Fluctuating Boltzmann equation and large deviations for a hard sphere gas

Thierry Bodineau

Joint work with
Isabelle Gallagher, Laure Saint-Raymond, Sergio Simonella

Introduction

Microscopic
Newtonian dynamics

Kinetic limit →

Mesoscopic
Boltzmann equation

Deterministic description

- Hamiltonian dynamics
- Reversible

Stochastic description

- Dissipative equation
- Irreversible

Finer scales beyond the Boltzmann equation ?

Irreversibility & microscopic correlations

Outline.

- Deterministic microscopic dynamics
- Convergence to the Boltzmann equation
- Fluctuations and cumulants
- Large deviations

Dilute gas of hard spheres

Gas of N hard spheres with deterministic Newtonian dynamics (elastic collisions).

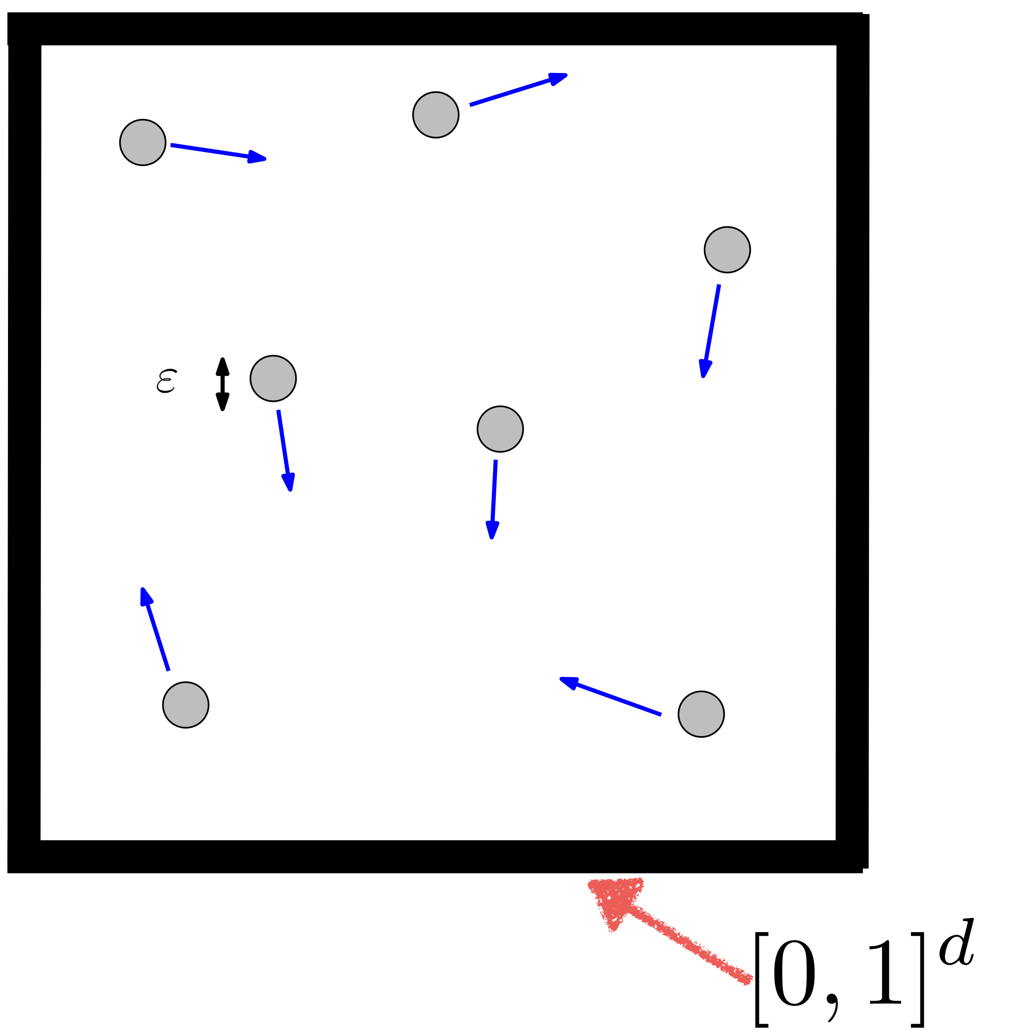
Microscopic scale :

$$Z_N(t) = (x_i(t), v_i(t))_{i \leq N}$$

Dimension : $d \geq 2$

Periodic domain: $\mathbb{T}^d = [0,1]^d$

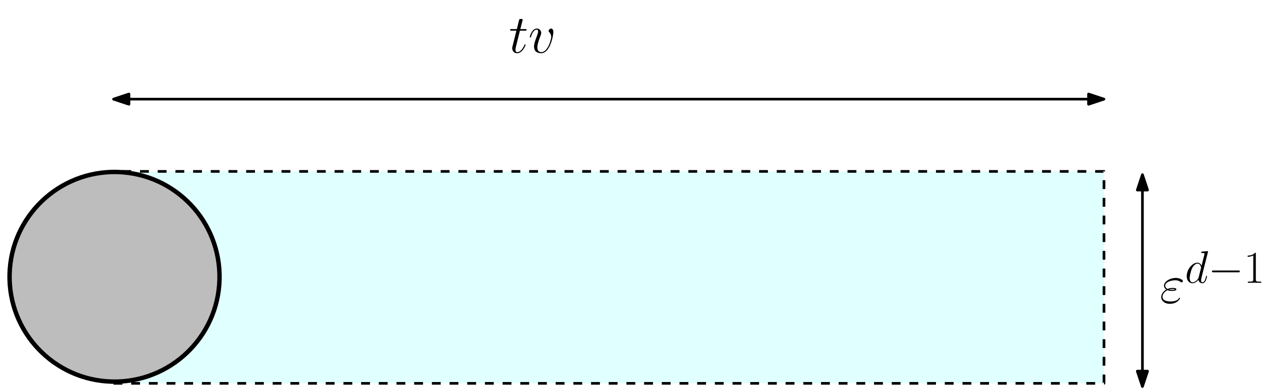
Sphere radius = ε



Strongly unstable dynamics

Boltzmann-Grad scaling $N\varepsilon^{d-1} = 1$

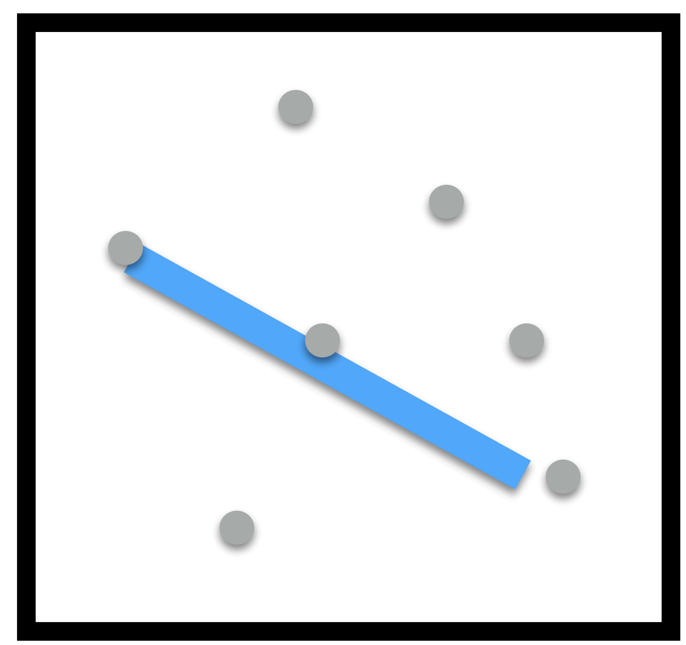
Boltzmann-Grad scaling



- Volume covered by a particle $= tv\varepsilon^{d-1}$
- N particles per unit volume

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

Dilute gas



$t = 1$
$v = 1$

On average, a particle has 1 collision per unit of time

Hard sphere dynamics

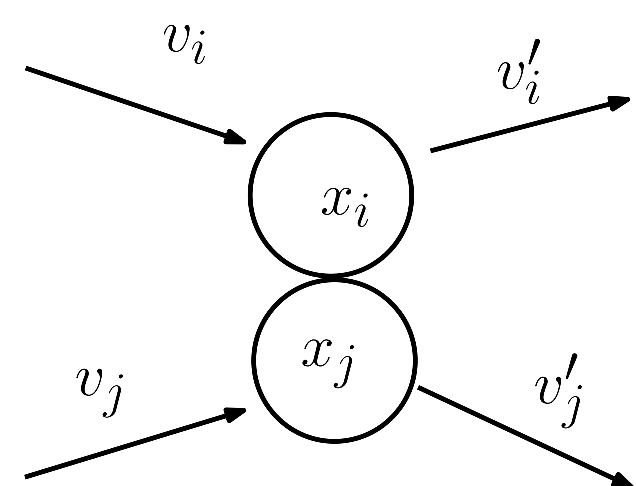
Deterministic

Gas of hard spheres $Z_N = \{(x_i(t), v_i(t)\}_{i\leq N}$

$$\frac{dx_i}{dt} = v_i, \quad \frac{dv_i}{dt} = 0 \quad \text{as long as} \quad |x_i(t) - x_j(t)| > \varepsilon$$

and elastic collisions if $|x_i(t) - x_j(t)| = \varepsilon$

$$\begin{cases} v_i' + v_j' = v_i + v_j \\ |v_i'|^2 + |v_j'|^2 = |v_i|^2 + |v_j|^2 \end{cases}$$



Liouville equation for the particle density $W_N(t, Z_N)$

$$\partial_t W_N + \sum_{i=1}^{N} v_i \cdot \nabla_{x_i} W_N = 0$$

in the phase space

$$\mathcal{D}_\varepsilon^N := \{Z_N \in \mathbf{T}^{dN} \times \mathbb{R}^{dN} \, / \, \forall i \neq j \,, \quad |x_i - x_j| > \varepsilon\}$$

with specular reflection on the boundary $\partial \mathcal{D}_\varepsilon^N$.

Initial density.

$$W_N(0,Z_N) = \prod_{i=1}^{N} f^0(z_i) \times \frac{1}{\mathcal{Z}_N} \prod_{i\neq j} 1_{|x_i - x_j| > \varepsilon}$$

Dilute gas : *almost product measure*

Grand canonical formalism :

N random : $\mu_\varepsilon = \mathbb{E}(N)$ *with* $\mu_\varepsilon \varepsilon^{d-1} = 1$

Boltzmann-Grad scaling

Typical density of a particle at time t : $F_1^\varepsilon(t, z_1)$

Typical density of k particles at time t : $F_k^\varepsilon(t, Z_k)$

Question. Convergence $F_1^\varepsilon(t, z_1) \xrightarrow[\mu_\varepsilon \varepsilon^{d-1} = 1]{\varepsilon \to 0} f(t, z_1)$

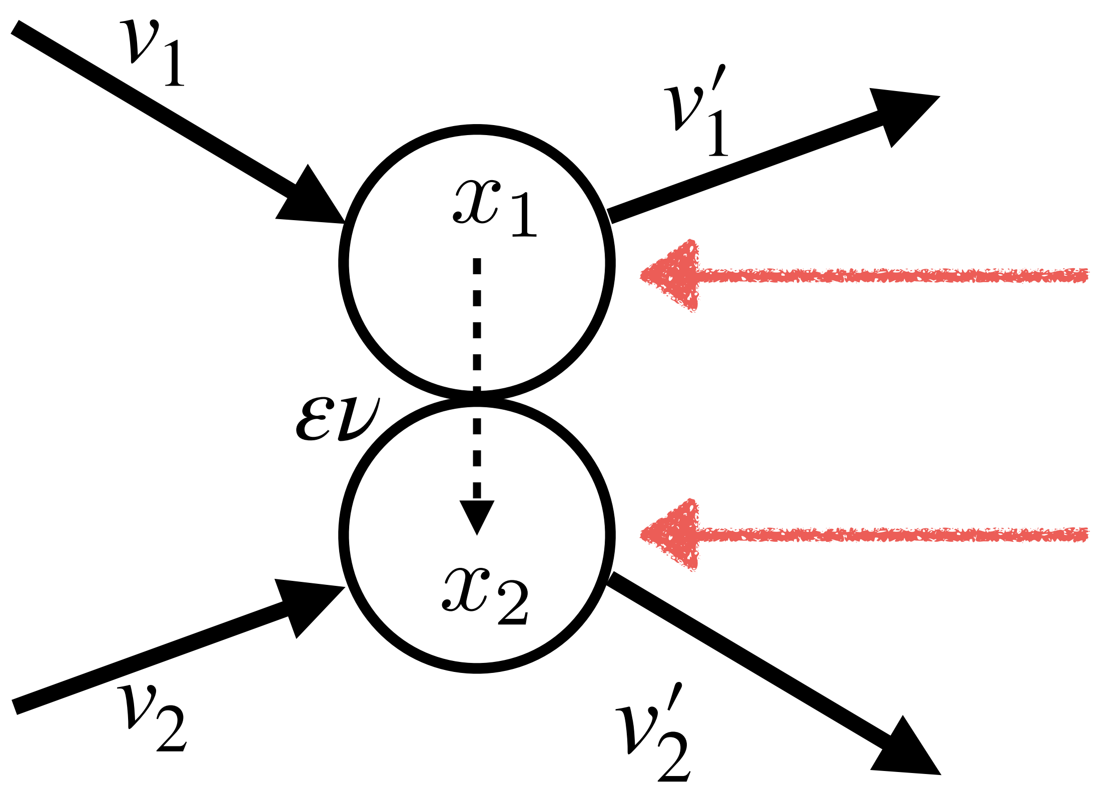
Evolution of the first marginal

$$(\partial_t + v_1 \cdot \nabla_{x_1}) F_1^\varepsilon(t, z_1) = \left(C_{1,2}\, F_2^\varepsilon\right)(t, z_1)$$

Collision operator

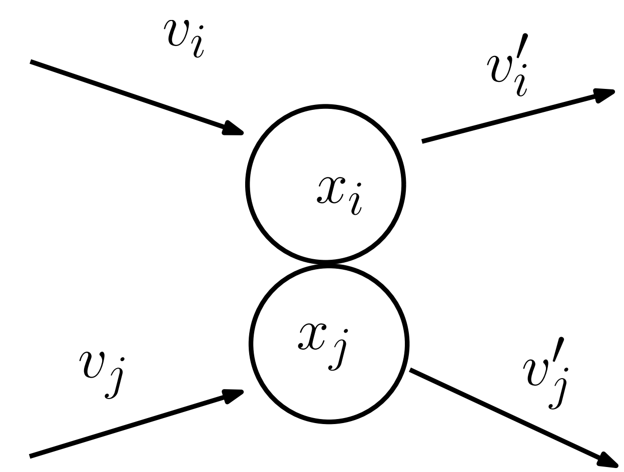
$$\left(C_{1,2} F_2^\varepsilon\right)(z_1) := \int_{\mathbf{S}^{d-1}\times\mathbb{R}^d} F_2^\varepsilon(x_1, v_1', x_1 + \varepsilon\nu, v_2') \Big((v_2 - v_1)\cdot\nu \Big)_+ d\nu dv_2$$

$$- \int_{\mathbf{S}^{d-1}\times\mathbb{R}^d} F_2^\varepsilon(x_1, v_1, x_1 + \varepsilon\nu, v_2) \Big((v_2 - v_1)\cdot\nu \Big)_- d\nu dv_2$$



- the collision occurs on a surface of area ε^{d-1}
- N-1 possible particles

Evolution of the first marginal



$$(\partial_t + v_1 \cdot \nabla_{x_1}) F_1^\varepsilon(t, z_1) = \left(C_{1,2} F_2^\varepsilon\right)(t, z_1)$$

Collision operator

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$$- \int_{\mathbf{S}^{d-1}\times\mathbb{R}^d} F_2^\varepsilon(x_1, v_1, x_1 + \varepsilon\nu, v_2) \Big((v_2 - v_1)\cdot\nu\Big)_- d\nu dv_2$$

CLAIM : microscopic chaos assumption

$$F_2^\varepsilon(x_1, v_1, x_1 + \varepsilon\nu, v_2) \simeq F_1^\varepsilon(x_1, v_1) F_1^\varepsilon(x_1 + \varepsilon\nu, v_2)$$

Consequence: Boltzmann equation

$$\partial_t f + v \cdot \nabla_x f = \iint [f(x, v') f(x, v_2') - f(x, v) f(x, v_2)] \Big((v - v_2)\cdot\nu\Big)_+ dv_2 d\nu$$

The reversibility paradox

Newtonian dynamics **Reversible**	Boltzmann-Grad limit → Molecular chaos	Boltzmann equation **Irreversible** **H**-theorem

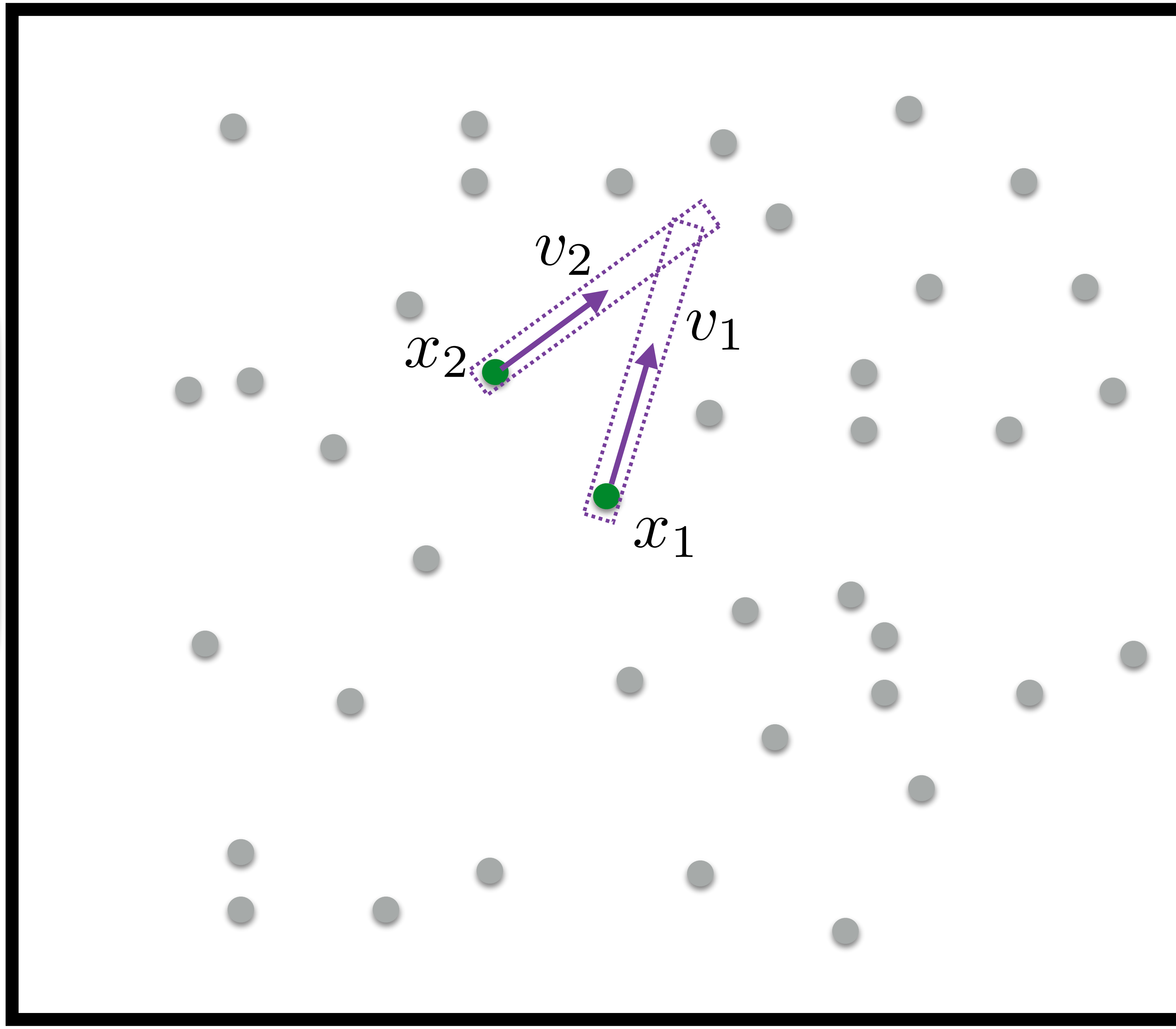
- Boltzmann equation (1872)
- Loschmidt : reversibility paradox
- Zermelo : Poincaré recurrence Theorem

Propagation of chaos

Singular set

$$F_2^\varepsilon(x_1, v_1, x_1 + \varepsilon\nu, v_2) \simeq F_1^\varepsilon(x_1, v_1) F_1^\varepsilon(x_1 + \varepsilon\nu, v_2)$$

Factorization if two particles didn't meet in the past

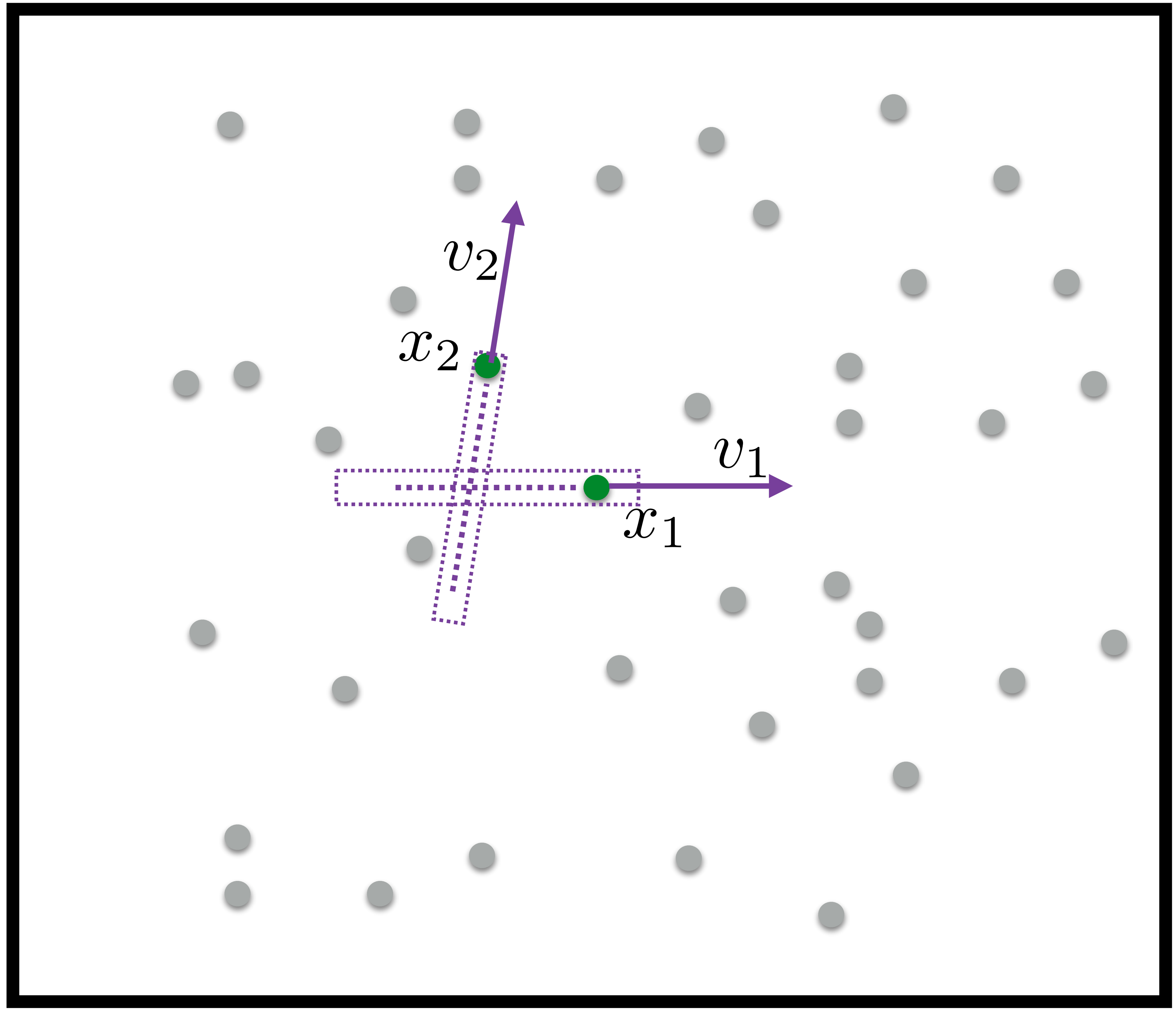


$$F_2^\varepsilon(x_1, v_1, x_2, v_2) \simeq F_1^\varepsilon(x_1, v_1) F_1^\varepsilon(x_2, v_2)$$

Memory effect

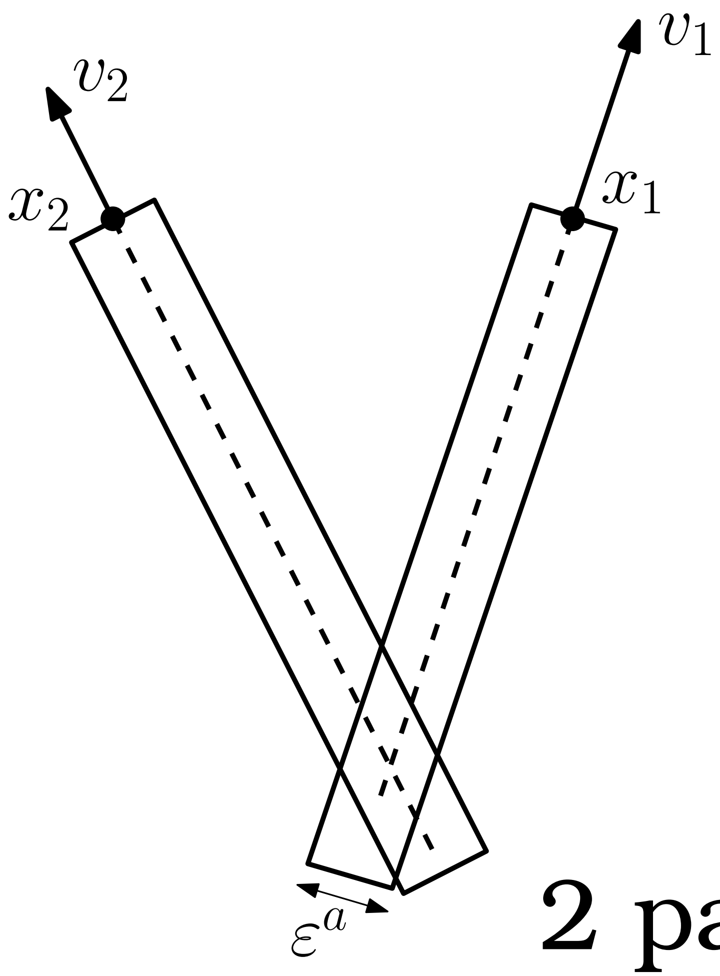
↓

No factorization



$$F_2^{\varepsilon}(x_1, v_1, x_2, v_2) \not\simeq F_1^{\varepsilon}(x_1, v_1) F_1^{\varepsilon}(x_2, v_2)$$

Excluded configurations



Given $T^* > 0$ and $a \in (0,1)$

$$\mathcal{B}_\varepsilon^k = \Big\{ Z_k ; \quad \exists u \in [0,T^*], \exists i \neq j \leq k, \\ |(x_i - uv_i) - (x_j - uv_j)| \leq \varepsilon^a \Big\}$$

2 particles were close to each other in the past

The measure of $\mathcal{B}_\varepsilon^k$ tends to 0 when $\varepsilon \to 0$

Theorem (*Convergence to the Boltzmann equation*)

Initial distribution $W_N(0, Z_N) = \prod_{i=1}^{N} f^0(z_i) \times exclusion$

with f^0 smooth and bounded $\|f^0\|_\infty \leq C$.

There exists $T^* > 0$ such that the marginals of the particle system converge to the solution of the Boltzmann equation in the time interval $[0, T^*]$

$$t \leq T^*, \qquad \|F_1^\varepsilon(t) - f(t)\|_\infty = \gamma(\varepsilon) \underset{\varepsilon \to 0}{\longrightarrow} 0$$

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

The Boltzmann equation :

$$\partial_t f + v \cdot \nabla_x f = \iint [f(x, v') f(x, v_2') - f(x, v) f(x, v_2)] \left((v - v_2) \cdot \nu\right)_+ dv_2 d\nu$$

with initial data $f(0,z) = f^0(z)$

Theorem (*Convergence to the Boltzmann equation*)

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$$t \le T^*, \qquad \|F_1^\varepsilon(t) - f(t)\|_\infty = \gamma(\varepsilon) \underset{\varepsilon \to 0}{\longrightarrow} 0$$

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

(one sided) **Propagation of chaos**

$$\forall t \in [0,T^*], \qquad \left| \Big(F_k^\varepsilon(t, Z_k) - \prod_{i=1}^{k} f(t, z_i)\Big) 1_{\{Z_k \notin \mathcal{B}_\varepsilon^k\}} \right| \le c^k \gamma(\varepsilon)$$

Derivation of the convergence:

Lanford; King; Alexander;
van Beijeren, Lanford, Lebowitz, Spohn;
Uchiyama; Cercignani, Illner, Pulvirenti; Simonella …

Quantitative convergence :

Gallagher, Saint-Raymond, Texier; Pulvirenti, Saffirio, Simonella; Denlinger; Pulvirenti, Simonella

Remarks:

- Short time convergence
- One-sided propagation of chaos

Loss of the reversibility

Convergence as a law of large numbers

Test function $h(z) = h(x, v)$

$$\mathbb{E}\left[\Big(\frac{1}{N}\sum_{i=1}^{N} h(z_i(t)) - \int f(t,z)h(z)dz\Big)^2\right] \underset{\varepsilon\to 0}{\longrightarrow} 0$$

Assuming N constant

$$= \frac{N}{N^2}\mathbb{E}\left[\Big(h(z_1(t)) - \int f(t)hdz\Big)^2\right] \underset{\varepsilon\to 0}{\longrightarrow} 0$$

$$+\frac{2N(N-1)}{N^2}\underbrace{\mathbb{E}\left[\Big(h(z_1(t)) - \int f(t)hdz\Big)\Big(h(z_2(t)) - \int f(t)hdz\Big)\right]}_{\text{correlations}}$$

$$\simeq \int F_N^{(2)}(t, z_1, z_2)h(z_1)h(z_2) - \Big(\int f(t)hdz\Big)^2 \underset{\varepsilon\to 0}{\longrightarrow} 0$$

chaos property

Central limit theorem

Test function $h(z) = h(x, v)$

Assuming
N constant

$$\mathbb{E}\left[\left(\frac{1}{\sqrt{N}}\sum_{i=1}^{N}\left(h(z_i(t)) - \int f(t,z)h(z)dz\right)\right)^2\right]$$

$$= \frac{N}{N}\mathbb{E}\left[\left(h(z_1(t)) - \int f(t)hdz\right)^2\right]$$

$$+\frac{2N(N-1)}{N}\underbrace{\mathbb{E}\left[\left(h(z_1(t)) - \int f(t)hdz\right)\left(h(z_2(t)) - \int f(t)hdz\right)\right]}_{\text{the decay needs to be quantified}}$$

the decay needs to be quantified [Spohn]

For fluctuations the correlations matter

Central limit theorem

Test function $h(z) = h(x, v)$

Grand canonical formalism

$$\mathbb{E}\left[\left(\frac{1}{\sqrt{\mu_\varepsilon}}\sum_{i=1}^{N}\left(h(z_i(t)) - \int f(t,z)h(z)dz\right)\right)^2\right]$$

$$= \mathbb{E}\left[\left(h(z_1(t)) - \int f(t)hdz\right)^2\right]$$

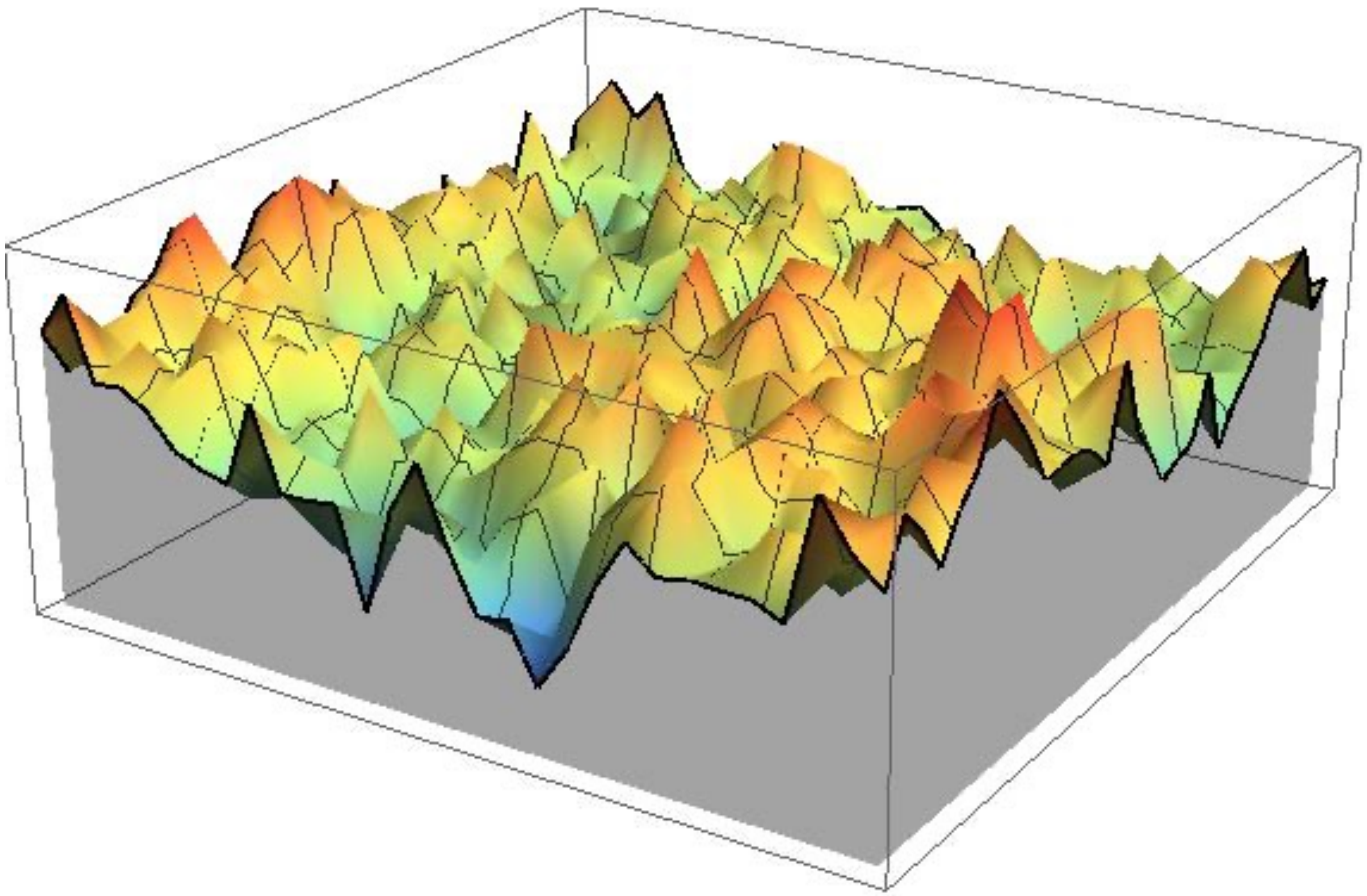
$$+2\mu_\varepsilon \underbrace{\mathbb{E}\left[\left(h(z_1(t)) - \int f(t)hdz\right)\left(h(z_2(t)) - \int f(t)hdz\right)\right]}_{\text{the decay needs to be quantified}}$$

[Spohn]

For fluctuations the correlations matter

Fluctuating Boltzmann equation

Fluctuation field. $$\zeta_t^{\varepsilon}(h) = \frac{1}{\sqrt{\mu_\varepsilon}} \sum_{i=1}^{N} \left(h\big(z_i(t)\big) - \int dz\, h(z) f(t,z) \right)$$



Question:
Time evolution of the fluctuations

Fluctuating Boltzmann equation

Fluctuation field. $$\zeta_t^{\varepsilon}(h) = \frac{1}{\sqrt{\mu_\varepsilon}} \sum_{i=1}^{N} \Big(h\big(z_i(t)\big) - \int dz\, h(z) f(t,z) \Big)$$

Theorem. [B., Gallagher, Saint-Raymond, Simonella]

Grand canonical distribution $W_N(0, Z_N) = \prod_{i=1}^{N} f^0(z_i) \times exclusion$

Convergence to a generalised Ornstein-Uhlenbeck process in the time interval $[0,T^*]$

$$\zeta_t^{\varepsilon} \xrightarrow[\varepsilon \to 0]{} \zeta_t \qquad \text{with} \qquad d\zeta_t = \mathscr{L}_t \zeta_t + d\eta_t$$

SPDE

Conjecture. [Spohn]

Model with stochastic collisions : [Rezakhanlou]

$$d\zeta_t = \mathscr{L}_t \zeta_t + d\eta_t$$

Linearised Boltzmann operator

Noise

$$\zeta_t^{\varepsilon}(h) = \frac{1}{\sqrt{\mu_\varepsilon}} \sum_{i=1}^{N} \Big(h\big(z_i(t)\big) - \int dz\, h(z) f(t,z) \Big) \xrightarrow[\varepsilon \to 0]{(law)} \zeta_t(h) = \text{“} \int dz \zeta_t(z) h(z) \text{”}$$

$\zeta_t(h)$ is a random variable (but ζ_t is a distribution)

weak formulation

$$d\zeta_t(h) = \zeta_t(\mathscr{L}_t^* h) + dB_t^{(h)}$$

Brownian motion with variance depending on h and $f(t)$

Holley-Stroock method at equilibrium

$$d\zeta_t = \mathscr{L}_t \zeta_t + d\eta_t$$

Linearised Boltzmann operator

- Dissipation

Noise

- Creates entropy
- Variance given by the recollisions [Spohn]

Analogy with the 1D Ornstein-Uhlenbeck process

$$dx_t = -x_t + dB_t$$

$$d\zeta_t = \mathscr{L}_t \zeta_t + d\eta_t$$

Example : initial data at equilibrium

$$W_N(0, Z_N) = \prod_{i=1}^{N} M(v_i) \times \frac{1}{\mathcal{Z}_N} \prod_{i \neq j} 1_{|x_i - x_j| > \varepsilon} \qquad M(v) = \frac{1}{c_d} \exp\Big(- \frac{v^2}{2} \Big)$$

invariant under the dynamics

Fluctuation field : $\zeta_t^{\varepsilon}(h) = \frac{1}{\sqrt{\mu_\varepsilon}} \sum_{i=1}^{N} \Big(h\big(z_i(t)\big) - \int dz\, h(z) M(v) \Big)$

$$d\zeta_t = \mathcal{L}_t \zeta_t + d\eta_t$$

Example : initial data at equilibrium

$$W_N(0, Z_N) = \prod_{i=1}^{N} M(v_i) \times \frac{1}{\mathcal{Z}_N} \prod_{i \neq j} 1_{|x_i - x_j| > \varepsilon} \qquad M(v) = \frac{1}{c_d} \exp\Big(-\frac{v^2}{2} \Big)$$

invariant under the dynamics

Fluctuation field :

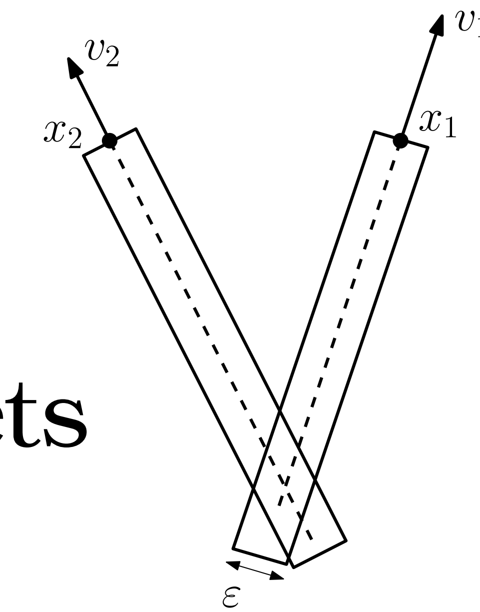
$$\zeta_t^\varepsilon(h) = \frac{1}{\sqrt{\mu_\varepsilon}} \sum_{i=1}^{N} \Big(h\big(z_i(t)\big) - \int dz\, h(z) M(v) \Big)$$

$$\lim_{\varepsilon \to 0} \mathbb{E}\Big(\zeta_0^\varepsilon(h) \zeta_0^\varepsilon(g) \Big) = \int dz h(z) g(z) M(v)$$

$$\lim_{\varepsilon \to 0} \mathbb{E}\Big(\zeta_0^\varepsilon(h) \zeta_t^\varepsilon(g) \Big) = \mathbb{E}\Big(\zeta_0(h) \zeta_t(g) \Big) \xrightarrow{t \to \infty} 0$$

- Time correlations decay
- Noise preserves the invariant measure

Cumulants



$$f_2^{\varepsilon}(t, z_1, z_2) = F_2^{\varepsilon}(t, z_1, z_2) - F_1^{\varepsilon}(t, z_1)\, F_1^{\varepsilon}(t, z_2)$$

$$\underset{\varepsilon \to 0}{\longrightarrow} 0 \qquad \text{except on the bad sets}$$

Theorem (grand canonical formalism)

$a = 1$

There exists $T^* > 0$ such that

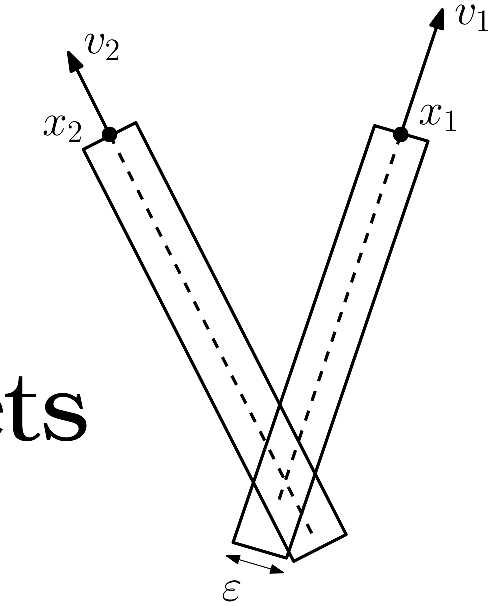
$$\forall t \in [0, T^*], \qquad \left\| f_2^{\varepsilon}(t) \right\|_1 \leq C \varepsilon^{(d-1)}$$

$$f_3^{\varepsilon}(z_1, z_2, z_3) = F_3^{\varepsilon}(z_1, z_2, z_3) - F_1^{\varepsilon}(z_1)\, F_2^{\varepsilon}(z_2, z_3) - F_1^{\varepsilon}(z_2)\, F_2^{\varepsilon}(z_1, z_3)$$
$$- F_1^{\varepsilon}(z_3)\, F_2^{\varepsilon}(z_1, z_2) + 2\, F_1^{\varepsilon}(z_1)\, F_1^{\varepsilon}(z_2)\, F_1^{\varepsilon}(z_3)$$

Cumulants

$$f_2^\varepsilon(t,z_1,z_2) = F_2^\varepsilon(t,z_1,z_2) - F_1^\varepsilon(t,z_1)\,F_1^\varepsilon(t,z_2)$$

$$\underset{\varepsilon\to 0}{\longrightarrow} 0 \qquad \text{except on the bad sets}$$



Theorem (grand canonical formalism)

singular support

There exists $T^* > 0$ such that $n \geq 2$

$$\forall t \in [0,T^*], \qquad \left\| f_n^\varepsilon(t) \right\|_1 \leq C^n\, \varepsilon^{(d-1)(n-1)}\, n!$$

$$f_3^\varepsilon(z_1,z_2,z_3) = F_3^\varepsilon(z_1,z_2,z_3) - F_1^\varepsilon(z_1)\,F_2^\varepsilon(z_2,z_3) - F_1^\varepsilon(z_2)\,F_2^\varepsilon(z_1,z_3)$$
$$-F_1^\varepsilon(z_3)\,F_2^\varepsilon(z_1,z_2) + 2\,F_1^\varepsilon(z_1)\,F_1^\varepsilon(z_2)\,F_1^\varepsilon(z_3)$$

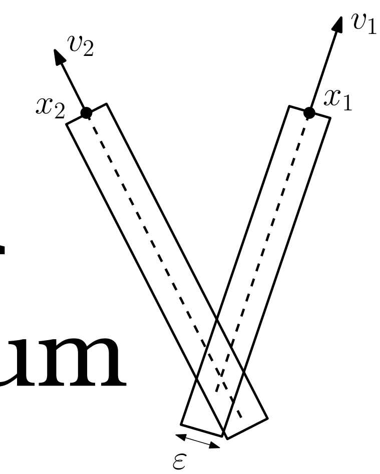
The cumulant f_n^ε encodes $n-1$ recollisions

Cumulants record the recollisions

Theorem (grand canonical formalism)

There exists $T^* > 0$ such that $n \geq 2$

$$\forall t \in [0, T^*], \qquad \left\| f_n^\varepsilon(t) \right\|_1 \leq C^n \, \frac{n!}{\mu_\varepsilon^{(n-1)}}$$



Proof. based on a **dynamical cluster expansion**

- Interactions more complicated than at equilibrium
- Consequence : precise controls on the measure

$$\frac{1}{\mu_\varepsilon} \log \mathbb{E}_\varepsilon\left(\exp\left(\sum_{i=1}^{N} h\big(z_i(t)\big) \right) \right) = \sum_{n=1}^{\infty} \frac{\mu_\varepsilon^{n-1}}{n!} \int dZ_n \, f_n^\varepsilon(t, Z_n) \prod_{\ell=1}^{n} \left(e^{h(z_\ell)} - 1\right)$$

A similar decomposition holds for sample paths

Convergence to the Ornstein-Uhlenbeck process

No stochastic process at the microscopic level

1/ *Convergence in law of the process* :

- Control of the characteristic function by the cumulants

$$\lambda \mapsto \mathbb{E}_\varepsilon \left(\exp\Big(\frac{\mathbf{i}\lambda}{\sqrt{\mu_\varepsilon}} \sum_{i=1}^{N} \Big(h\big(z_i(t)\big) - \int dz\, h(z) M(v) \Big) \Big) \right)$$

- Estimates on the size of the cumulants imply that only f_2^ε is relevant
- Identification of the variance by controlling the time evolution of $f_2 = \lim_{\varepsilon \to 0} f_2^\varepsilon$ [Spohn]

2/ *Tightness of the process.*

Large deviations

Let $\varphi \neq f$ be an atypical evolution on $[0,T^*]$

$$\mathbb{P}_\varepsilon\Big(observing\ \varphi\Big) \underset{\varepsilon\to 0}{\simeq} \exp\Big(-\mu_\varepsilon \widehat{\mathscr{F}}_{[0,T^*]}(\varphi)\Big)$$

The empirical measure concentrates on φ

Model with stochastic collisions : [Rezakhanlou]

Conjecture : [Bouchet]

$$\widehat{\mathscr{F}}_{[0,T^*]}(\varphi) := \sup_p \left\{ \int_0^{T^*} ds \Big[\int_{[0,1]^d} dx \int_{\mathbb{R}^d} dv\, p(s,x,v)\, D_s\varphi(s,x,v) - \mathscr{H}\big(\varphi(s), p(s)\big) \Big] \right\}$$

with

$$\mathscr{H}(\varphi,p) := \frac{1}{2}\int \varphi(x,v_1)\varphi(x,v_2)\big(\exp\big(\Delta p\big)-1\big)((v_1-v_2)\cdot\omega)_+ d\omega dv_1 dv_2 dx$$

Does this extends to the deterministic dynamics ?

Theorem. There exists $T^* > 0$, a functional $\mathcal{F}_{[0,T^*]}$ and a restricted set of functions $\mathcal{R}$ such that

$$\forall \varphi \in \mathcal{R}, \qquad \mathbb{P}_\varepsilon\Big(\textit{observing } \varphi\Big) \underset{\varepsilon\to 0}{\simeq} \exp\Big(-\mu_\varepsilon \mathcal{F}_{[0,T^*]}(\varphi)\Big)$$

For functions φ in a subset $\hat{\mathcal{R}} \subset \mathcal{R}$ then

$$\mathcal{F}_{[0,T^*]}(\varphi) = \widehat{\mathcal{F}}_{[0,T^*]}(\varphi)$$

Standard methods for stochastic processes don't apply :

- The randomness is only in the initial data
- No obvious way to tilt the dynamics directly

Fun facts.

$$\frac{1}{\mu_\varepsilon}\log \mathbb{E}_\varepsilon\Big(\exp\Big(\sum_{i=1}^N h\big(z_i(t)\big)\Big)\Big) = \sum_{n=1}^\infty \frac{\mu_\varepsilon^{n-1}}{n!}\int dZ_n\, f_n^\varepsilon(t,Z_n)\prod_{\ell=1}^n (e^{h(z_\ell)}-1)$$

control of the series

Let $H\big(z([0,T^*])\big)$ be a function on the trajectories

$$\frac{1}{\mu_\varepsilon}\log \mathbb{E}_\varepsilon\Big(\exp\Big(\sum_{i=1}^N H\big(z_i([0,T^*])\big)\Big)\Big) = \sum_{n=1}^\infty \frac{\mu_\varepsilon^{n-1}}{n!} f^\varepsilon_{n,[0,T^*]}\big((e^H-1)^{\otimes n}\big)$$

Laplace transform is linked to large deviations

involves a control of recollisions

Question. Can this be related to a stochastic structure ?

Hamilton-Jacobi equation

Claim. There exists $T^* > 0$ such that for "suitable" h

$$\frac{1}{\mu_\varepsilon} \log \mathbb{E}_\varepsilon\left(\exp\left(\sum_{i=1}^{N} h\big(z_i(t)\big)\right)\right) \xrightarrow[\varepsilon\to 0]{} \mathcal{J}(t,h)$$

The limit satisfies an Hamilton-Jacobi equation:

$$\partial_t \mathcal{J}(t,h) = \mathcal{H}\left(\frac{\partial \mathcal{J}(t,h)}{\partial h}, h\right) + \int v \cdot \nabla_x h(z)\, \frac{\partial \mathcal{J}(t,h)}{\partial h}(z)\, dz$$

$$\mathcal{H}(\varphi, h) := \frac{1}{2}\int \varphi(x_1,v_1)\varphi(x_1,v_2)\big(\exp\big(\Delta h\big) - 1\big)((v_1 - v_2)\cdot\omega)_+ d\omega dv_1 dv_2 dx_1$$

same structure as the stochastic model

Proof. *(for a modified HJ equation)*

The cumulants have a limiting structure $f_n(t)$ satisfying a hierarchy of (singular) equations.

Conclusion

Deterministic dynamics of a diluted gas of hard spheres :

- Microscopic correlations & reversibility
- Cumulants and singular correlation structure
- Stochastic description holds also at *very small scales* :
    - Fluctuations around Boltzmann equation
    - Large deviations

Open problems.

- Local equilibrium vs memory effects ?
- Understanding the entropy cascade in the microscopic dynamics
- Long time dynamics