Entropy and irreversibility in gas dynamics

Joint work with
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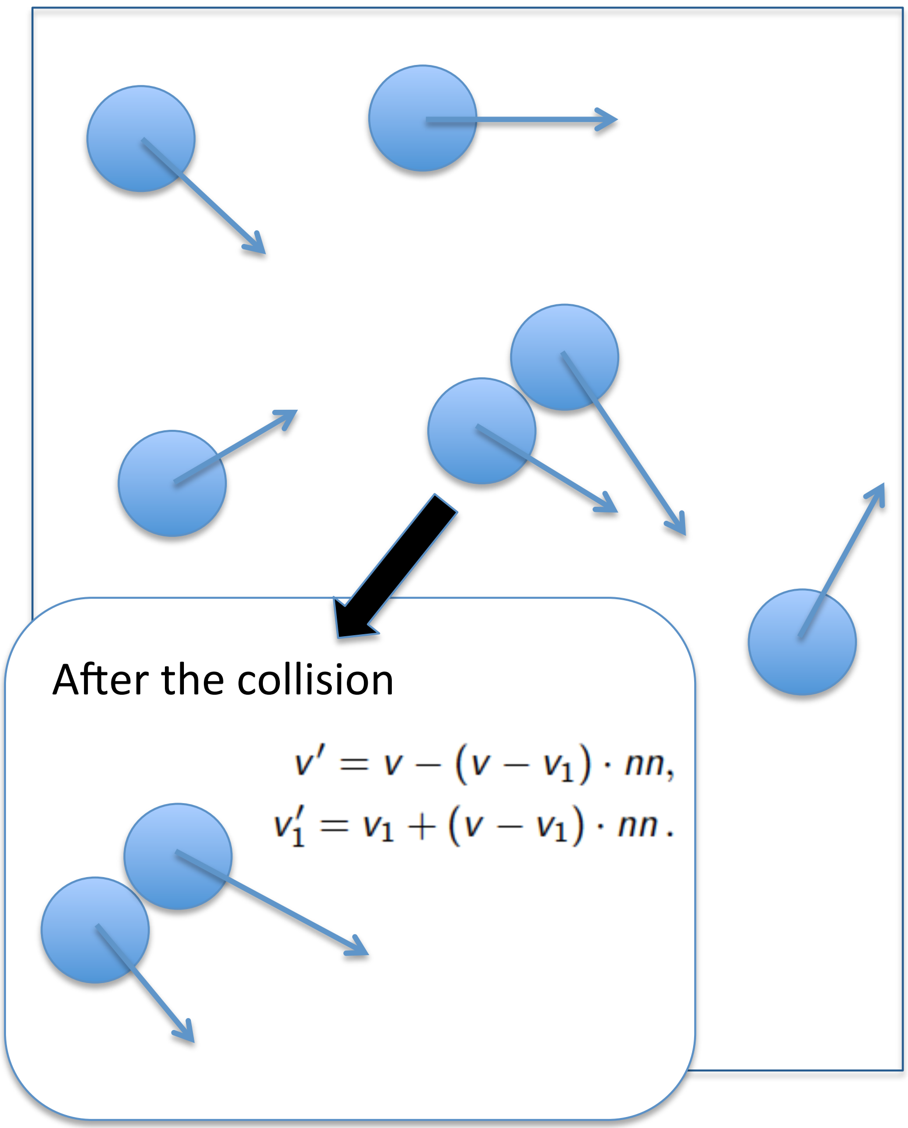
Kinetic description for a gas of hard spheres

Hard sphere dynamics



The system evolves under the combined effects of free transport and collisions.

Collisions are supposed to be elastic, i.e. to preserve momentum and kinetic energy.

Together with the non penetration condition, these conservations determine the evolution of two spheres.

Boltzmann's model

The unknown

$$f \equiv f(t,x,v)$$

Probability of having a particle with position x and velocity v at time t.

The chaos assumption

$$\mathbb{P}[(t,x,v) \text{ et } (t,x,v_1)] = f(t,x,v)f(t,x,v_1)$$

Pre-collisional particles are independent.

The evolution equation

Accounts for the effects of transport and collisions.

$$\underbrace{\partial_t f + \sum_i v_i \partial_{x_i} f}_{\text{transport}} = \underbrace{C^+ - C^-}_{\text{collisions}}$$

$$C^+(t,x,v) = \int \mathbb{P}[(t,x,v') \text{ et } (t,x,v_1')]|(v-v_1)\cdot n|dndv_1,$$

$$C^-(t,x,v) = \int \mathbb{P}[(t,x,v) \text{ et } (t,x,v_1)]|(v-v_1)\cdot n|dndv_1.$$

Physical features

Because of

- microscopic **exchangeability**,
- **microreversibility** of collisions,

the collision integral has symmetries, with important implications.

The second principle of thermodynamics

$$S(t) = -\int f \log f(t,x,v)\,dxdv \text{ increasing function of } t.$$

When t>>1, f converges to some equilibrium.

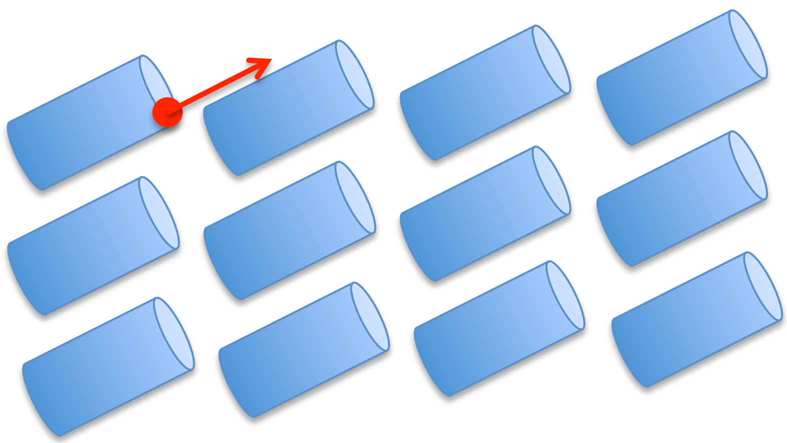
Loschmidt's paradox

Boltzmann's equation predicts an irreversible evolution while the dynamics is reversible.

The low density limit

The scaling

N spheres of size ε on a lattice



Volume covered by a particle of velocity v during a time t : |v|t ε

The transport and collision process have the same time scale if the (inverse) mean free path is of order 1 :

$$N\varepsilon^{d-1} = \alpha \sim 1$$

which only holds for perfect gases.

A statistical description

The N particle density f_N is governed by a simple **transport equation** in a domain encoding the non overlapping condition.

The quantity we are interested in is the first marginal

$$f_N^{(1)}(z_1) = \int f_N(Z_N) dz_2 \dots dz_N.$$

By integration, it is shown to satisfy some **collisional equation** (similar to the Boltzmann equation), but involving some joint probability in the collision term.

The chaos assumption

The joint probability can be expressed in terms of the one particle distribution under some independence assumption

$$f_N^{(2)}(t, z_1, z_2) = f_N^{(1)}(t, z_1) f_N^{(1)}(t, z_2).$$

This identity cannot be true for all times!
- At time 0, small error due to the exclusion.
- For further times, we expect propagation of chaos with small error in the **low density limit**.

Theorem (Lanford)

Consider N hard spheres on $\mathbb{T}^d \times \mathbb{R}^d$, initially "independent" and identically distributed according to f_0

$$f_0(x,v) \leq \exp\left(-\mu - \frac{\beta}{2}|v|^2\right) .$$

Then, in the Boltzmann-Grad limit $N \to \infty$ with $N\varepsilon^{d-1} = \alpha$, the distribution $f_N^{(1)}(t,x,v)$ of a typical particle converges almost everywhere to the solution f of the Boltzmann equation

$$\partial_t f + v \cdot \nabla_x f = \alpha Q(f,f)$$

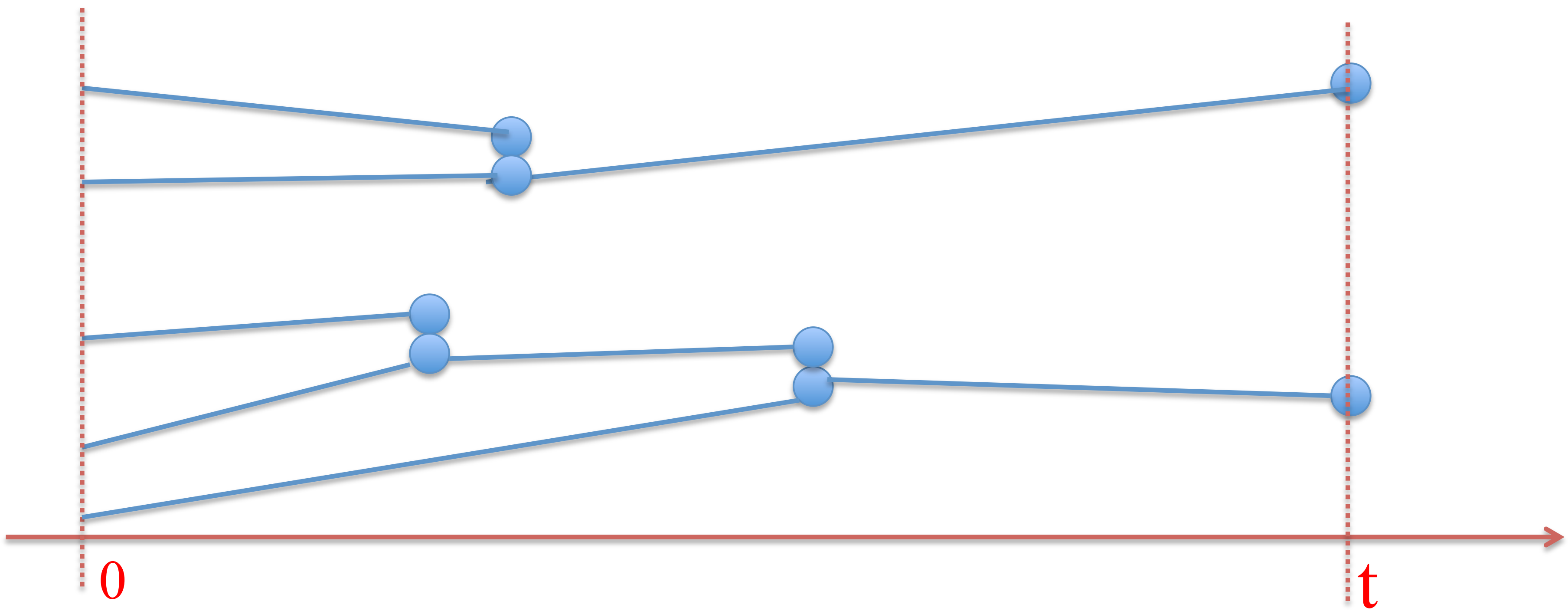
on a short time interval $[0, T^*(\beta,\mu)/\alpha[$.

Some elements of proof

Collision trees

Solutions of the molecular dynamics can be represented by **collision trees**, with transport and scattering operators.

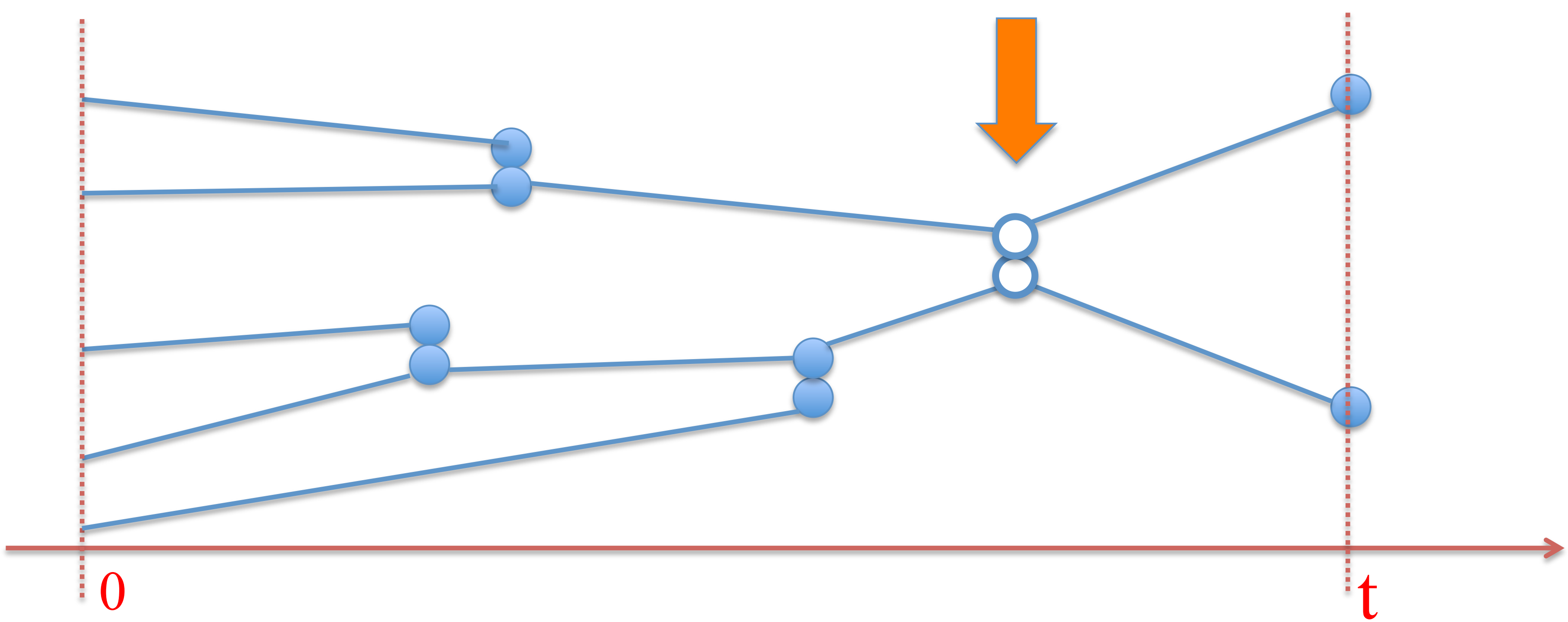
This representation is a reformulation of the BBGKY hierarchy.



Propagation of chaos

Solutions of the Boltzmann equation provide a good approximation as long as there is **no recollision** (i.e. no collision between two particles which are not independent).

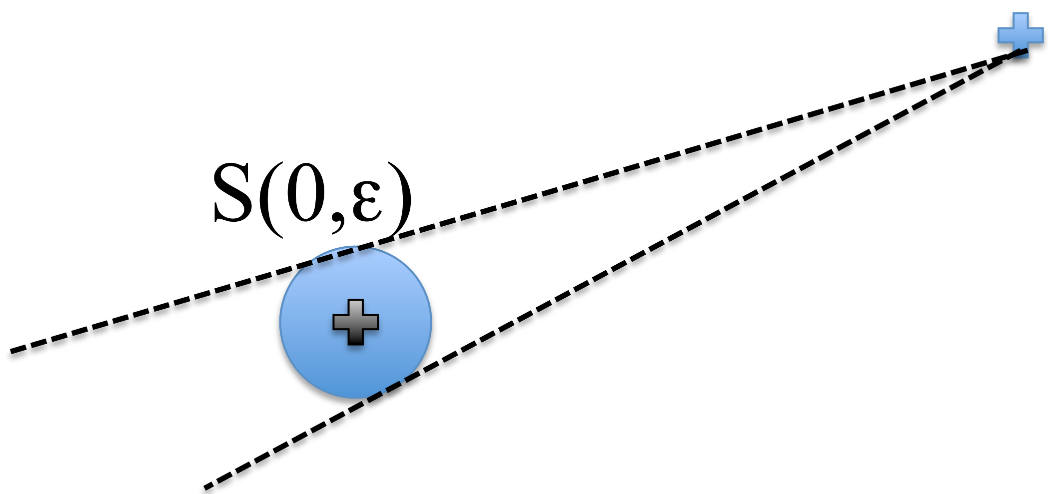
This is the crucial observation by Lanford (see also CIP).



Geometric control of recollisions

To avoid recollisions, we **remove a small set** of bad parameters from each collision integral.

These estimates have been quantified only recently (see GSRT, PSS).



This decomposition of collision integrals can be done as long as the size of collision trees remains controlled (giant components might lead to phase transition).

Bad geometrical sets and irreversibility

Bad sets

Collisional free flow

No convergence of the first term in the series expansion if the backward free flow involves a collision.

$$\mathcal{B}_{\varepsilon_0}^{n-} = \Big\{ Z_n \in (\mathbb{T}^d \times B_R)^n, \qquad \exists s \in [0,T], \exists i,j, \qquad |x_i - x_j - s(v_i - v_j)| \leq \varepsilon_0 \Big\}$$

Outside from these bad sets, one can show that all terms in the series expansion converge (by averaging over bad integration parameters).

Small measure

At least one colliding pair in the past.

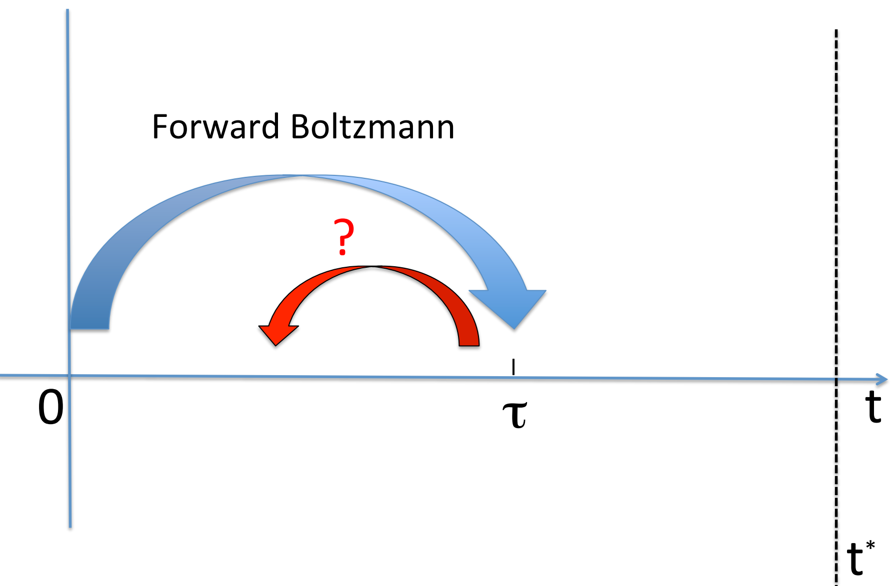
$$|\mathcal{B}_\varepsilon^{n\pm}| \leq C n^2 R T \varepsilon^{d-1}\,.$$

Time symmetry

For negative times, bad sets are defined with the forward free flow.

$$|\mathcal{B}_\varepsilon^{n+} \cap \mathcal{B}_\varepsilon^{n-}| \leq C n^2 \varepsilon^d\,.$$

Irreversibility



The solution of the molecular dynamics is described as a superposition of (red) **pseudo-trajectories between time t and time τ.**

By definition, all « red » pseudo-trajectories involving at least one collision will reach at time τ **a configuration belonging to some bad set.**

→ No information on the convergence

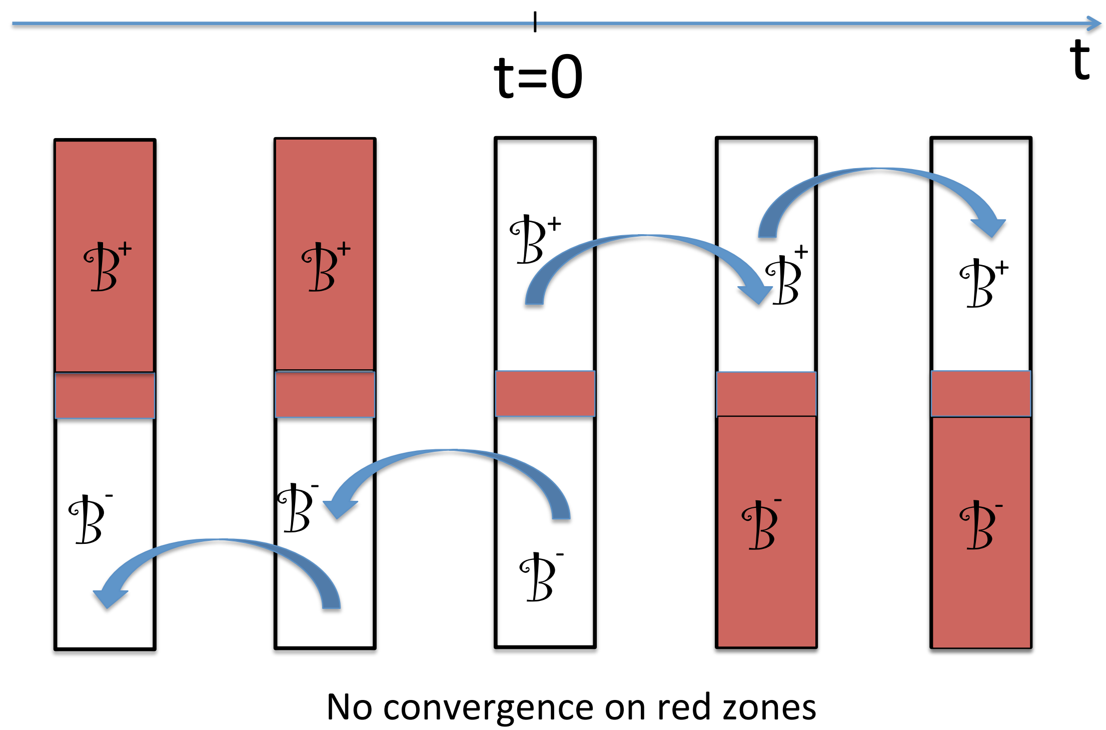
A singular averaging process

Irreversibility is NOT due to

- An arbitrary choice in writing the collision operator
- The chaos assumption
- Forgetting about relative positions of collisional particles

Convergence and chaos hold only outside singular sets.

And these singular sets govern the reverse dynamics!



Correlations and entropy

The linearized entropy

For fluctuations around the equilibrium $M_{N,\beta}$,

- the chaos assumption at time 0 states

$$\delta f_{N,0}(x,v) = M_{N,\beta} \sum_{i=1}^{N} g_0(z_i) \text{ with } \int M g_0 \, dx dv = 0;$$

- the entropy then reduces to the weighted L^2 norm

$$\int \frac{(\delta f_{N,0})^2}{M_{N,\beta}} dZ_N \leq CN \|g_0\|^2_{L^2(Mdz)} < +\infty \, .$$

Cumulant decomposition

An algebraic computation (extracting averages) gives the following **cumulant identity**

$$f_N^{(s)}(t, Z_s) = M_\beta^{\otimes s} \sum_{m=1}^{s} \sum_{\sigma \in \mathfrak{S}_s^m} g_N^m(t, Z_\sigma)$$

The L^2 bound combined with **exchangeability** then shows that higher order cumulants are small

$$\|g_N^m\|^2_{L^2_\beta(\mathbb{D}^m)} \leq \frac{CN \exp(C\alpha^2)}{C_N^m} \|g_0\|^2_{L^2_\beta} \cdot$$

Tracking the information

More precisely, the following identity holds

$$N\|g_N^{(1)}(t)\|^2_{L^2(Mdz)} + \sum_{k=2}^{N} C_N^k \|g_N^{(k)}(t)\|^2_{L^2(M^{\otimes k} dZ_k)} \leq CN\|g_0\|^2_{L^2(Mdz)} \, .$$

To be compared with the « entropy » inequality for the linearized Boltzmann equation

$$\|g(t)\|^2_{L^2(Mdz)} + \alpha \int_0^t \int M g \mathcal{L} g(s,z) dz ds \leq \|g_0\|^2_{L^2(Mdz)} \, .$$

This shows that the **information is not dissipated but transferred to higher order cumulants** (correlations are localized in small sets, but contain a macroscopic part of the information).