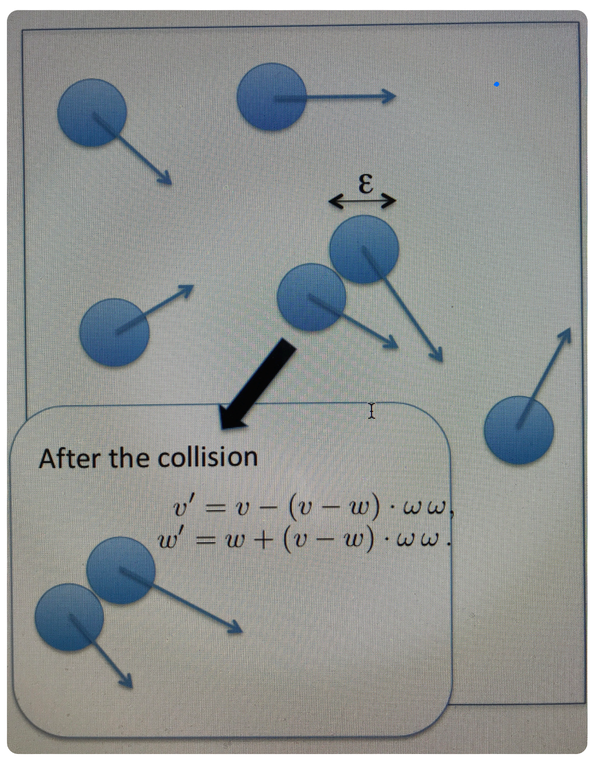
Particle systems in the low density regime.

Part 1. Law of large numbers

1 Perfect gases

The microscopic dynamics is a combination of transport and elastic collisions.
(Hamiltonian dynamics)



$$\begin{cases} \dfrac{dx_i}{dt} = v_i \quad \text{as long as } |x_i - x_j| > \varepsilon \\ \text{elastic reflection when } |x_i - x_j| = \varepsilon \end{cases}$$

The dynamics is deterministic, but we will average over initial configurations in $\mathcal{D}_N^\varepsilon = \{ (x_i, v_i)_{1\leq i\leq N} \,/\, \forall i\neq j \; |x_i - x_j| > \varepsilon \}$

<u>In the canonical setting</u>, the number N of particles is fixed and the probability density satisfies the Liouville equation

$$\partial_t W_N + \sum_{i=1}^N v_i \cdot \nabla_{x_i} W_N = 0 \quad \text{on } \mathcal{D}_N^\varepsilon$$

<u>In the grand canonical setting</u>, the number of particles is distributed according a Poisson process

$$\frac{1}{Z_\varepsilon} \frac{\mu_\varepsilon^N}{N!} \mathbb{1}_{\mathcal{D}_N^\varepsilon} \prod_{i=1}^N f_0(x_i, v_i)$$

<u>The Boltzmann-Grad scaling</u> is the regime where each particle undergoes one collision per unit of time in average.

A simple computation due to Maxwell shows that $\mu_\varepsilon \varepsilon^{d-1} \sim 1$

$$\boxed{\begin{aligned} &i \text{ and } j \text{ collide on } [0,T] \\ \Leftrightarrow\ & \exists s \in [0,T] \mid |x_i - x_j - (v_i - v_j)s| \leq \varepsilon \\ \Leftrightarrow\ & x_j \in C_i \text{ with } |C_i| \lesssim \varepsilon^{d-1} t \end{aligned}}$$

This regime describes perfect gases (no excluded volume)

Questions

$\boxed{Q1}$: what is the almost sure dynamics as $\mu_\varepsilon \to \infty$? (law of large numbers)

$\boxed{Q2}$: how does the system fluctuate around this dynamics ? (central limit theorem)

$\boxed{Q3}$: what is the probability of observing another dynamics ? (large deviations)

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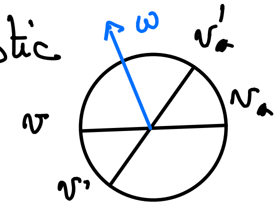
② The Boltzmann equation

The unknown is the probability density $f = f(t,x,v)$ of finding a particle with position x and velocity v at time t.

It evolves under the combined effect of transport and collisions

$$\begin{cases} \partial_t f + v \cdot \nabla_x f = Q(f,f) \\ Q(f,f)(v) = \iint \Big(\underbrace{f(v')\, f(v_*')}_{\text{gain term}} - \underbrace{f(v)\, f(v_*)}_{\text{loss term}} \Big) \underbrace{\big((v-v_*)\cdot\omega\big)_+}_{\text{hard sphere jump rate}} \, dv_*\, d\omega \end{cases}$$

Collisions are assumed to be pointwise and elastic



$$\begin{cases} v' + v'_* = v + v_* \\ |v'|^2 + |v'_*|^2 = |v|^2 + |v_*|^2 \end{cases}$$

They are parametrized by the deflection angle ω, which is random

Using the exchangeability $(v, v_*) \longmapsto (v_*, v)$ and the micro-reversibility $(v, v_*, \omega) \longmapsto (v', v'_*, \omega)$ we can prove the identity

$$\int Q(f,f)\, \varphi(v)\, dv = \frac{1}{4} \iint \big(f(v') f(v'_*) - f(v) f(v_*) \big) \big((v - v_*) \cdot \omega \big)_+ \big(\varphi(v) + \varphi(v_*) - \varphi(v') - \varphi(v'_*) \big)\, dv_*\, dv\, d\omega$$

Choosing φ to be a collision invariant $1, v_1, \dots v_d, |v|^2$ we obtain the conservation laws (mass, momentum and energy)

$$\begin{cases} \partial_t \int f\, dv + \nabla_x \cdot \int f v\, dv = 0 \\ \partial_t \int f v\, dv + \nabla_x \cdot \int f\, v \otimes v\, dv = 0 \\ \partial_t \int f |v|^2\, dv + \nabla_x \cdot \int f |v|^2 v\, dv = 0 \end{cases}$$

Applying the same identity with $\varphi = \log f$ shows that $\int Q(f,f) \log f\, dv \leq 0$

from which we deduce the H-theorem (second principle)

$$\partial_t \int f \log f\, dv + \nabla_x \cdot \int f \log f\, v\, dv \leq 0.$$

The a priori bounds coming from these physical estimates are not strong enough to make sense of the collision operator (which is essentially a multiplication of L^1 functions of (t,x))

To solve the Cauchy problem, there are 3 settings

- local solutions in some weighted L^∞ space
- global solutions in the vincinity of equilibrium
- global renormalized solutions

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③ Lanford's theorem → a partial answer to Q1

Theorem: In the Boltzmann-Grad limit $\mu_\varepsilon \to \infty$, the empirical measure π_t^ε defined by

$$\pi_t^\varepsilon(h) = \frac{1}{\mu_\varepsilon} \sum_{i=1}^{N} h(z_i(t))$$

concentrates on the solution to the Boltzmann equation

$$\begin{cases} \partial_t f + v \cdot \nabla_x f = Q(f,f) \\ Q(f,f) = \int \big(f(v')f(v_*') - f(v)f(v_*)\big)\big((v-v_*)\cdot\omega\big)_+ \, dv_* \, d\omega \end{cases}$$

on a time interval $[0,T]$ (depending only on f_0)

This statement raises many issues.

$\boxed{P1}$: the limiting equation is irreversible (H-theorem)
What do we loose in the limiting process?
Is it possible to retrieve some reversibility?

$\boxed{P2}$: the convergence holds only for short times.
Where does this limitation come from?
What would we need to iterate the result?

The proof relies on the study of correlation functions F_n^ε defined as projections of the probability measure

$$\int F_n^\varepsilon h_n \, dZ_n = \mathbb{E}_\varepsilon \left(\frac{1}{\mu_\varepsilon^n} \sum_{(i_1, \dots i_n)} h_n(z_{i_1}(t), \dots z_{i_n}(t)) \right)$$

F_n^ε encodes the joint probability of finding n particles in the state $(z_1, \dots z_n)$ at time t.

We will prove that $F_n^\varepsilon \longrightarrow F_n$ where (F_n) solves a hierarchy of equations which has a factorized solution $F_n = f^{\otimes n}$ with f solving the Boltzmann equation.

⚠ chaos is not proved directly, nor the concentration of π_t^ε

4) Sketch of proof

The BBGKY hierarchy (Bogoliubov, Born, Green, Kirkwood, Yvon)

By integration of the Liouville equation, we get that

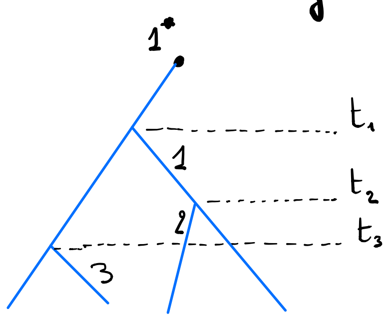
$$\partial_t F^\varepsilon_n + \sum_{i=1}^{n} v_i \cdot \nabla_{x_i} F^\varepsilon_n = \sum_{i=1}^{n} C^{i,n+1} F^\varepsilon_{n+1}$$

Iterating Duhamel's formula leads to

$$\left\{ \begin{array}{l} F^\varepsilon_n(t) = \sum\limits_{m=0} Q^\varepsilon_{n,n+m}(t)\, F^\varepsilon_{n+m}(0) \\ Q^\varepsilon_{n,n+m}(t) = \int dT_m\, S_n(t-t_1) C_n S_{n+1}(t_1-t_2) \dots C_{n+m-1} S_{n+m}(t_m) \end{array} \right.$$

Geometric representation:

The combinatorics of collisions is encoded in trees with n roots, m branchings



For all admissible parameters $(t_i, v_i, \omega_i)_{1\le i\le m}$ we construct pseudo-trajectories $\Psi^\varepsilon_{n,m}$ starting from Z_n^*

- backward transport on $[t_i, t_{i-1}]$
- addition of particle i at t_i : $x_i = x_{a_i} + \varepsilon \omega_i$
  + scattering if $(v_i, v_{a_i}(t_i))$ is post-collisional

$$F^\varepsilon_n(t) = \sum_{m=0}^{\infty} \sum_{a \in \mathcal{A}_{n,m}} \int dT_m\, dV_m\, d\Omega_m\, \mathcal{C}(\Psi^\varepsilon_{n,m})\, F^{\varepsilon,0}_{n+m}(\Psi_{n,m}(0))$$

Short time estimate

The number of trees is given by $|\mathcal{A}_{n,m}| = n(n+1)\dots(n+m-1)$
Each elementary integral involves a simplex in time $t_1 < t_2 \dots < t_m$
Forgetting for the sake of simplicity that collision cross sections diverge at large energies, we get

$$\left| Q^{\varepsilon}_{n,n+m}(t)\, F^{\varepsilon,0}_{n+m} \right| \leq (C_0 t)^m \frac{(n+m-1)!}{(n-1)!\; m!}$$

The series expansion therefore makes sense for short times, it converges uniformly and it is enough to study the convergence as $\mu_\varepsilon \to \infty$ term by term.

Removing recollisions

When the size of particles $\varepsilon \to 0$, we expect the pseudo-trajectories $\Psi^{\varepsilon}_{n,m}$ will converge to some $\Psi_{n,m}$

- backward free transport on $[t_i, t_{i-1}]$
- addition of particle i at t_i : $x_i = x_{a_i}$ no shift (+ scattering)

This convergence can be proved provided that $\Psi^{\varepsilon}_{n,m}$ has no recollision
A careful geometric analysis shows that it happens for a small set of parameters (negligible in the limit)