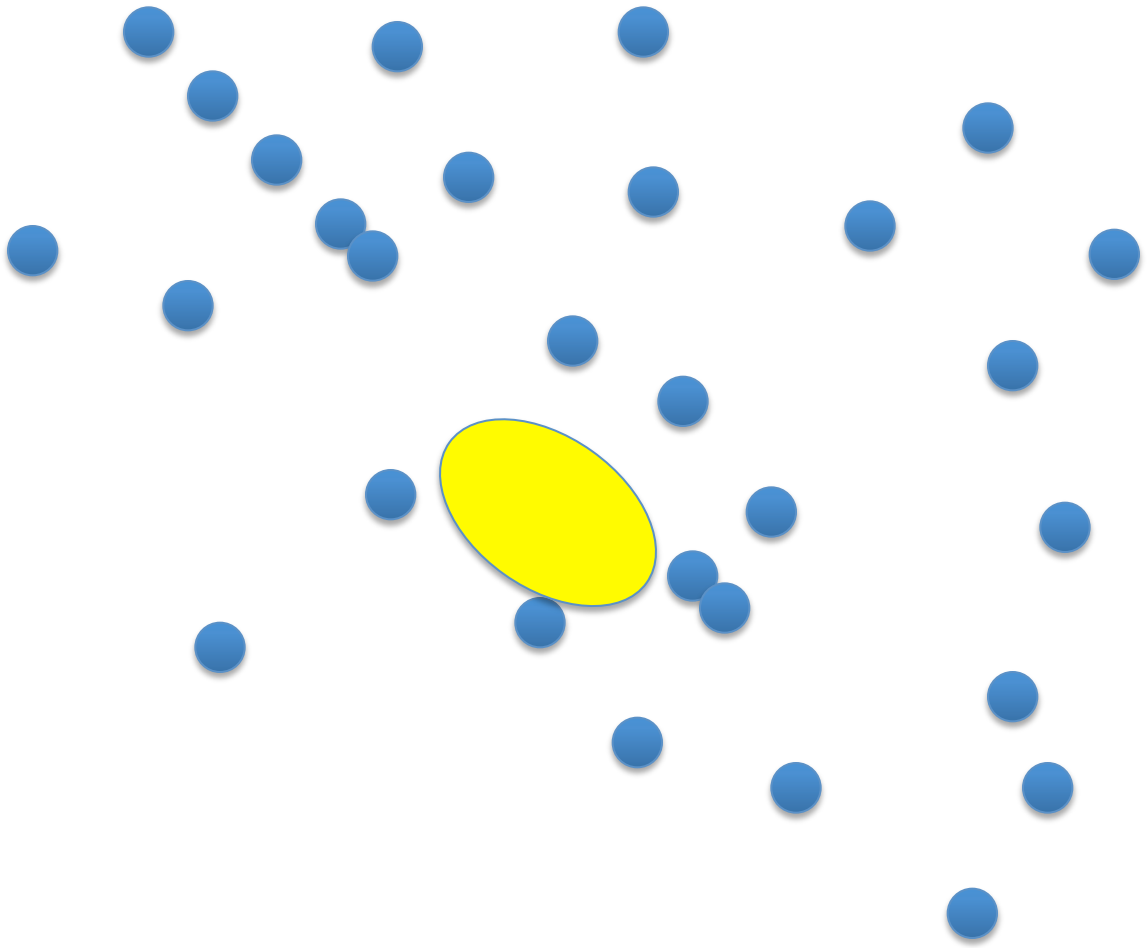
Motion of a massive particle in a rarefied gas.

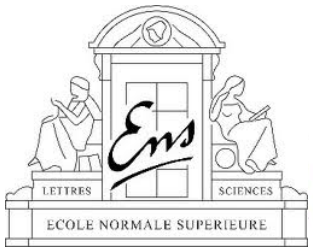
Work in progress
with Thierry Bodineau
and Isabelle Gallagher



A simple system :
- N solid balls of diameter ε
- One big (non spherical) particle of size ε/α interacting only by contact.

Question : can we say something about the macroscopic motion of the molecule?

The microscopic dynamics



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Admissible configurations

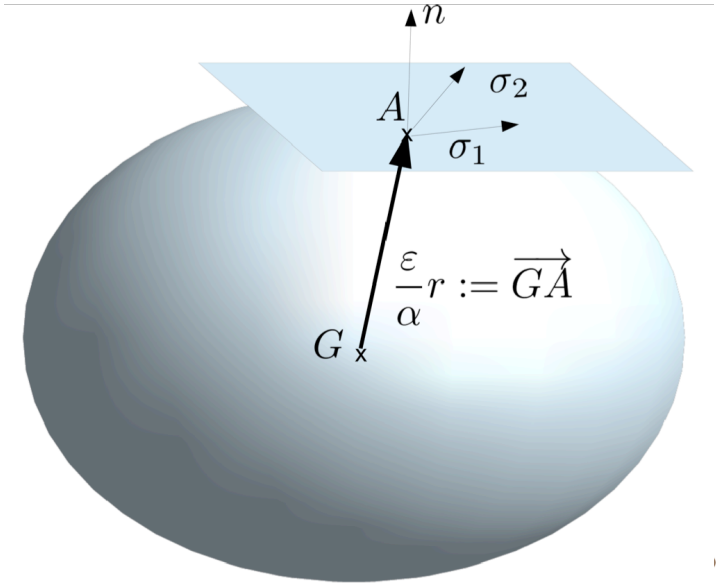
- Positions of the atoms $X_N := (x_1, \ldots, x_N)$

$$\forall i \neq j\,, \quad |x_i - x_j| > \varepsilon$$

- Position and orientation of the molecule (X, Θ)

$$\forall i \quad d\big(x_i, X + \frac{\varepsilon}{\alpha} R_\Theta \bar{\Sigma}\big) > \varepsilon$$

The surface of the reference convex body $\partial\bar{\Sigma}$ is parametrized by $\bar{\sigma}$.



Newton's laws

- Velocities of the atoms $V_N := (v_1, \ldots, v_N)$
- Velocity of the center of mass and angular velocity of the molecule $(V, \hat{\Omega})$

are constant except at collisions.

Collision laws for the atoms

$$v_i' := v_i - \frac{1}{\varepsilon^2}(v_i - v_j) \cdot (x_i - x_j)\,(x_i - x_j)$$

$$v_j' := v_j + \frac{1}{\varepsilon^2}(v_i - v_j) \cdot (x_i - x_j)\,(x_i - x_j)$$

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Collision laws for the molecule

- The collision produces a force f in the direction n

which is a Dirac mass in time → jump conditions

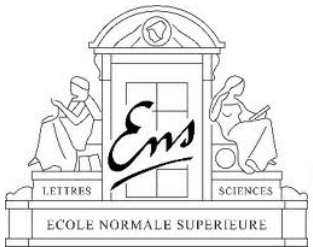
- The total energy is conserved.

$$v' - v = \frac{2}{A+1}(V + \hat{\Omega} \wedge \frac{\varepsilon}{\alpha} r - v) \cdot n \, n$$

$$V' - V = -\frac{2m}{M(A+1)}(V + \hat{\Omega} \wedge \frac{\varepsilon}{\alpha} r - v) \cdot n \, n$$

$$\hat{\Omega}' - \hat{\Omega} = -\frac{2m}{(A+1)}(V + \hat{\Omega} \wedge \frac{\varepsilon}{\alpha} r - v) \cdot n \, \hat{I}^{-1} \frac{\varepsilon}{\alpha} r \wedge n \, .$$

with $$A := \frac{m}{M} + m \left(\frac{\varepsilon}{\alpha}\right)^2 (r \times n \cdot \hat{I}^{-1} r \times n)$$



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Collision invariants

The following quantities are conserved

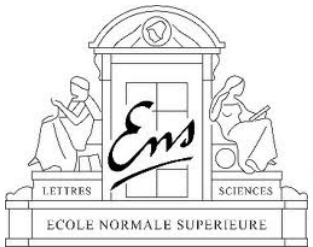
$$\mathcal{P} := mv + MV \quad \text{(total momentum)}$$

$$\mathcal{E} := \frac{1}{2}(m|v|^2 + M|V|^2 + \hat{\Omega}\hat{I}\hat{\Omega}) \quad \text{(total energy)}$$

$$\hat{\mathcal{I}} := \hat{I}\cdot\hat{\Omega} + MV \wedge \frac{\varepsilon}{\alpha} r \quad \text{(angular momentum at the contact point)}\,.$$

Due to the smallness of the molecule, it is natural to rescale the angular velocity and the moment of inertia :

$$I := \left(\frac{\alpha}{\varepsilon}\right)^2 \hat{I} \quad \text{and} \quad \Omega := \frac{\varepsilon}{\alpha}\hat{\Omega}$$



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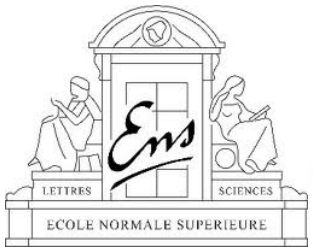
The low density asymptotics



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A statistical point of view

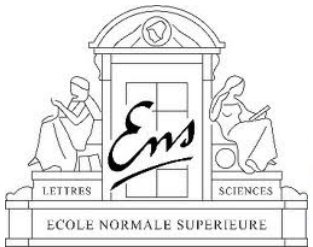
We are interested in the probability distribution of the molecule

$$f_N^{(1)}(t, X, V, \Theta, \Omega) := \int f_N(t, X, V, \Theta, \Omega, Z_N)\, dZ_N$$

where f_N satisfies the **Liouville equation**

$$\partial_t f_N + V \cdot \nabla_X f_N + \sum_{i=1}^{N} v_i \cdot \nabla_{x_i} f_N + \frac{\alpha}{\varepsilon} \Omega \cdot \nabla_\Theta f_N = 0$$

supplemented with reflection conditions on $\partial \mathcal{D}_N^\varepsilon$.



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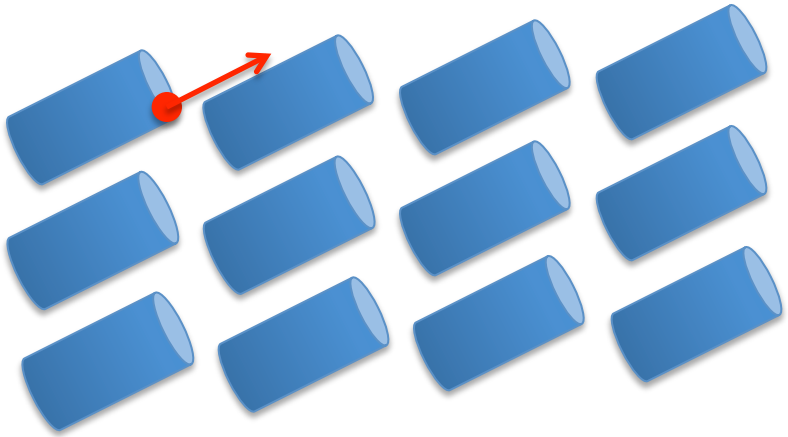
The Boltzmann-Grad scaling

The transport and collision process for the atoms have the same time scale if

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

which only holds for **rarefied gases**.



N spheres of size ε on a lattice

Volume covered by one particle of velocity v during a time t : $|v|t\ \varepsilon^{d-1}$

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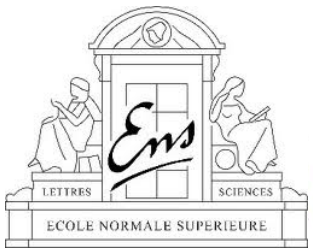
The BBGKY hierarchy

By **Green's formula** and the symmetry,

$$\partial_t f_N^{(s)} + V \cdot \nabla_X f_N^{(s)} + \sum_{i=1}^{s-1} v_i \cdot \nabla_{x_i} f_N^{(s)} + \frac{\alpha}{\varepsilon} \Omega \cdot \nabla_\Theta f_N^{(s)}$$
$$= C_{s,s+1} f_N^{(s+1)} + D_{s,s+1} f_N^{(s+1)} \qquad \text{on } \mathcal{D}_{s-1}^{\varepsilon}$$

where $C_{s,s+1}$ is the boundary term describing the **collision between two atoms**

$$C_{s,s+1} f^{(s+1)} := (N-s+1)\varepsilon^{d-1} \sum_{i=1}^{s-1} \int f^{s+1}(\ldots, x_i+\varepsilon\nu, v_s)((v_i-v_s)\cdot\nu) d\nu dv_s$$



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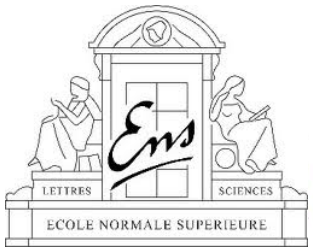
and $D_{s.s+1}$ holds for **collisions with the molecule**

$$D_{s,s+1}f^{(s+1)} := (N-s+1)\left(\frac{\varepsilon}{\alpha}\right)^{d-1}\sum_{i=1}^{s-1}\int f^{s+1}(\ldots, X+\frac{\varepsilon}{\alpha}R_\Theta\bar{r}+\varepsilon R_\Theta\bar{n}, v_s)$$
$$((V+\Omega\wedge R_\Theta\bar{r})-v_s)\cdot R_\Theta\bar{n}d\bar{\sigma}dv_s$$

The normal to the collision surface in the (X, x, Θ) space is indeed given by $(-R_\Theta\bar{n}, R_\Theta\bar{n}, R_\Theta(\bar{r}\wedge\bar{n}))$

Both collision integrals can be split according to the sign of the integrand. We then use the scattering to express the gain part in terms of **precollisional configurations**.



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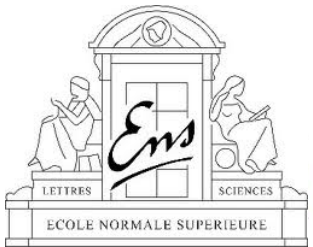
Close to equilibrium

To get an equation for the motion of the molecule, we need a closure for the hierarchy. Here we will assume that **atoms are almost at equilibrium**

$$f_{N,0}(X,V,\Theta,\Omega,X_N,V_N) := M_N(V,\Omega,V_N)g_0(X,V,\Theta,\Omega)$$

$$M_N(V,\Omega,V_N) = \left(\frac{\beta}{2\pi}\right)^{\frac{d}{2}(N+1)+\frac{d(d-1)}{4}} m^{\frac{dN}{2}} (\det I)^{1/2} \exp\left(-\frac{\beta}{2}(|V|^2+m|V_N|^2+\Omega\cdot I\cdot\Omega)\right)\frac{1_{\mathcal{D}_N}}{\mathcal{Z}_N}$$

As the Gibbs measure M_N is a stationary solution to the Liouville equation, we expect this form to be **stable under the dynamics** in the low density limit.



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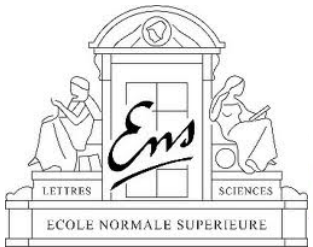
The grazing collision limit



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A weak coupling scaling

We are interested in the motion of a **big molecule surrounded by a fluid** (rarefied gas), i.e.

$$\frac{m}{M} = \alpha^{2(d-1)}, \quad \alpha << 1,$$

The molecule will therefore undergo a lot of collisions, but each one of these collisions will generate an **infinitesimal deflection**:

$$V_n' = V_n - \frac{2m}{A+1} b \quad \text{and} \quad \Omega' = \Omega - \frac{2m}{(A+1)} b I^{-1}(r \wedge n)$$

$$\text{with } b = (V + \Omega \wedge r - v) \cdot n$$

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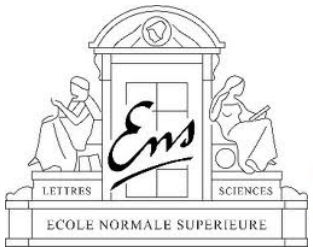
The Boltzmann equation

Provided that we get uniform convergence estimates in α as $\varepsilon \to 0$, the dynamics should be approximated by the **Boltzmann equation**

$$\partial_t g_\alpha + V \cdot \nabla_X g_\alpha = \frac{1}{\alpha^{d-1}} \int d\Theta \int_{\partial\bar{\Sigma}_\alpha \times \mathbb{R}^d} \left(\frac{\beta m}{2\pi}\right)^{\frac{d}{2}} e^{-\frac{\beta}{2} m|v|^2}$$
$$\Big(g_\alpha(X, V', \Omega')\big((V' - v' + \Omega' \times R_\Theta \bar{r}) \cdot R_\Theta \bar{n}\big)_-$$
$$- g_\alpha(X, V, \Omega)\big((V - v + \Omega \times R_\Theta \bar{r}) \cdot R_\Theta \bar{n}\big)_- \Big)\, d\bar{\sigma} dv\,.$$

Note the **angular average** coming from the singular perturbation in the transport.



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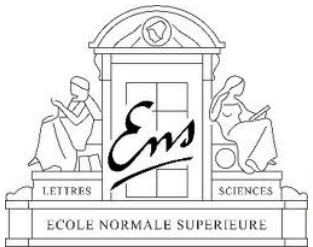
The collision term in weak form

We have now to exhibit **cancellations between the gain and loss parts** in the collision integral.

We use a **duality argument** and compute

$$F := \frac{1}{\alpha^{d-1}} \int \left(\frac{\beta m}{2\pi}\right)^{\frac{d}{2}} e^{-\frac{\beta}{2}(|V|^2+m|v|^2+\Omega\cdot I\cdot\Omega)} g_\alpha(X,V,\Omega)\big((V-v+\Omega\times r)\cdot n\big)_-$$
$$\times\big(\varphi(X,V',\Omega')-\varphi(X,V,\Omega)\big)\, d\sigma dv dX\, d\Omega dV\, d\Theta\,.$$

Note that because atoms are lighter, they move faster and we expect $v = O(m^{-1/2})$.



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A generalized Ornstein-Uhlenbeck process

At leading order in α, the two terms cancel by

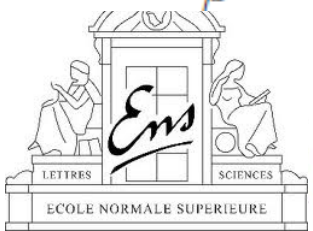
Stokes formula

$$\int_{\partial\Sigma_\alpha} n \cdot e d\sigma = \int_{\Sigma_\alpha} \nabla \cdot e dr = 0,$$

$$\int_{\partial\Sigma_\alpha} r \wedge n \cdot e d\sigma = \int_{\Sigma_\alpha} \nabla \cdot (e \wedge r) dr = 0\,.$$

We then get, for some N,K,T depending only on $\bar{\Sigma}$

$$F = \left(\frac{2}{\pi\beta}\right)^{1/2} \int dX\, d\Omega dV\, e^{-\frac{\beta}{2}(|V|^2 + \Omega\cdot I\cdot\Omega)} g_\alpha(X,V,\Omega)$$
$$\times \Big((VN + \Omega K)\nabla_V \varphi(X,V,\Omega) + (VK^t + \Omega T) I^{-1} \nabla_\Omega \varphi(X,V,\Omega)$$
$$+ \frac{2}{\beta}(\nabla_V \cdot N \cdot \nabla_V + I^{-1}\nabla_\Omega \cdot T \cdot I^{-1}\nabla_\Omega + 2\nabla_V \cdot K^t \cdot I^{-1}\nabla_\Omega)\varphi(X,V,\Omega)\Big)$$



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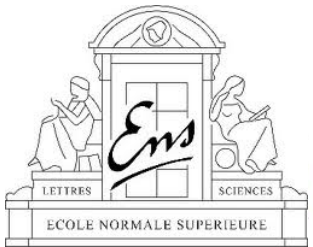
Strategy of the proof



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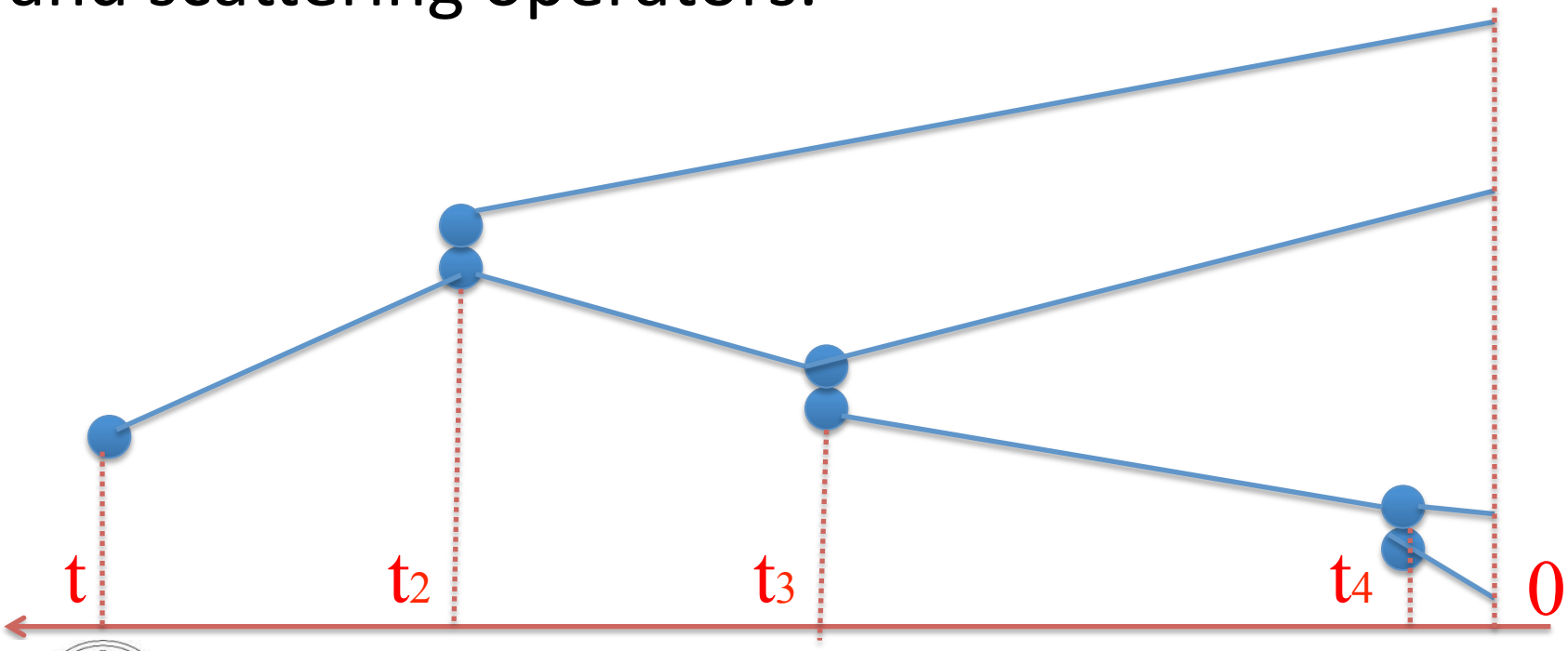
Collision trees

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



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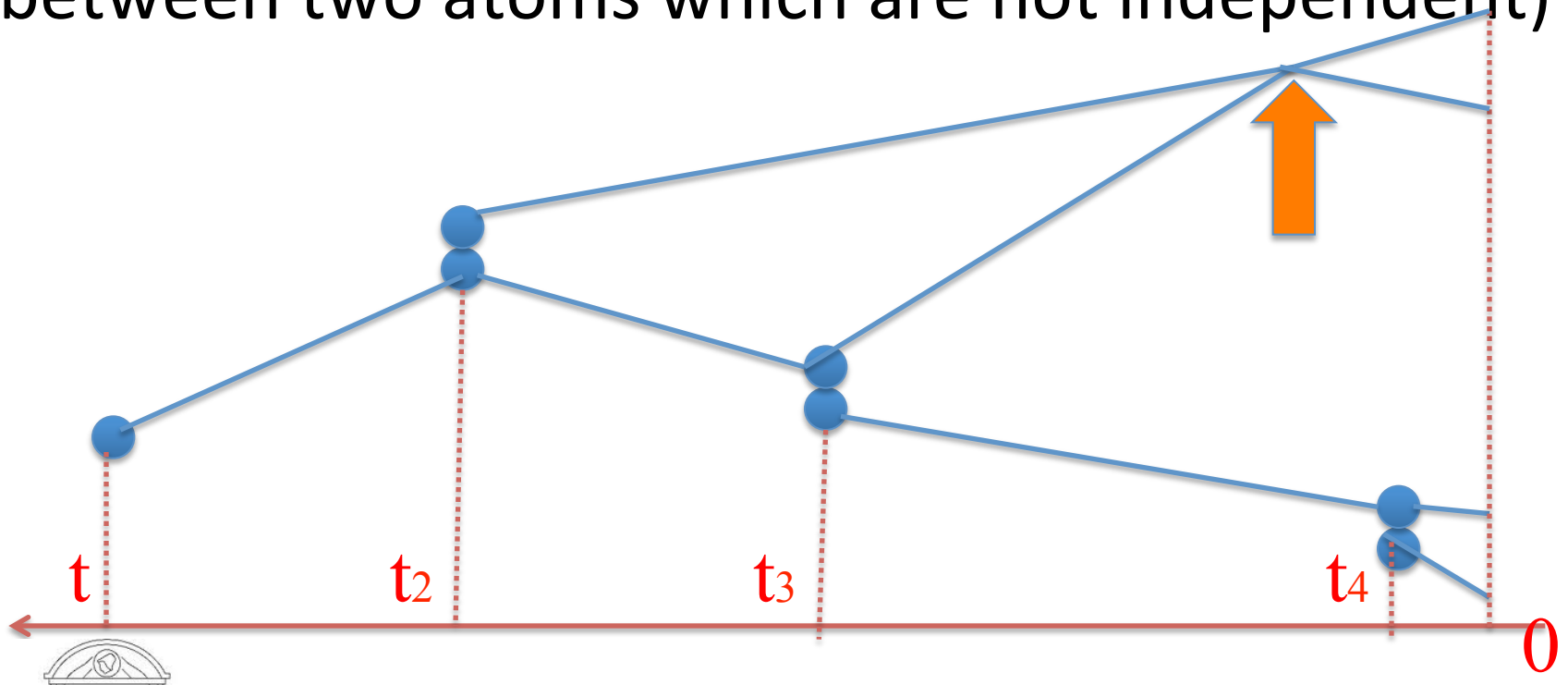
Recollisions

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



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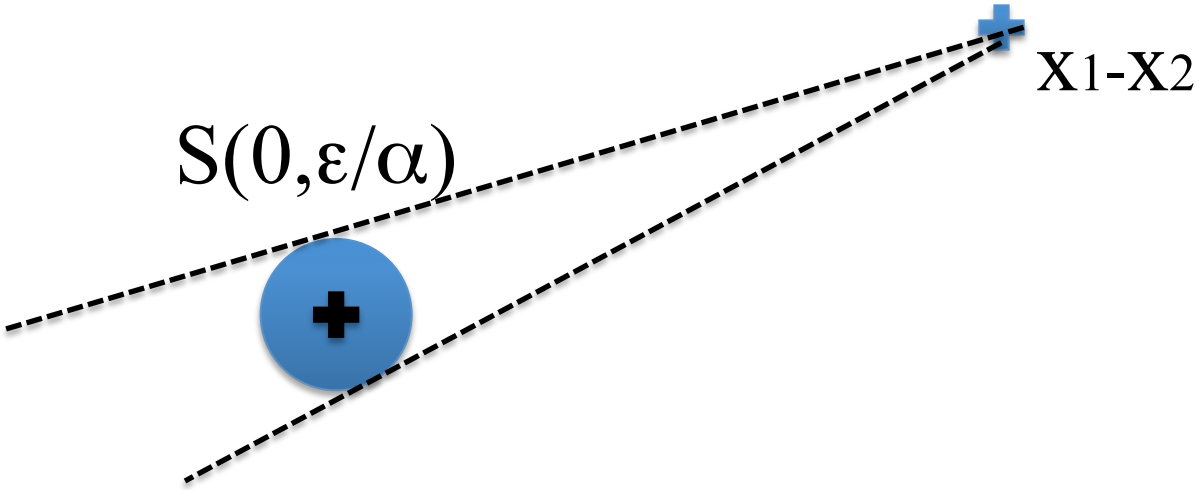
Geometric control of recollisions

- By a **geometric study** of the free transport (with precession), we can prove that recollisions are of small probability when $\varepsilon << 1$, $\alpha >> \varepsilon^{1/d}$



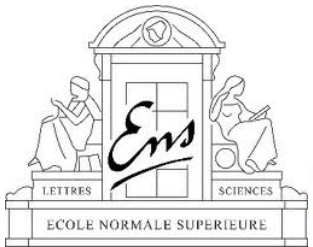
- We therefore **remove a small set** of bad parameters from each collision integral.

About the size of the trees

- The truncation is admissible only for **relatively small trees** (of size at most log N).

- In Lanford's proof, the size of the trees is controlled only for very short times, by some **Cauchy-Kowalewski estimate.**

- Close to equilibrium, we use global a priori estimates to **discard superexponential trees**.



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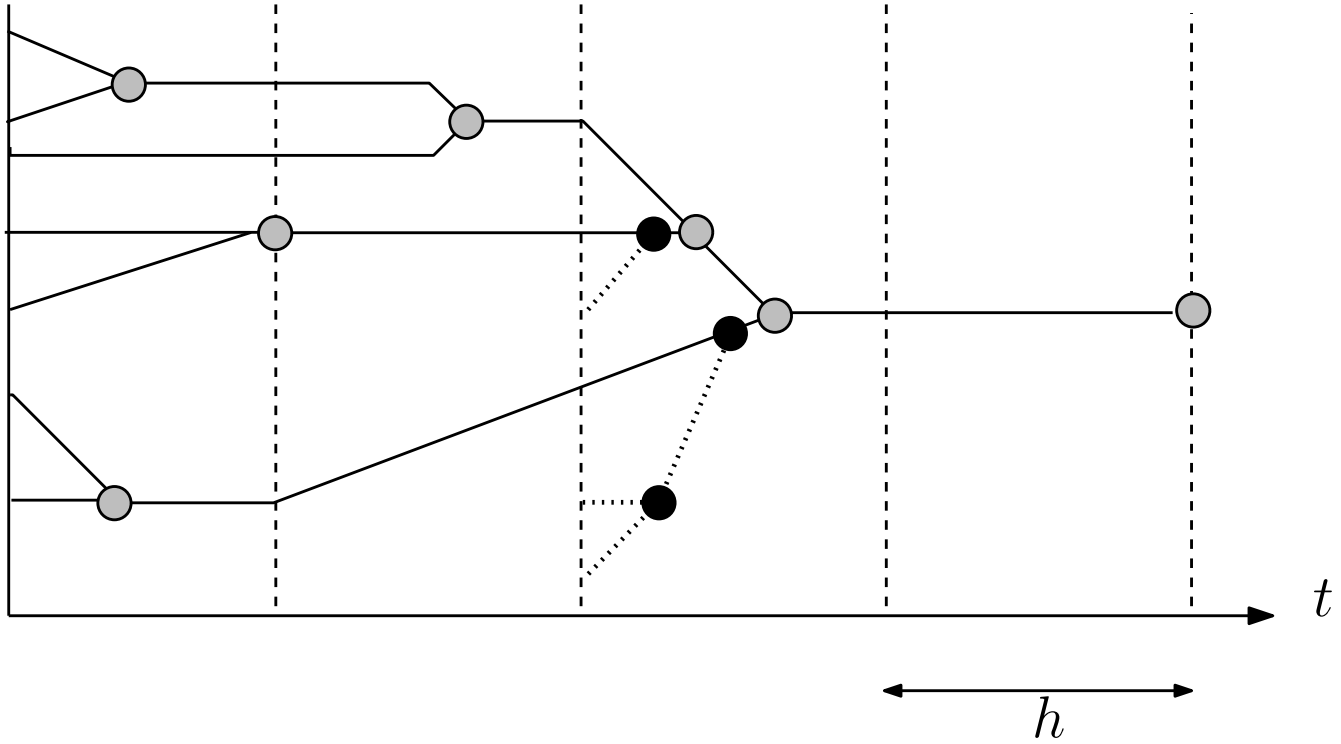
A sampling in time

Superexponential trees are negligible if $h << \frac{t}{\alpha^{2(d-1)}}$



The error coming from the geometric surgery is

$$C^{2^K} \varepsilon^{1/2} \text{ with } K = \frac{t}{h}$$

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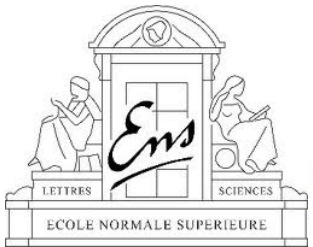
What can be said about macroscopic molecules?



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