Dynamical Connectivity of Hard Spheres

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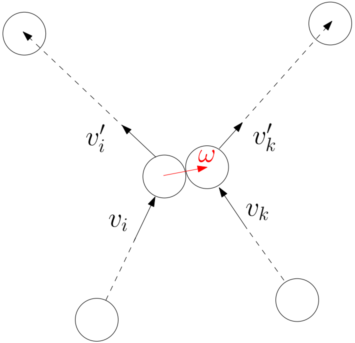
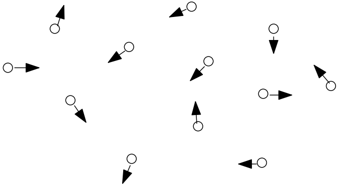
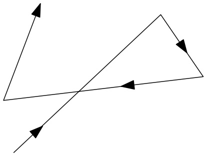


v_i'
v_k'
ω
v_i
v_k

$$\begin{cases} \dot{x}_i = v_i \\ \dot{v}_i = 0 \end{cases} \quad \text{in} \quad \Omega_N^\varepsilon := \left\{ |x_i - x_k| > \varepsilon \text{ for } i \neq k \right\} \subset \left(\mathbb{R}^d \times \mathbb{R}^d\right)^N \qquad d \geq 2$$

$$\begin{cases} v_i' = v_i - \omega[\omega \cdot (v_i - v_k)] \\ v_k' = v_k - \omega[\omega \cdot (v_j - v_k)] \end{cases} \quad \text{if} \quad x_k - x_i = \varepsilon\,\omega\,, \quad \omega \in S^{d-1}$$





N = number of spheres ; ε = sphere diameter

rate of coll. $\simeq N\varepsilon^{d-1} \sim 1$; ‘volume’ density $N\varepsilon^d \sim \varepsilon$

$\varepsilon \ll 1$: low density gas

Configuration $Z_N = (z_1, z_2, \cdots, z_N) \qquad z_i = (x_i, v_i)$.

Density distribution: $W_N^\varepsilon = W_N^\varepsilon(t, Z_N)$, symmetric in the particle labels.

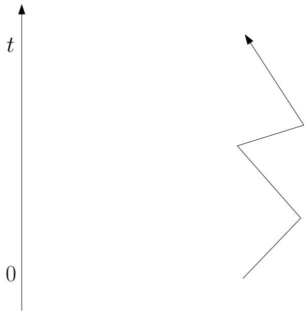
$$\left(\partial_t + \sum_{i=1}^N v_i \cdot \nabla_{x_i}\right) W_N^\varepsilon = 0 \qquad \text{in} \qquad \Omega_N^\varepsilon$$

$$W_N^\varepsilon(\cdots, x_i, v_i', \cdots, x_k, v_k' \cdots) = W_N^\varepsilon(\cdots, x_i, v_i, \cdots, x_k, v_k \cdots)\,, \qquad x_k - x_i = \varepsilon\,\omega$$

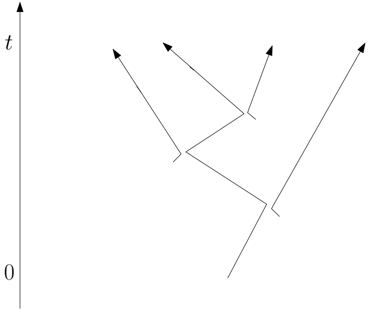
$$W_N^\varepsilon|_{t=0} = W_{0,N}^\varepsilon$$

Liouville equation

$W_N^\varepsilon|_{t=0} = W_{0,N}^\varepsilon$
$W_{0,N}^\varepsilon$ “chaotic” (finite marginals almost tensorized)



Trajectory of particle 1 *in* $[0, t]$



Forward cluster of particle 1 *in* $[0, t]$

$$FC(1) = \text{Forward-Cluster}(1) = \left\{1, k_1, k_2, k_3\right\}$$

Problem: given $t > 0$, $|FC(1)| = ?$, uniformly in ε, N with $\varepsilon^{d-1} N \sim 1$.

* After the *Boltzmann-Grad limit* $\varepsilon \to 0$, $N = \varepsilon^{-(d-1)}$ one gets:

$$\mathbb{E}(|FC(1)|) \simeq e^{Ct}, C > 0$$

(using the homogeneous Boltzmann equation, or numerical simulations; e.g. as in [Aoki, Pulvirenti, S., Tsuji. ('15)]).

* For $\varepsilon > 0$: difficult. Rough bound:

$$\mathbb{P}_N^\varepsilon(|FC(1)| = k) \leq \frac{(Ct)^k k!}{k!} .$$

The *equilibrium state* can be handled at least.

Theorem. [Pulvirenti, S. ('20)]

We consider the system of hard spheres of unit mass and diameter $\varepsilon > 0$, moving in $\mathbb{R}^3$, in the equilibrium state with density

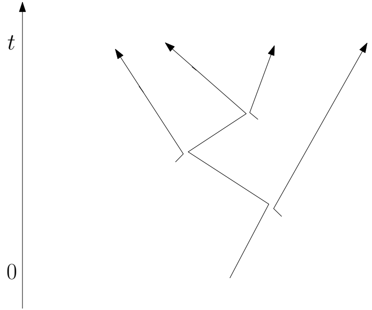
$$W_N^\varepsilon(Z_N) = \frac{1}{\mathcal{Z}_N} e^{-\frac{\beta}{2}\sum_i v_i^2} \prod_{i<k} \mathbb{1}_{|x_i - x_k| > \varepsilon} ,$$

($\beta > 0$, $\mathcal{Z}_N$ normalization constant). Then, $\exists k_0$ such that, for $k > k_0$, the probability of finding a forward cluster of size k at time t is

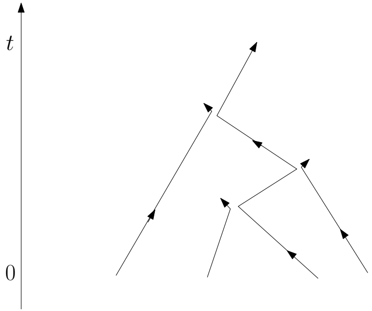
$$\mathbb{P}_{N,eq}^\varepsilon(|FC(1)| = k) \leq (1+2t)e^{-\frac{1}{2}k^{\frac{1}{2t}}} .$$

In particular, $\mathbb{E}_{N,eq}^\varepsilon(|FC(1)|)$ is bounded uniformly in ε in any bounded interval of time.

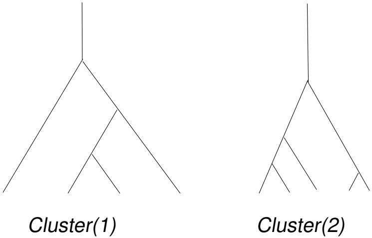
Remark. Not optimal. Expected: $\mathbb{P}_{N,eq}^\varepsilon(|FC(1)| = k) \leq e^{-ct}(1 - e^{-c't})^k$, $(c, c' > 0)$.



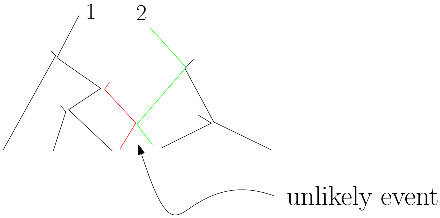
Forward cluster of particle 1 *in* $[0, t]$



Backward cluster of particle 1 *in* $[0, t]$
("Wild sums" for the Boltzmann equation)

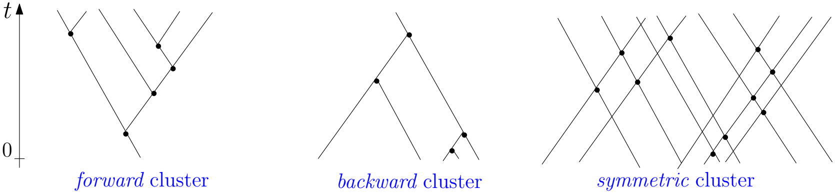


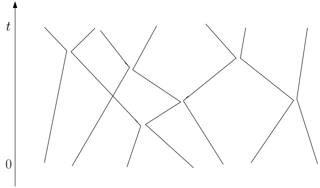
"Typically", $\text{Cluster}(1) \bigcap \text{Cluster}(2) = \emptyset$ *(chaos propagation)*



Mathematical derivation of the Boltzmann equation from Newton laws

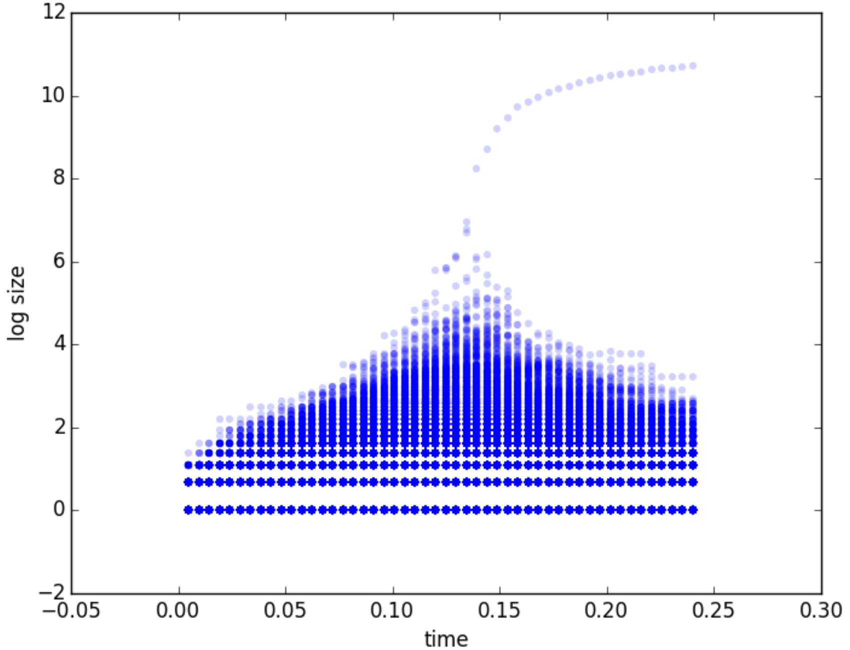
[Lanford, Spohn, Illner, Pulvirenti, ... Bodineau, Gallagher, Saint-Raymond, Texier, S. ...]

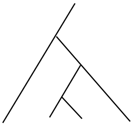


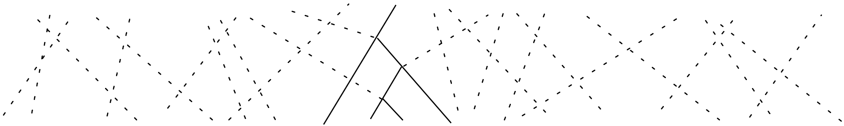


Definition. *We call two spheres "$t-$neighbours" if they collided during the time interval $[0,t]$. Any connected component of this neighbour relation is called a symmetric cluster at time t.*

[Sinai ('70), Gabrielov, Keilis-Borok, Sinai, Zaliapin ('08)]


12
10
8
6
4
2
0
−2
log size
−0.05
0.00
0.05
0.10
0.15
0.20
0.25
0.30
time





Results. [Patterson, S., Wagner ('16,'17)]

* In the Boltzmann-Grad limit, there exist kinetic equations for the symmetric cluster dynamics:

$$\frac{\#(\text{clusters of size } k \text{ at time } t)}{N} \longrightarrow n^{(k)}(t)\,;$$

* The equations exhibit the phase transition in finite time.

Symmetric cluster distribution: $\left\{ f^{(k)} = f^{(k)}(t, Z_k) \right\}_{k \geq 1}^{\infty}$

Boltzmann cluster equations:

$$\left(\partial_t + \sum_{i=1}^{k} v_i \cdot \nabla_{x_i} \right) f^{(k)}$$

$$= \frac{1}{2} \sum_{\substack{Q \subset \{1, \cdots, k\} \\ Q = \{\alpha_1, \cdots, \alpha_q\} \\ Q^c = \{\beta_1, \cdots, \beta_{k-q}\}}} \frac{1}{\binom{k}{q}} \sum_{\substack{\alpha \in Q \\ \beta \in Q^c}} \delta(x_\alpha - x_\beta) \int_{S^2} \left(\omega \cdot (v_\alpha - v_\beta) \right)_+$$

$$\times f^{(q)} \left(z_{\alpha_1}, \cdots, x_\alpha, v'_\alpha, \cdots, z_{\alpha_q} \right) f^{(k-q)} \left(z_{\beta_1}, \cdots, x_\beta, v'_\beta, \cdots, z_{\beta_q} \right) d\omega$$

$$- \sum_{\alpha=1}^{k} \int_{S^2 \times \mathbb{R}^3} (\omega \cdot (v_\alpha - v_*))_+ f^{(k)}(z_1, \cdots, x_\alpha, v_\alpha, \cdots, z_j) f(x_\alpha, v_*) d\omega dv_*$$

$f(x, v)$ = Boltzmann density $\geq \sum_{k \geq 1} k \int_{\mathbb{R}^{6(k-1)}} f^{(k)}(x, v, z_2, \cdots, z_k) dz_2 \cdots dz_k$

equality holds only up to $t \leq t_c$ *(giant cluster)*

Integrating all variables Z_k we get, for $t \leq t_c$,

$$\partial_t n^{(k)}(t) = \frac{1}{2} \sum_{q=1}^{k-1} \mathcal{K}_t(q, k-q)\, n^{(q)}(t)\, n^{(k-q)}(t) - \sum_{q \geq 1} \mathcal{K}_t(k,q)\, n^{(k)}(t)\, n^{(q)}(t)$$

with kernel

$$\mathcal{K}_t(k,q) = k\, q \int dv_1\, dv_2\, dx\, d\omega\, ((v_1 - v_2) \cdot \omega)_+\, f^{(k)}(t; x, v_1)\, f^{(q)}(t; x, v_2)\,,$$

where $f^{(k)}(t; x, v)$ = normalized $1-$particle phase-space distribution in clusters of size k.

Remark. $\mathcal{K}_t(k,q) \neq kq$, unless we replace $\int d\omega\, ((v_1 - v_2) \cdot \omega)_+$ with a constant, namely:

Maxwell mol. with Grad cutoff $\longleftrightarrow$ *Smoluchowski eq. with product kernel*

Consider the Boltzmann equation for Maxwell molecules with Grad cutoff:

$$\partial_t f(v) = -Rf + \int_{\mathbb{R}^d \times S^{d-1}} dv_1 d\omega \; b\left(\frac{(v-v_1)}{|v-v_1|} \cdot \omega\right) f(v_1') f(v'), \qquad R > 0.$$

Then:

– The associated cluster size distribution is

$$n^{(k)}(t) = k^{-\beta} e^{-k/\gamma(t)} (1 + O(1/k))$$

with $\beta = 5/2$ and $\gamma(t) = |\ln(eRte^{-Rt})|^{-1}$.

– Its normalization constant has discontinuous second derivative at the critical time $t_c = R^{-1}$.

– The density of particles in a $k-$cluster is not normalized: $m_1(t) = \sum_{k\geq 1} k\, n^{(k)}(t) < 1$ for $t > t_c$, and $m_1(t) \to 0$ exponentially as $t \to \infty$.

– $\partial_t f^{(k)}(t; x, v) = 0$ and $\partial_t E^{(k)}(t) = \partial_t \left(\int dv \frac{v^2}{2} f^{(k)}(t; x, v) \right) = 0$.

THANK YOU!

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