

The Brownian motion as the limit of a deterministic system of hard-spheres

T. Bodineau

Joint work with I. Gallagher and L. Saint-Raymond

April 2, 2014

Outline

- Linear Boltzmann equation & Brownian motion
- Lanford's strategy & pruning procedure
- Coupling with the Boltzmann hierarchy

Hard sphere dynamics

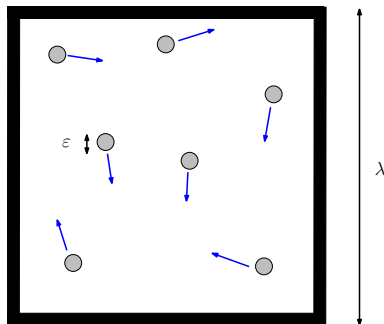
Gas of N hard spheres with deterministic Newtonian dynamics (elastic collisions).

Periodic domain: $\mathbf{T}_\lambda^d = [0, \lambda]^d$

Sphere radius = ε

Dilute gas : $N\varepsilon^{d-1}\lambda^{-d} \equiv 1$

Boltzmann-Grad scaling



Hard sphere dynamics

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

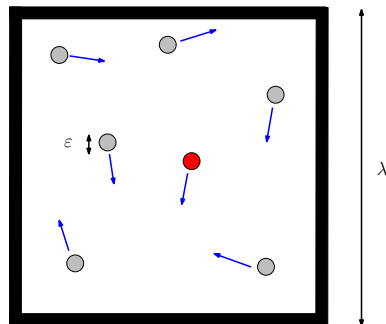
Initial data at equilibrium
and a tagged particle (x_1, v_1)

Questions.

In the Boltzmann-Grad limit

$$N \rightarrow \infty, \quad N \varepsilon^{d-1} \lambda^{-d} \equiv 1$$

$\Rightarrow$ Distribution of the tagged particle
 $(x_1(t), v_1(t))$ for $t > 0$?



Hard sphere dynamics

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

Initial data at equilibrium
and a tagged particle (x_1, v_1)

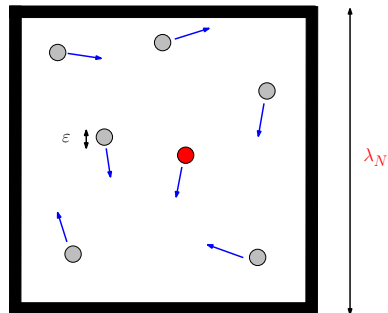
Questions.

In the Boltzmann-Grad limit

$$N \rightarrow \infty, \quad N \varepsilon^{d-1} \lambda^{-d} \equiv 1$$

⇒ Distribution of the tagged particle
 $(x_1(t), v_1(t))$ for $t > 0$?

⇒ Position the tagged particle
 $\frac{1}{\lambda_N} x_1(\lambda_N^2 \tau)$ for $\tau > 0$?



Hard sphere dynamics

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

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

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

$$\begin{cases} v_i(t^+) = v_i(t^-) - \frac{1}{\varepsilon^2} (v_i - v_j) \cdot (x_i - x_j)(x_i - x_j)(t^-) \\ v_j(t^+) = v_j(t^-) + \frac{1}{\varepsilon^2} (v_i - v_j) \cdot (x_i - x_j)(x_i - x_j)(t^-) \end{cases}$$

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

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

in the phase space

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

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

The tagged particle

Equilibrium distribution

$$M_{N,\beta}(Z_N) = \frac{1}{Z_{N,\beta}} \exp\left(-\frac{\beta}{2} \sum_{i=1}^N |v_i|^2\right) \prod_{i \neq j} 1_{|x_i - x_j| > \varepsilon}$$

Particle $Z_1 = (x_1, v_1)$ is tagged. Initial distribution :

$$f_N^0(Z_N) = M_{N,\beta}(Z_N) \varphi_N^0((x_1, v_1))$$

Uniform bound: $\varphi_N^0((x_1, v_1)) \leq \mu_N$

Notation: Marginals

$$t \geq 0, \forall s \geq 1, \quad f_N^{(s)}(t, Z_s) = \iint f_N(t, Z_N) dz_{s+1} \dots dz_N$$

Tagged particle distribution $f_N^{(1)}(t, (x_1, v_1))$

Linear Boltzmann equation

Large time convergence : [van Beijeren, Lanford, Lebowitz, Spohn]
[Lebowitz, Spohn]

N -particle system

$$f_N^{(1)}(t, (\mathbf{x}_1, \mathbf{v}_1))$$

$$\xrightarrow{N \rightarrow \infty}$$

$$\forall t > 0$$

Linear Boltzmann equation

$$g(t, (\mathbf{x}_1, \mathbf{v}_1))$$

Linear Boltzmann equation

$$\begin{cases} \partial_t g + \mathbf{v} \cdot \nabla_{\mathbf{x}} g = -Lg, \\ Lg(\mathbf{v}) := \iint [g(\mathbf{v})M_\beta(\mathbf{v}_1) - g(\mathbf{v}')M_\beta(\mathbf{v}'_1)] ((\mathbf{v} - \mathbf{v}_1) \cdot \boldsymbol{\nu})_+ d\mathbf{v}_1 d\boldsymbol{\nu}, \\ \mathbf{v}' = \mathbf{v} + (\boldsymbol{\nu} \cdot (\mathbf{v}_1 - \mathbf{v}))\boldsymbol{\nu} \quad \mathbf{v}'_1 = \mathbf{v}_1 - (\boldsymbol{\nu} \cdot (\mathbf{v}_1 - \mathbf{v}))\boldsymbol{\nu} \end{cases}$$

with $M_\beta(\mathbf{v}) := \left(\frac{\beta}{2\pi}\right)^{\frac{d}{2}} \exp\left(-\frac{\beta}{2}|\mathbf{v}|^2\right)$

Linear Boltzmann equation

Large time convergence : [van Beijeren, Lanford, Lebowitz, Spohn]
[Lebowitz, Spohn]

N -particle system

$$f_N^{(1)}(t, (x_1, v_1))$$

$$\xrightarrow{N \rightarrow \infty}$$

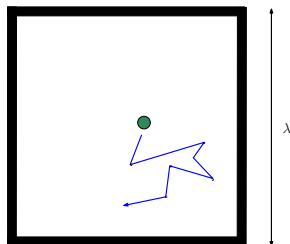
$$\forall t > 0$$

Linear Boltzmann equation

$$g(t, (x_1, v_1))$$

Markov process on the velocities
 $\{v(t)\}_{t \geq 0}$ with generator L .

Position : $x(t) = \int_0^t v(u) du$



Linear Boltzmann equation

Large time convergence : [van Beijeren, Lanford, Lebowitz, Spohn]
[Lebowitz, Spohn]

N -particle system

$$f_N^{(1)}(t, (x_1, v_1))$$

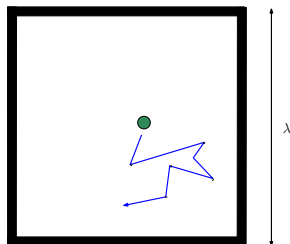
$$\xrightarrow{N \rightarrow \infty}$$

$$\forall t > 0$$

Linear Boltzmann equation

$$g(t, (x_1, v_1))$$

- Probabilist approaches :
Tanaka, Sznitman, Meleard,
Graham, Fournier ...
- Quantum brownian motion



Convergence to a Brownian motion

N -particle
system

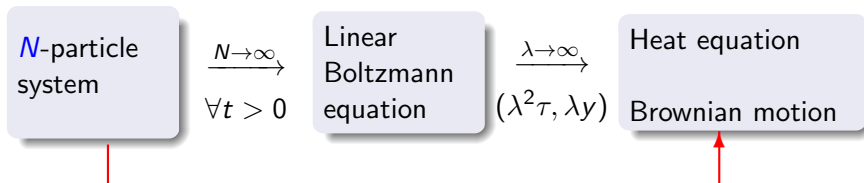
$\xrightarrow{N \rightarrow \infty}$
 $\forall t > 0$

Linear
Boltzmann
equation

$\xrightarrow{\lambda \rightarrow \infty}$
 $(\lambda^2 \tau, \lambda y)$

Heat equation
Brownian motion

Convergence to a Brownian motion



$$\lambda_N = o((\log \log N)^{1/5}), \quad N \varepsilon^{d-1} \lambda_N^{-d} \equiv 1, \quad (\lambda_N^2 \tau, \lambda_N y)$$

Key : quantitative convergence to the Linear Boltzmann equation

For $t_N = o(\mu_N^{-1/2} \sqrt{\log \log N})$

$$\|\lambda^d f_N^{(1)} - g\|_{L^\infty([0, t_N] \times \mathbf{T}_\lambda^d \times \mathbb{R}^d)} \leq C \mu_N^2 \left(\frac{t_N^2}{\log \log N} \right)^2$$

with $f_N^0(Z_N) = M_{N, \beta}(Z_N) \varphi_N^0(z_1)$, $g^0(Z_N) = \lambda^d M_\beta(v_1) \varphi^0(z_1)$.

Convergence to a Brownian motion

Rescaled position of the tagged particle

$$\mathcal{X}(\tau) = \frac{1}{\lambda_N} \mathbf{x}_1(\lambda_N^2 \tau) \quad \text{with} \quad \lambda_N = o((\log \log N)^{1/5})$$

Initial distribution

$$f_N^0(Z_N) = M_{N,\beta}(Z_N) \mu_N \varphi_N^0 \left(\frac{\mathbf{x}_1}{\lambda_N^{1-\zeta}} \right), \quad \text{with} \quad \zeta \in]0, \frac{1}{4d}[$$

Theorem. [B, Gallagher, Saint-Raymond]

$\mathcal{X}$ converges weakly to a brownian motion with variance κ

The distribution $\lambda_N^d f_N^{(1)}(\lambda_N^2 \tau, \lambda_N y, \nu)$ of the tagged particle converges as $N \rightarrow \infty$ to $M_\beta \rho$

$$\partial_\tau \rho = \kappa \Delta_y \rho \quad \text{on } \mathbb{R}^+ \times [0, 1]^d, \quad \rho|_{\tau=0} = \delta_0$$

Boltzmann equation

Theorem. [Lanford; Uchiyama; Cercignani, Illner, Pulvirenti; Gallagher, Saint-Raymond, Texier]

For chaotic initial data $f_N^0(Z_N) \simeq \prod_{i=1}^N f^0(z_i)$ the density of the particle system converges up to a time $t > 0$ to the solution of the Boltzmann equation when $N \rightarrow \infty$, $N\varepsilon^{d-1}\lambda^{-d} \equiv 1$

$$\begin{aligned} & \partial_t f + v \cdot \nabla_x f \\ &= \iint_{\mathbf{S}^{d-1} \times \mathbb{R}^d} [f(v')f(v'_1) - f(v)f(v_1)] ((v - v_1) \cdot \nu)_+ dv_1 d\nu \end{aligned}$$

with $v' = v + \nu \cdot (v_1 - v) \nu$, $v'_1 = v_1 - \nu \cdot (v_1 - v) \nu$

⇒ Lanford's strategy leads to a short time convergence which depends on f^0 . The convergence time remains short even if initially the system starts from equilibrium $f_N^0 = M_{N,\beta}$!!

BBGKY hierarchy for the marginals

For $s < N$ and on $\mathcal{D}_\varepsilon^s = \{Z_s = (x_i, v_i)_{i \leq s} \mid i \neq j, \quad |x_i - x_j| > \varepsilon\}$

$$(\partial_t + \sum_{i=1}^s v_i \cdot \nabla_{x_i}) f_N^{(s)}(t, Z_s) = (C_{s,s+1} f_N^{(s+1)})(t, Z_s)$$

where the collision term is defined by

$$\begin{aligned} & (C_{s,s+1} f_N^{(s+1)})(Z_s) \\ &:= (N-s) \varepsilon^{d-1} \sum_{i=1}^s \int_{\mathbf{S}^{d-1} \times \mathbb{R}^d} f_N^{(s+1)}(\dots, x_i, v_i^*, \dots, x_i + \varepsilon \nu, v_{s+1}^*) \left((v_{s+1} - v_i) \cdot \nu \right)_+ d\nu dv_{s+1} \\ & \quad - (N-s) \varepsilon^{d-1} \sum_{i=1}^s \int_{\mathbf{S}^{d-1} \times \mathbb{R}^d} f_N^{(s+1)}(\dots, x_i, v_i, \dots, x_i + \varepsilon \nu, v_{s+1}) \left((v_{s+1} - v_i) \cdot \nu \right)_- d\nu dv_{s+1} \end{aligned}$$

where $\mathbf{S}^{d-1}$ denotes the unit sphere in $\mathbb{R}^d$.

Duhamel Formula

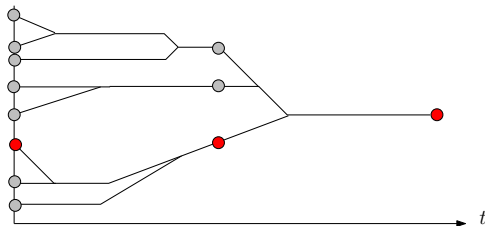
Denote by $\mathbf{S}_s$ the semi-group associated to free transport in $\mathcal{D}_\varepsilon^s$

Duhamel Formula

$$f_N^{(1)}(t) = \mathbf{S}_1(t)f_N^{(1)}(0) + \int_0^t \mathbf{S}_1(t-t_1)C_{1,2}f_N^{(2)}(t_1) dt_1 ,$$

Collision tree :

- Transport operator $\mathbf{S}_s$ (possible recollisions)
- Addition of a particle to the tree after each collision



Duhamel Formula

Denote by $\mathbf{S}_s$ the semi-group associated to free transport in $\mathcal{D}_\varepsilon^s$

Duhamel Formula

$$f_N^{(1)}(t) = \mathbf{S}_1(t)f_N^{(1)}(0) + \int_0^t \mathbf{S}_1(t-t_1)C_{1,2}f_N^{(2)}(t_1) dt_1,$$

Iterated Duhamel formula

$$f_N^{(1)}(t) = \sum_{n=0}^{N-1} Q_{1,1+n}(t)f_N^{(1+n)}(0)$$

with

$$Q_{s,s+n}(t) := \int_0^t \int_0^{t_1} \dots \int_0^{t_{n-1}} dt_n \dots dt_1 \mathbf{S}_s(t-t_1)C_{s,s+1} \\ \mathbf{S}_{s+1}(t_1-t_2)C_{s+1,s+2} \dots \mathbf{S}_{s+n}(t_n)$$

Key issue. Convergence of the series when $N \rightarrow \infty$

Continuity estimates for the collision operators

Weighted norms :

$$\|f_k\|_{\varepsilon,k,\beta} := \sup_{Z_k \in \mathcal{D}_\varepsilon^k} \left| f_k(Z_k) \exp\left(\frac{\beta}{2} \sum_{i=1}^k |v_i|^2\right) \right| < \infty$$

The initial data satisfy : $\lambda^{ds} \|f_N^{0,(s)}\|_{\varepsilon,s,\beta} \leq \mu_N^2 C^s$

Collision operators estimates

$$\left\| Q_{s,s+n}(t) f_{s+n} \right\|_{\varepsilon,s,\beta/2} \leq e^{s-1} \left(C_d(\beta) \lambda^d t \right)^n \|f_{s+n}\|_{\varepsilon,s+n,\beta}$$

Thus

$$f_N^{(1)}(t) = \sum_{n=0}^{N-1} Q_{1,1+n}(t) f_N^{(1+n)}(0)$$

can be controlled only up to short times

$\mathbb{L}^\infty$ bound

Initial distribution :

$$f_N^0(Z_N) = M_{N,\beta}(Z_N) \varphi_N^0((x_1, v_1))$$

Uniform bound: $\varphi_N^0((x_1, v_1)) \leq \mu_N$

The measure $M_{N,\beta}(Z_N)$ is **stationary** thus the maximum principle implies bounds **uniform in time**

For any $s \geq 1$

$$\sup_{t \geq 0} f_N^{(s)}(t, Z_s) \leq \mu_N M_{N,\beta}^{(s)}(Z_s) \leq \lambda^{-ds} \mu_N (1 - \varepsilon \kappa_d)^{-s} M_\beta^{\otimes s}(V_s)$$

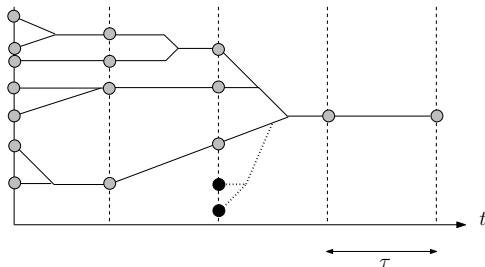
In this way the cancellations in the collision operator are recovered.

Pruning procedure

Decompose : $[0, t] = \bigcup_{k=1}^K [(k-1)\tau, k\tau]$ for some $\tau > 0$

Good collision trees.

Less than $n_k = 2^k$ collisions during $[(K-k)\tau, (K-k+1)\tau]$



In each time interval $[(K-k)\tau, (K-k+1)\tau]$

$$\left\| Q_{s,s+n}(\tau) f_{s+n} \right\|_{\varepsilon,s,\beta/2} \leq e^{s-1} \left(C_d(\beta) \lambda^d \tau \right)^n \|f_{s+n}\|_{\varepsilon,s+n,\beta}$$

Pruning procedure

Truncated iterated Duhamel formula:

$$f_N^{(1)}(t) = \sum_{j_1=0}^2 \dots \sum_{j_K=0}^{2^K} Q_{1,J_1}(\tau) Q_{J_1,J_2}(\tau) \dots Q_{J_{K-1},J_K}(\tau) f_N^{0(J_K)} + R_N^K(t)$$

with $J_\ell = 1 + j_1 + \dots + j_\ell$

- The main contribution is given by the good collision trees with $j_k \leq 2^k$ during the time interval $[(K-k)\tau, (K-k+1)\tau]$
- The contribution of the large trees $R_N^K(t)$ is controlled

$$\|R_N^K(t)\|_{\mathbb{L}^\infty} \leq \mu_N \frac{t^2}{K}$$

⇔ If t is large, then K has to be very large and τ very small.

Boltzmann Hierarchy

For $s \geq 1$ and $Z_s \in \mathbf{T}^{ds} \times \mathbb{R}^{ds}$

$$(\partial_t + \sum_{i=1}^s v_i \cdot \nabla_{x_i}) g^{(s)}(t, Z_s) = (C_{s,s+1}^0) g^{(s+1)}(t, Z_s)$$

where the collision term is defined by

$$\begin{aligned} & (C_{s,s+1}^0 g^{(s+1)})(Z_s) \\ &:= \sum_{i=1}^s \int_{\mathbf{S}^{d-1} \times \mathbb{R}^d} g^{(s+1)}(\dots, x_i, v_i^*, \dots, x_i, v_{s+1}^*) \left((v_{s+1} - v_i) \cdot \nu \right)_+ d\nu dv_{s+1} \\ &\quad - \sum_{i=1}^s \int_{\mathbf{S}^{d-1} \times \mathbb{R}^d} g^{(s+1)}(\dots, x_i, v_i, \dots, x_i, v_{s+1}) \left((v_{s+1} - v_i) \cdot \nu \right)_- d\nu dv_{s+1} \end{aligned}$$

This is the **limit** hierarchy when $\varepsilon \rightarrow 0$ and $N \rightarrow \infty$.

Boltzmann Hierarchy

For $s \geq 1$ and $Z_s \in \mathbf{T}^{ds} \times \mathbb{R}^{ds}$

$$(\partial_t + \sum_{i=1}^s v_i \cdot \nabla_{x_i}) g^{(s)}(t, Z_s) = (C_{s,s+1}^0) g^{(s+1)}(t, Z_s)$$

Iterated Duhamel formula

$$g^{(1)}(t) = \sum_{n=0}^{\infty} Q_{1,1+n}^0(t) g^{(1+n)}(0)$$

Explicit solution : $g^{(s)}(t) = g(t, \mathbf{z}_1) \prod_{i=2}^s M_{\beta}(v_i)$

with $g(t, \mathbf{z}_1)$ solution of the **Linear Boltzman equation**

$$\partial_t g + v \cdot \nabla_x g = -Lg$$

and $M_{\beta}(v) := \left(\frac{\beta}{2\pi}\right)^{\frac{d}{2}} \exp\left(-\frac{\beta}{2}|v|^2\right)$

Comparing the BBGKY and Boltzmann hierarchies

As $N \rightarrow \infty$ in the scaling $N\varepsilon^{d-1}\lambda^{-d} \equiv 1$,

$$\left| \left(\lambda^{ds} f_N^{0(s)} - g_N^{0(s)} \right) \prod_{i \neq j} 1_{|x_i - x_j| > \varepsilon} \right| \leq C \varepsilon \mu_N^2 s M_\beta^{\otimes s}$$

for the **initial distributions**

$$f_N^0(Z_N) = M_{N,\beta}(Z_N) \varphi_N^0(\mathbf{z}_1), \quad g_N^{0(s)}(Z_s) = \left(\prod_{i=1}^s M_\beta(v_i) \right) \varphi_N^0(\mathbf{z}_1)$$

and

$$M_{N,\beta}(Z_N) = \frac{1}{\mathcal{Z}_{N,\beta}} \exp \left(-\frac{\beta}{2} \sum_{i=1}^N |v_i|^2 \right) \prod_{i \neq j} 1_{|x_i - x_j| > \varepsilon}$$

Main Goal

$$\|\lambda^d f_N^{(1)} - g_N^{(1)}\|_{L^\infty([0,t] \times \mathbf{T}_\lambda^d \times \mathbb{R}^d)} \rightarrow 0, \quad \text{as } N \rightarrow \infty$$

Comparing the truncated hierarchies

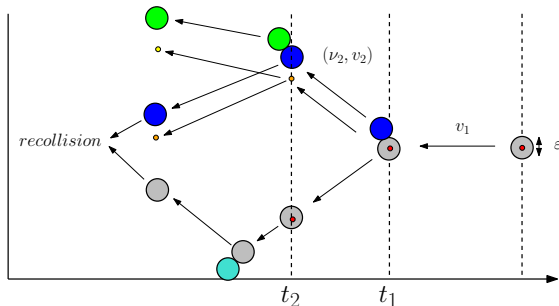
$$f_N^{(1,K)}(t) = \sum_{j_1=0}^2 \dots \sum_{j_K=0}^{2^K} Q_{1,J_1}(\tau) Q_{J_1,J_2}(\tau) \dots Q_{J_{K-1},J_K}(\tau) f_N^{0(J_K)}$$

$$g_N^{(1,K)}(t) = \sum_{j_1=0}^2 \dots \sum_{j_K=0}^{2^K} Q_{1,J_1}^0(\tau) Q_{J_1,J_2}^0(\tau) \dots Q_{J_{K-1},J_K}^0(\tau) g_N^{0(J_K)}$$

Geometric interpretation of the collisions operators:

Backward dynamics

Coupling
trajectories



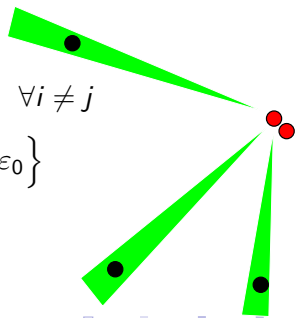
Removing recollisions

BBGKY and Boltzmann trajectories can be coupled if there are no recollisions

- Truncating high velocities
- Truncating collisions in short time intervals
- Recursive construction of the **good trajectories**

$$\mathcal{G}_k(\varepsilon_0) = \left\{ Z_k \in \mathbf{T}_\lambda^{dk} \times \mathbb{R}^{dk} / \forall s \in [0, t], \quad \forall i \neq j \right. \\ \left. d(x_i - sv_i, x_j - sv_j) \geq \varepsilon_0 \right\}$$

Up to a small set of velocities, the system is stable by addition of the $k + 1$ particle



Removing recollisions

Choosing the velocities such that the particles in both hierarchies remain at distance less than $2^K \varepsilon$ and that there are no recollisions. This boils down to remove a set of velocities with small probability.

Quantitative controls : [Gallagher, Saint-Raymond, Texier]

$$\text{Error} \leq (Ct)^{\mathcal{N}_t} \varepsilon \quad \text{with} \quad \mathcal{N}_t \quad \text{particles in the tree at time } t$$

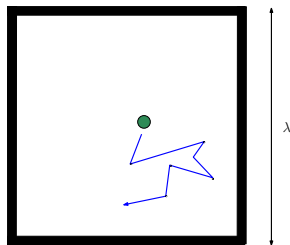
Estimates are valid up to times : $t_N = o\left(\mu_N^{-1/2} \sqrt{\log \log(N)}\right)$

$$\|\lambda^d f_N^{(1)} - g_N^{(1)}\|_{L^\infty([0, t_N] \times \mathbf{T}_\lambda^d \times \mathbb{R}^d)} \leq C \mu_N^2 \left(\frac{t_N^2}{\log \log N} \right)^2$$

Coupling both hierarchies

Position : $x_1^0(t) = \int_0^t v(u) du$

Markov process on the velocities
 $\{v(t)\}_{t \geq 0}$ with generator $\mathcal{L}$



$$\begin{cases} \mathcal{L}g(v) := \iint M_\beta(v_1)[g(v') - g(v)] ((v - v_1) \cdot v)_+ dv_1 dv, \\ v' = v + (\nu \cdot (v_1 - v))\nu \quad v'_1 = v_1 - (\nu \cdot (v_1 - v))\nu \end{cases}$$

Central limit Theorem for additive functionals of Markov chains
 ($\mathcal{L}$ has a spectral gap)

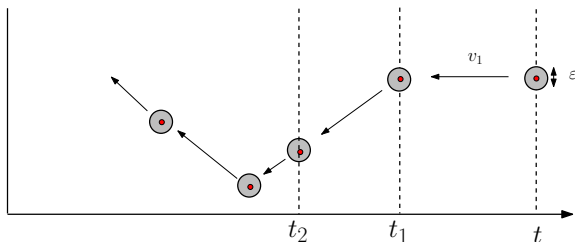
$$\lim_{N \rightarrow \infty} \mathbb{E} \left(h \left(\frac{1}{\lambda_N} x_1^0(\lambda_N^2 \tau) \right) \right) = \mathbb{E} \left(h(B(\tau)) \right)$$

$$\begin{aligned} \lim_{N \rightarrow \infty} \mathbb{E} \left(h_1 \left(\frac{1}{\lambda_N} x_1^0(\lambda_N^2 \tau_1) \right) \dots h_\ell \left(\frac{1}{\lambda_N} x_1^0(\lambda_N^2 \tau_\ell) \right) \right) \\ = \mathbb{E} \left(h_1(B(\tau_1)) \dots h_\ell(B(\tau_\ell)) \right) \end{aligned}$$

The diffusion coefficient κ is given by

$$\kappa = \lim_{t \rightarrow \infty} \frac{1}{d} \mathbb{E}_{M_\beta} \left[\left(\frac{1}{\sqrt{t}} \int_0^t v_1^0(s) ds \right)^2 \right]$$

Coupling the trajectories x_1 and x_1^0 to get estimates at different times



Conclusion

- Brownian motion for deterministic hard sphere dynamics

Conclusion

- Brownian motion for deterministic hard sphere dynamics
- Linearized Boltzmann equation for large times
[work in progress]