vec{\omega}_{12}\cdot(\vec{p}_2 - \vec{p}_1)\; \rho^{(a)}_{2,t}(\vec{q}_1, \vec{p}_1, \vec{q}_1 + a\vec{\omega}_{12}, \vec{p}_2)$$

and after a few further manipulations he derived a new collision operator: the *BBGKY* collision operator*

$$\widehat{\mathcal{C}}^{(a)}_{1,2}\rho^{(a)}_{2,t} = Na^2 \int_{\vec{\omega}_{12}\cdot(\vec{p}_1-\vec{p}_2)\geq 0} d\vec{p}_2\, d\vec{\omega}_{1,2}(\vec{\omega}_{12}\cdot\vec{p}_2 - \vec{p}_1)$$
$$[\rho^{(a)}_{2,t}(\vec{q}_1, \vec{p}_1{}', \vec{q}_1 - a\vec{\omega}_{12}, \vec{p}_2{}') - \rho^{(a)}_{2,t}(\vec{q}_1, \vec{p}_1, \vec{q}_1 + a\vec{\omega}_{12}, \vec{p}_2)]$$

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Compare again with the *Boltzmann collision operator*

$$\mathcal{C}f^{(2)}_t = Na^2 \int d\vec{p}_2 \int_{\vec{\omega}_{12}\cdot(\vec{p}_1-\vec{p}_2)\geq 0} d\vec{\omega}_{12}\, \vec{\omega}_{12}\cdot(\vec{p}_1 - \vec{p}_2)$$
$$\left[f^{(2)}_t(\vec{q}, \vec{p}_1{}', \vec{q}, \vec{p}_2{}') - f^{(2)}_t(\vec{q}, \vec{p}_1, \vec{q}, \vec{p}_2)\right]$$

Deriving the Boltzmann equation from the BBGKY hierarchy

From the above one expects that

$$\widehat{\mathcal{C}}_{1,2}^{(a)} \longrightarrow \mathcal{C} \quad \text{if} \quad a \longrightarrow 0.$$

More precisely, one expects this in the so-called Boltzmann-Grad limit: $a \longrightarrow 0$, while simultaneously $N \longrightarrow \infty$, $Na^2 =$constant.

Lanford's theorem spells out under what conditions this is the case.

Assumptions in Lanford's Theorem

Let $h_\beta(\vec{p}_i) = (\frac{\beta}{2\pi m})^{\frac{3}{2}} z\, e^{-\frac{\beta \vec{p}_i^2}{2m}}$ be the equilibrium Maxwellian distribution for a gas of density $z = 1/|\Lambda|$ at inverse temperature β.

(1) Regularity assumption

There is a positive real constant M such that for all $k = 1, \ldots, N$

$$\rho^{(a)}_{k,0}(x_1, ..., x_k) \leq M \prod_{i=1}^{k} h_\beta(\vec{p}_i)$$

This assumption rules out certain initial $\rho^{(a)}_{k,0}$ which are "too" far away from equilibrium

(2) Convergence assumption

$$\lim_{a \to 0} \rho^{(a)}_{k,0}(x_1, ..., x_k) = \prod_{i=1}^{k} f_0(x_i)$$

Lanford's theorem

LANFORD'S THEOREM

If assumptions (1) and (2) are satisfied at $t = 0$, there exists a strictly positive real number τ such that for all $t \in [0, \tau]$

$$\lim_{a \to 0} \rho^{(a)}_{k,t}(x_1, ..., x_k) = \prod_{i=1}^{k} f_t(x_i)$$

Where $\rho_{k,t}$ is a solution of the the BBGKY hierarchy (with BBGKY* collision operator!) and f_t a solution of the Boltzmann equation with initial condition f_0.

Where does irreversibility come from?

Lanford's theorem shows the validity of the Boltzmann equation can be derived from Hamitonian dynamics in the BBGKY formalism in the Boltzmann-Grad limit, for times $0 \leq t \leq \tau$.

But the solutions of the Boltzmann equation typically behave irreversibly $dH[f_t]/dt < 0$. The Hamiltonian dynamics is time-reversal invariant. Hence, there must be some additional time-asymmetric ingredient in the theorem.

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- Assumptions (1) and (2) are clearly neutral under time-reversal.
- the BBGKY hierarchy is time-reversal invariant
- Lanford (1981) argued that irreversibility is due to the Boltzmann-Grad limit.
- We believe that this limit is also neutral under time-reversal.
- We claim that the BBGKY* hierarchy is not time-reversal invariant. Hence, the time-asymmetric ingredient is the insistence on the incoming collision configurations.

Conclusions

The source of irreversibility lies in the passage from the BBGKY hierarchy to the BBGKY* hierarchy.

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Also, if one chose the outgoing configuration, one would instead obtain the “anti-Boltzmann equation’. This shows that

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- Adopting the incoming configuration is necessary to derive Boltzmann Equation

Moral: the choice of the incoming configuration is still the essential ingredient to obtain irreversibility in Lanford's theorem. But if we ask for a **motivation** for this choice, we are no further than Boltzmann was . . .