Motion of a big molecule in a rarefied gas close to equilibrium

Joint work with
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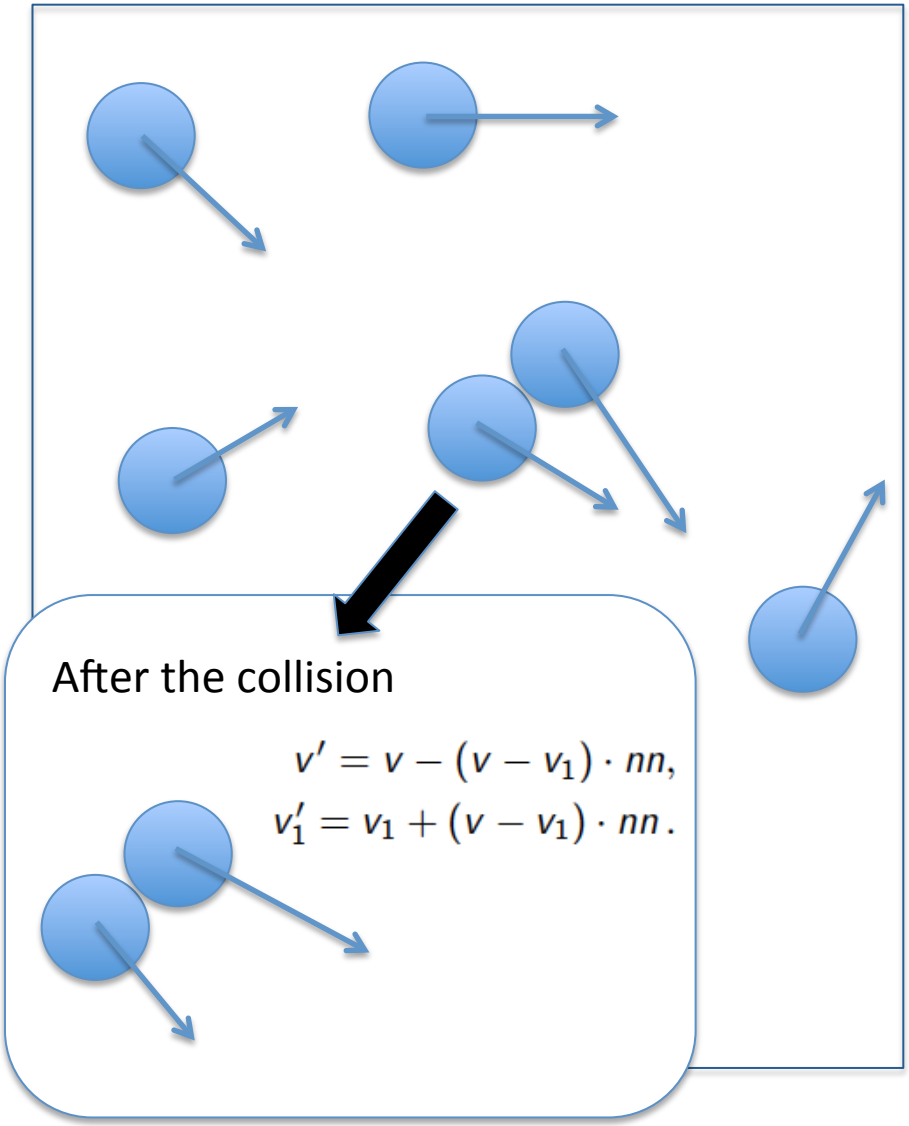
The dynamics of atoms

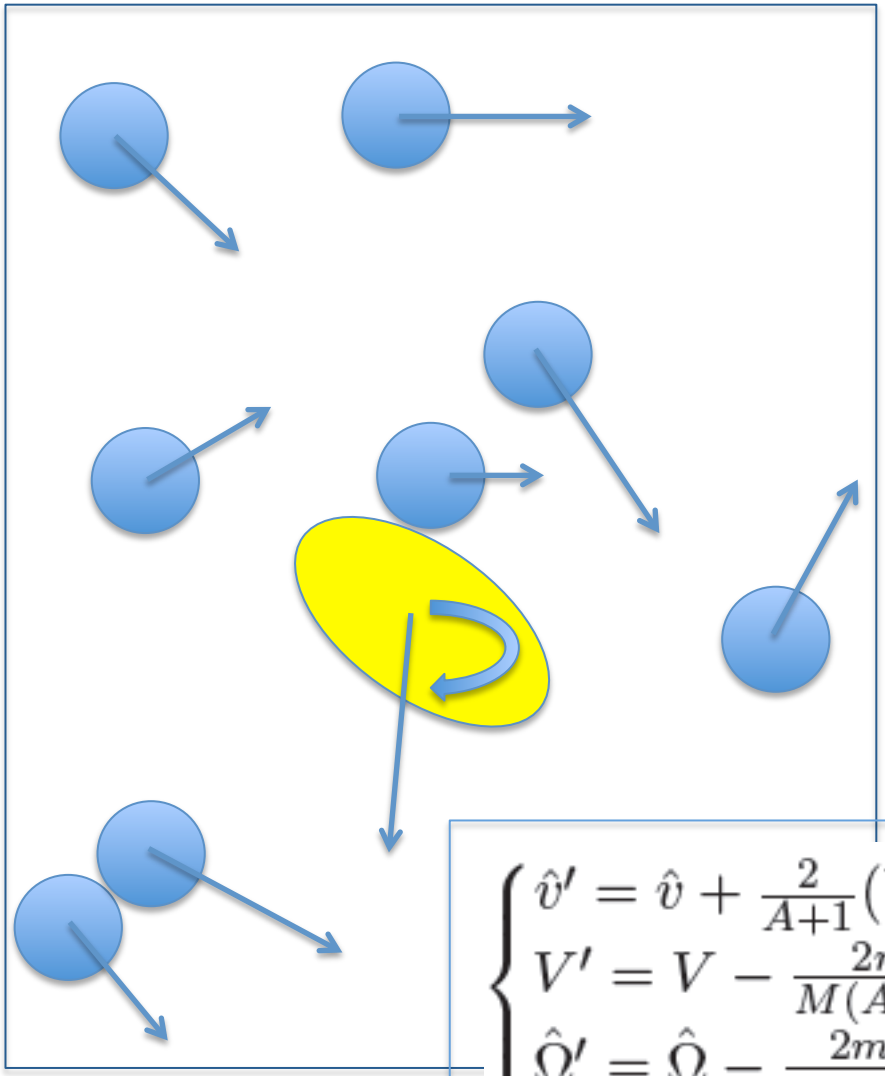


N atoms of diameter ε evolve under the combined effects of free transport and collisions.

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.

The dynamics of the molecule



The molecule is isometric to $(\varepsilon/\alpha)\Sigma$, it may translate and rotate.

The collision between the molecule and an atom produces a force in the normal direction, which is a Dirac mass in time.

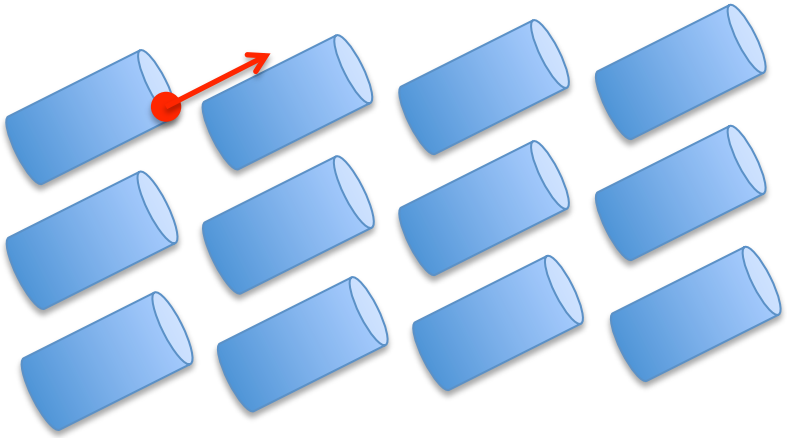
The conservation of energy gives the jump conditions :

$$\begin{cases} \hat{v}' = \hat{v} + \frac{2}{A+1}(V + \frac{\varepsilon}{\alpha}\hat{\Omega}\, r^{\perp} - \hat{v}) \cdot n\, n\,, \\ V' = V - \frac{2m}{M(A+1)}(V + \frac{\varepsilon}{\alpha}\hat{\Omega}\, r^{\perp} - \hat{v}) \cdot n\, n\,, \\ \hat{\Omega}' = \hat{\Omega} - \frac{2m}{(A+1)\hat{I}}\frac{\varepsilon}{\alpha}(n \cdot r^{\perp})\,(V + \frac{\varepsilon}{\alpha}\hat{\Omega}\, r^{\perp} - \hat{v}) \cdot n \end{cases}$$

The Ornstein-Uhlenbeck limit

The Boltzmann-Grad scaling

N spheres of size ε on a lattice



Volume covered by a particle of velocity $\hat{v}$ during a time t : $|\hat{v}|$ t ε

The transport and collision process have the same time scale if

$$N\varepsilon = 1$$

The relaxation rate is then proportional to the typical velocity

$$\hat{v}_{typ} = O(m^{-1/2}).$$

The « weak coupling » limit

Since the molecule is much bigger, it will undergo **a lot of collisions**, typically $1/\alpha$ more collisions.

Note that each one of these collisions will generate an **infinitesimal deflection**:

$$V' - V = -\frac{2m}{M(1+A)}(V + \frac{\varepsilon}{\alpha}\hat{\Omega} - \hat{v}) = O(m^{1/2})\,.$$

We thus choose the mass of atoms such that

$$\frac{m}{M} = \alpha^2, \quad \alpha << 1$$

The limiting equation

The unknown

$$f = f(t, X, V, \Theta, \Omega)$$

Probability that the molecule has position x, orientation θ, velocity v and angular momentum Ω at time t.

The equilibrium assumption

$$M_\beta(\hat{v}) = \frac{\beta\alpha^2}{2\pi} \exp(-\frac{\beta}{2}(\alpha\hat{v})^2)$$

Pre-collisional atoms are at equilibrium, independent of the molecule.

The evolution equation

Accounts for the effects of transport and collisions.

$$\partial_t g + V \cdot \nabla_X g = \left(\frac{8}{\pi\beta}\right)^{1/2} \mathcal{L} g \,.$$

$$\mathcal{L} g = \frac{1}{\beta}\left(\frac{L}{2}\Delta_V + \frac{\mathcal{K}}{I^2}\partial_\Omega^2\right) - \frac{L}{2} V \cdot \nabla_V - \frac{\mathcal{K}}{I}\Omega\partial_\Omega\Big),$$

with $L = |\partial\Sigma|$ and $\mathcal{K} := \int_0^L (r \cdot n^\perp)^2 d\sigma$.

Theorem (Bodineau, Gallagher, Saint-Raymond)

Consider a molecule $(\varepsilon/\alpha)\Sigma$ of mass 1, in a gas consisting of N atoms of diameter ε and mass α^2 initially at equilibrium :

$$f_{N+1,0} = \frac{1}{\mathcal{Z}_{N+1}} \exp\left(-\frac{\beta}{2}(V_N^2 + V^2 + I\Omega^2)\right) g_0(X, V, \Theta, \Omega),$$

denoting by $V_N = \alpha\hat{V}_N$ and $\Omega = (\varepsilon/\alpha)\hat{\Omega}$ the rescaled velocities of atoms and angular momentum of the molecule.

Then, in the limit $N \to \infty$, $\varepsilon \to 0$, $\alpha \to 0$, with $N\varepsilon = 1$ and $1/\alpha^4 << \log\log N$, the distribution of the molecule $f_{N+1}^{(1)}(t, X, V, \Theta, \Omega)$ converges to the solution of the Fokker-Planck equation

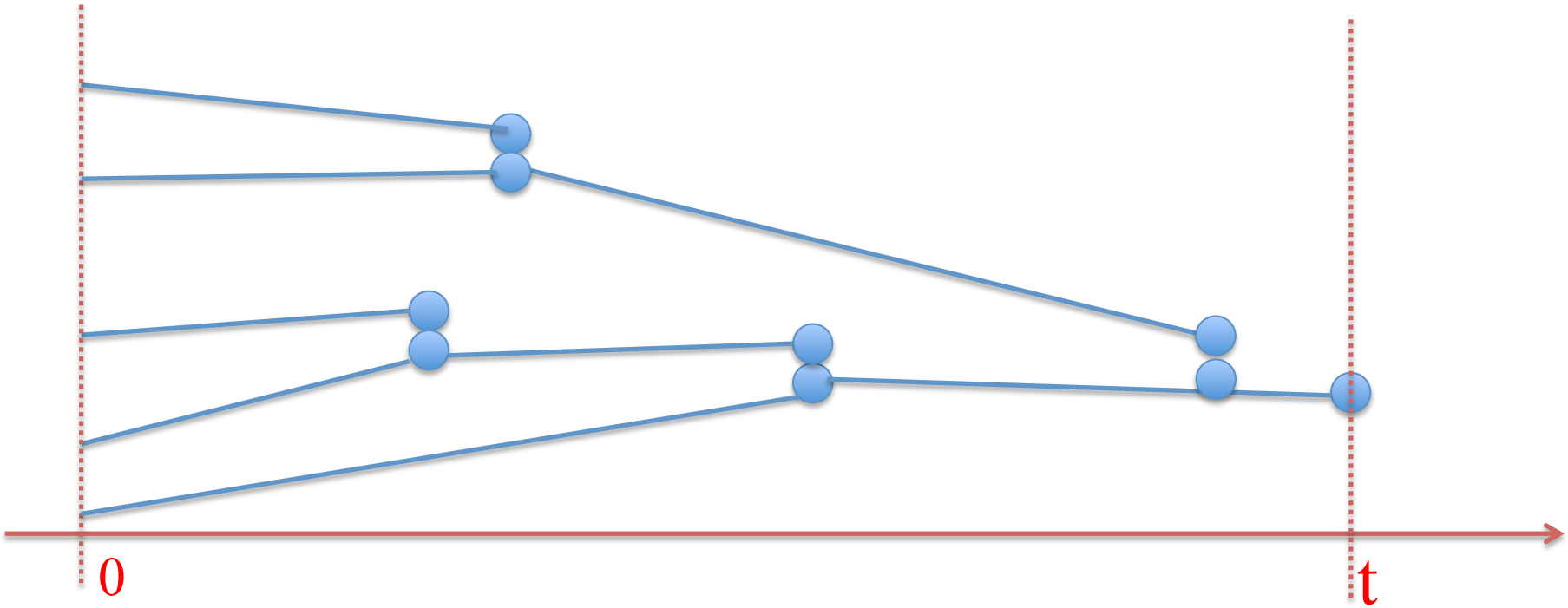
$$\partial_t g + V \cdot \nabla_X g = \left(\frac{8}{\pi\beta}\right)^{1/2} \mathcal{L} g\,.$$

Lanford's strategy

Collision trees

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

This representation is a reformulation of the BBGKY hierarchy.



A short-time uniform bound

The contribution of **collision trees of size s** to the evolution of the first marginal can be roughly estimated by

$$\underbrace{s!}_{\substack{\text{combinatorial factor}\\ \text{counting trees of size s}}} \times \underbrace{\left(\frac{Ct}{\alpha^2}\right)^s}_{\substack{\text{integration over}\\ \text{the simplex in time}}}$$

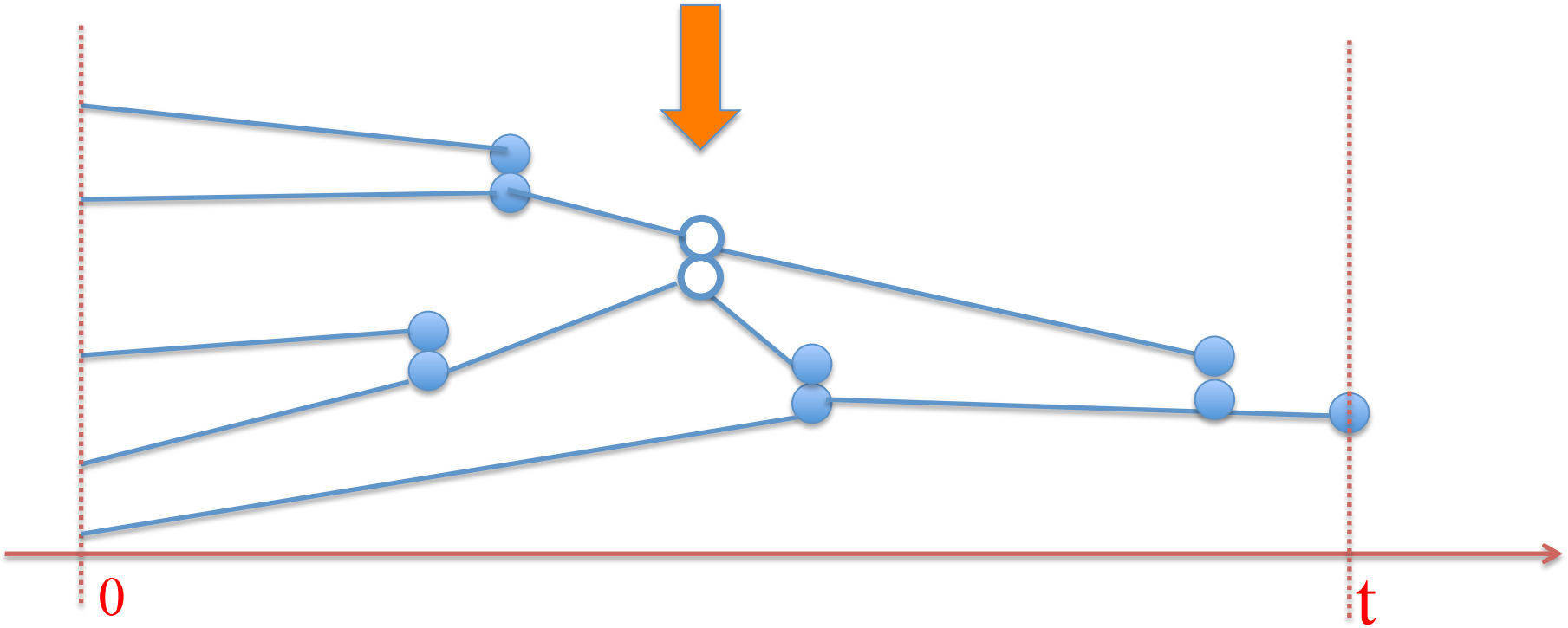
(up to some loss in the decay at large v).

The series expansion **converges only on a fraction of the mean free time**, i.e. for times of order $O(\alpha^2)$.
It is not enough to reach the diffusion limit.

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).

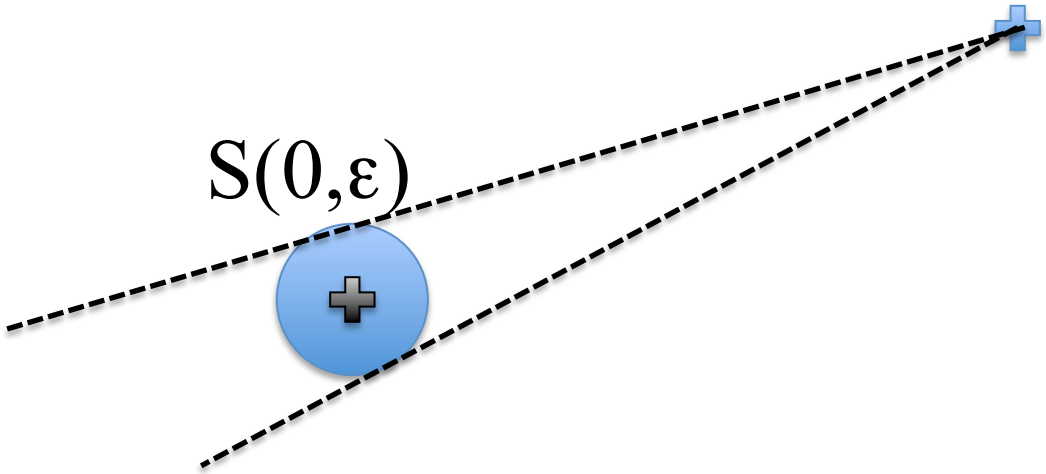
This is the crucial observation by Lanford (see also CIP).



Geometric control of recollisions

To avoid recollisions, the idea is to **remove a small set** of bad parameters from each collision integral.

These estimates have been quantified in the case of (identical) spheres (see GSRT, PSS).



One additional difficulty here is that, because of its geometry, the **molecule can collide twice with the same atom**. We will therefore have to condition the initial data.

The pruning procedure

The maximum principle

Because we consider a gas initially at equilibrium and only specify the distribution of the molecule at time 0,

$$f_{N+1,0} \leq C_0 M_{N+1} ,$$

where M_{N+1} is **invariant under the dynamics** (Gibbs measure).

The maximum principle implies that

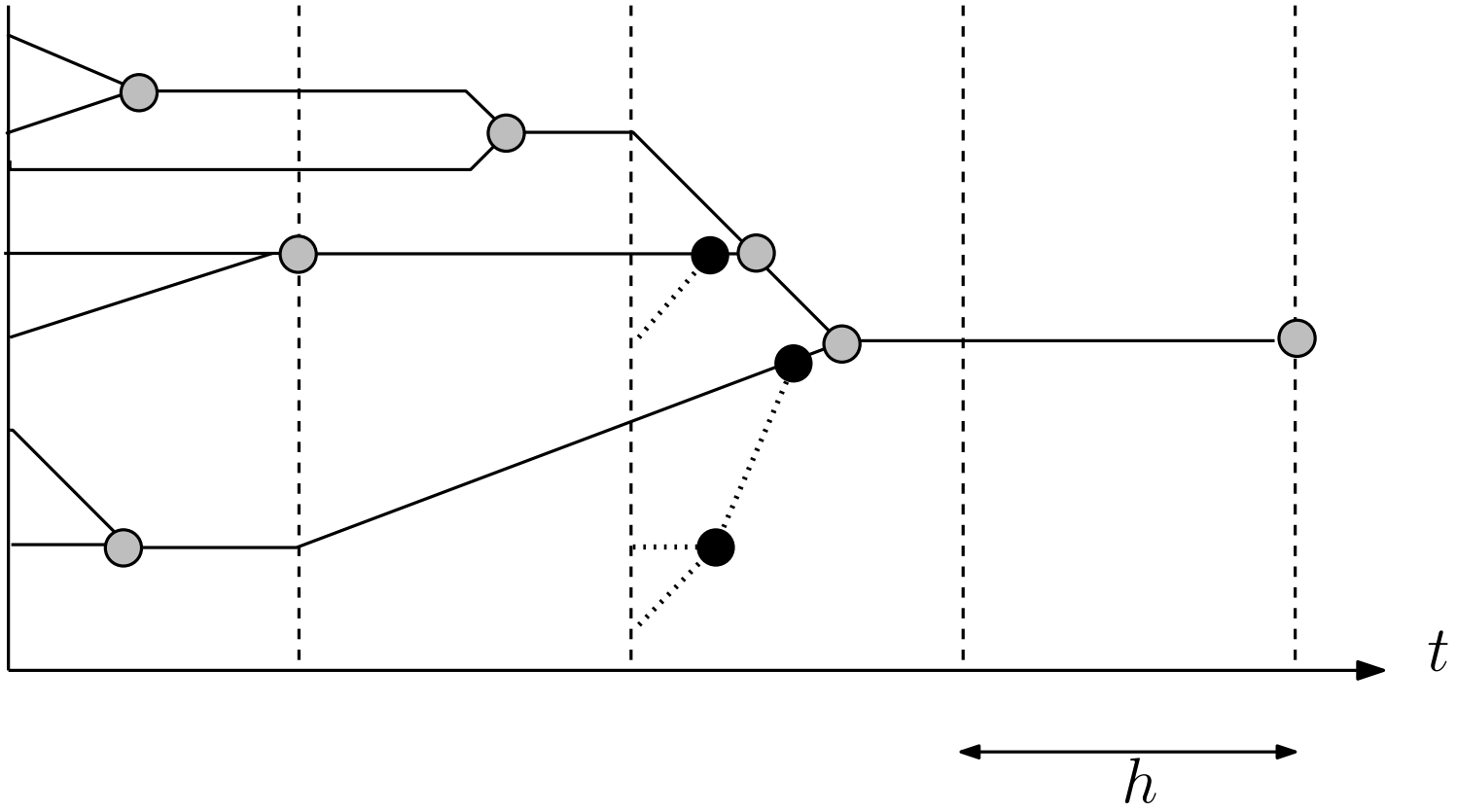
$$f_{N+1}(t) \leq C_0 M_{N+1} ,$$

and therefore a **uniform control on the marginals**

$$f_{N+1}^{(s)}(t) \leq C_0 C^s M^s .$$

A sampling in time

We can use these global in time a priori estimates to discard collision trees with super-exponential branching.



Control of the remainder

A refinement of the previous estimate shows that the contribution of collision trees with

- $J_{k-1} \leq \frac{2^k - 1}{2 - 1} \leq 2^k$ branching points on $[t - (k-1)h, t]$
- $j_k \geq 2^k$ branching points on $[t - kh, t - (k-1)h]$

is at most of order

$$\left(\frac{Ct}{\alpha^2}\right)^{J_{k-1}} \left(\frac{Ct}{\alpha^2}\right)^{n_k} \leq \left(\frac{Cth}{\alpha^4}\right)^{2^k}$$

The **contribution of super exponential trees** vanishes in the limit provided that $\frac{1}{\alpha^4} << \frac{1}{th}$

In order to control the remainders associated to the **geometric cut-off**, we further need that $K = \frac{t}{h} << \log\log N$.

Conditioning the initial data

The geometric conditions

To study the binary interaction between the molecule and an atom, we can rescale time and space so that

- the molecule has size $O(1)$ and the diameter of the atom is α;
- the velocity and angular velocity of the molecule are $O(1)$;
- the typical velocity of the atom is $O(1/\alpha)$.

We then use the **scale separation** together with the **strict convexity** of the molecule to prove that the atom will escape from a security ball before the molecule has really moved.

More precisely, we prove that there will be no recollision if at the first collision

$$|v' - \alpha V'| \geq \alpha^{2/3+\eta}$$

$$|\Omega'| \leq |\log \alpha| \quad \text{and} \quad |V' - V| > \alpha^{2+\eta}$$

Tracking the molecule

The space of trajectories can be endowed with the Skorohod topology. Then, starting from discrete time samplings, we can prove the following **correspondance between trajectories and pseudo-trajectories** :

Proposition. For any measurable event $\mathcal{C}$ in $D([0,T])$

$$\mathbb{P}_N\Big(\{Y_T \in \mathcal{C}\}\Big) = \int dY \sum_{m=0}^{N-1} Q_{1,1+m}(T)\, \mathbf{1}_{\{Y_T \in \mathcal{C}\}}\, f_{N+1}^{(1+m)}(0),$$

where the series are restricted to the pseudo-trajectories in $\mathcal{C}$.

In particular, iterating the argument on time intervals of size $o(\alpha^2)$, one can prove that the probability that the molecule has very small jumps or very large angular momentum converges to 0.

Untypical relative velocities

- Either an atom reaches slowly the molecule after travelling on a distance at least ε/α .
  By **Bienaymé-Tchebichev inequality**, we then get

$$\mathbb{P}_N(\mathcal{B}_1) \leq N\frac{T}{\varepsilon}\mathbb{P}_{M_{\beta,I,N}}\left(|x_1 - X| \leq \frac{2\varepsilon}{\alpha}\right)\,\mathbb{E}_{M_{\beta,I,N}}\left(|v_1 - \alpha V|\,\mathbf{1}_{\{|v_1-\alpha V|\leq \alpha^{5/6}\}}\right)$$
$$\leq N\frac{T}{\varepsilon}\frac{4\varepsilon^2}{\alpha^2}\alpha^{5/2} = 4T\alpha^{1/2}.$$

- Or a slow atom is created by a collision involving two atoms close to the molecule

$$\mathbb{P}_N(\mathcal{B}_2) \leq CN^2\frac{T}{\varepsilon}\mathbb{P}_{M_{\beta,I,N}}\left(|x_1 - X| \leq \frac{2\varepsilon}{\alpha}\right)^2\,\mathbb{E}_{M_{\beta,I,N}}\left(2|v_1 - \alpha V| + \alpha\right)$$
$$\leq CN^2\frac{T}{\varepsilon}\frac{16\varepsilon^4}{\alpha^4}\left|\log\varepsilon\right|^6 = \frac{CT\varepsilon}{\alpha^4}\left|\log\varepsilon\right|^6$$