HARD-SPHERE GASES: DETERMINISTIC DYNAMICS WITH RANDOM INITIAL DATA

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Sergio Simonella

Critical behaviour in spatial particle systems - Berlin, January 29-31 2025

- The large scale limit problem
 - Basic tools from statistical mechanics
 - A warm-up problem
- e Hard sphere dynamics
 - Hard sphere gas: law of large numbers
 - Hard sphere gas: CLT and large deviations
- Long time results
 - Fluctuating hydrodynamics

Material.

* H. Spohn. Large scale dynamics of interacting particles. Texts and Monographs in Physics, Springer, Heidelberg, 1991.

* C. Cercignani, R. Illner, M. Pulvirenti. *The Mathematical Theory of Dilute Gases.* Applied Math. Sci. **106**, Springer-Verlag, New York, 1994.

* T. Bodineau, I. Gallagher, L. Saint-Raymond, S. Simonella. Dynamics of dilute gases: a statistical approach.
Proceedings of the International Congress of Mathematicians 2022, 2, 750-795, Ed. D. Beliaev and S. Smirnov, EMS Press, 2023. 1. The large scale limit

deterministic dynamics



random initial data

deterministic dynamics



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motivation : macroscopic theory of matter based on first principles



N particles (e.g.
$$N \sim 10^{23}$$
)

label
$$i = 1, 2, \cdots, N$$

- $z_i = (x_i, v_i) \in \mathbb{T}^d \times \mathbb{R}^d$: position, velocity of particle i
- U : molecular potential (central)

$$\begin{cases} \frac{d}{dt}x_{i} = v_{i} \\ \frac{d}{dt}v_{i} = -\sum_{j \neq i} \nabla U \left(x_{i} - x_{j}\right) &, i = 1, \cdots, N \\ \left(x_{i}(0), v_{i}(0)\right) = \left(x_{i}^{0}, v_{i}^{0}\right) \end{cases}$$



deterministic dynamics: Newton's laws





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$$(z_i^0)_i \xrightarrow{T_t} (z_i(t))_i$$

Phase space : $(\mathbb{T}^d \times \mathbb{R}^d)^N$





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Properties : * $T_{t_1+t_2} = T_{t_1}T_{t_2}$

- * $dz_1 \cdots dz_N$ invariant
- * $(x_i(-t), -v_i(-t))_i$ solution
- * conservation of mass, momentum, energy





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$$N \longrightarrow \infty$$

$$\varepsilon \longrightarrow 0$$
MACRO



hydrodynamics

Euler, Navier-Stokes, heat...

(U coded in coefficients)

+ fluctuations

(revealing the coefficients)



observed macroscopic behaviour corresponds to "typical" configurations





A state is a probability measure on the N particle phase space. Initial measure : \mathcal{W}_0 . Evolution : $\mathcal{W}(t) = \mathcal{W}_0 \circ T_{-t}$.

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$$\frac{\bigvee_{\varepsilon \to 0}^{N \to \infty}}{\mathbf{MACRO}}$$





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random initial data

 $(z_i(t))_i$ random variables

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(Hilbert 1900)



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Scaling : $x^{\varepsilon}(t) = \varepsilon x \left(\frac{t}{\varepsilon^2}\right)$



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Theorem. [Bunimovich - Sinai '81] $x^{\varepsilon}(t) \Rightarrow \sqrt{2D} b(t)$ D positive diffusion matrix, b(t) standard Brownian motion.



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[&]quot;I will not discuss derivations which include some external randomness in the dynamics by the Varadhan school. I will also not discuss the derivation of a diffusion equation for non-interacting particles moving among Sinai billiards. Those cases show what we could do if only our mathematics was better." [J. Lebowitz]

 $N \longrightarrow \infty$ $\varepsilon \longrightarrow 0$

KIN

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Kinetic Limit $N\varepsilon^d \ll 1$ and/or $U_{\varepsilon} \ll 1$

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chaos propagation



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$$Kinetic Limit$$

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$$(\partial_{t} + v \cdot \nabla_{x}) f + F(x) \cdot \nabla_{v} f = Q(f, f)$$

$$long-range$$

$$mean-field$$

$$Collisions$$



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$$\begin{array}{c|c} \mathbf{KIN} \\ (\partial_t + v \cdot \nabla_x) f &+ \underbrace{F(x) \cdot \nabla_v f}_{\text{mean-field}} = \underbrace{\mathcal{Q}(f, f)}_{\text{collisions}} \mathcal{Q}_B(f, f)(z) = \int B(v - v_*, \omega) \left[f'f'_* - ff_*\right] \\ & \text{Boltzmann (gas dynamics)}_{N\varepsilon^d \ll 1, \ U_\varepsilon(x) = U(x/\varepsilon)} \\ & \mathcal{Q}_L(f, f)(z) = \nabla_v \int a(v - v_*) \left[f_* \nabla f - f \nabla f_*\right] \\ & \text{Landau (plasma physics, Balescu-Lenard)} \\ & N\varepsilon^d \sim 1, \ U_\varepsilon(x) = \sqrt{\varepsilon} U(x/\varepsilon) \end{array}$$

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Kinetic Limit (in any fixed time interval [0, t], t > 0)

- * reversible \rightarrow irreversible (time's arrow)
- * memory (unbounded order) \rightarrow Markov property
- * N-particle interaction \rightarrow nonlinearity (even small)



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Long times $(t \sim t_{\varepsilon} \rightarrow \infty \text{ gently})$



1.1. Basic tools from statistical mechanics

Grand canonical phase space : $\Omega = \bigcup_{n \ge 0} \Omega_n$, $\Omega_n = (\mathbb{T}^d \times \mathbb{R}^d)^n$.

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Average particle number : $\mathbb{E}[N] = \sum_{n \ge 0} n p_n$, $p_n = \frac{1}{n!} \int_{\Omega_n} W_n$.

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 $\text{Scaling}: W_n = W_n^{\boldsymbol{\varepsilon}} \ , \quad \mathbb{E} = \mathbb{E}_{\boldsymbol{\varepsilon}} \ , \quad \boldsymbol{\varepsilon} > 0 \ .$

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 $\label{eq:Low-density limit} \text{Low-density limit}: \varepsilon \to 0 \ , \ \mathbb{E}_{\varepsilon}[N] \to \infty \ , \ \mathbb{E}_{\varepsilon}[N] \varepsilon^{d-1} \to 1 \ (\mathbb{E}_{\varepsilon}[N] \varepsilon^d \sim \varepsilon).$



 $U_{\varepsilon}(x) = U\left(\frac{x}{\varepsilon}\right)$

Correlation functions :
$$\{\rho_j^{\varepsilon}\}_{j\geq 0}$$

 $\rho_j^{\varepsilon}: \Omega_j \to \mathbb{R}^+$
 $\rho_j^{\varepsilon}(z_1, \cdots, z_j) = \sum_{k\geq 0} \frac{1}{k!} \int_{\Omega_k} W_{j+k}^{\varepsilon}(z_1, \cdots, z_{j+k}) dz_{j+1} \cdots dz_{j+k}$

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Inverse formula :

$$W_j^{\varepsilon}(z_1,\cdots,z_j) = \sum_{k\geq 0} \frac{(-1)^k}{k!} \int_{\Omega_k} \rho_{j+k}^{\varepsilon}(z_1,\cdots,z_{j+k}) dz_{j+1} \cdots dz_{j+k}$$

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Moment formula :

$$\begin{cases} \rho_1^{\varepsilon}(z_1) = \mathbb{E}_{\varepsilon}[\sum_{i=1}^N \delta_{z_i^{\varepsilon}}(z_1)] \\ \rho_2^{\varepsilon}(z_1, z_2) = \mathbb{E}_{\varepsilon}[\sum_{i_1 \neq i_2} \delta_{z_{i_1}^{\varepsilon}}(z_1) \delta_{z_{i_2}^{\varepsilon}}(z_2)] \\ \dots \end{cases}$$

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 $\rho_j^{\varepsilon}(z_1, \cdots, z_j) = \sum_{k\geq 0} \frac{1}{k!} \int_{\Omega_k} W_{j+k}^{\varepsilon}(z_1, \cdots, z_{j+k}) dz_{j+1} \cdots dz_{j+k}$

Inverse formula :

$$W_j^{\varepsilon}(z_1, \cdots, z_j) = \sum_{k \ge 0} \frac{(-1)^k}{k!} \int_{\Omega_k} \rho_{j+k}^{\varepsilon}(z_1, \cdots, z_{j+k}) dz_{j+1} \cdots dz_{j+k}$$

Moment formula :

$$\begin{cases} \rho_1^{\varepsilon}(z_1) = \mathbb{E}_{\varepsilon}[\sum_{i=1}^N \delta_{z_i^{\varepsilon}}(z_1)] \\ \rho_2^{\varepsilon}(z_1, z_2) = \mathbb{E}_{\varepsilon}[\sum_{i_1 \neq i_2} \delta_{z_{i_1}^{\varepsilon}}(z_1) \delta_{z_{i_2}^{\varepsilon}}(z_2)] \\ \dots \\ \int_{\Omega_j} \rho_j^{\varepsilon} = \mathbb{E}_{\varepsilon}[N(N-1)\cdots(N-j+1)] \,. \end{cases}$$

Correlation functions :
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 $\text{Rescaled correlation functions}: F_j^\varepsilon = \varepsilon^{j(d-1)} \rho_j^\varepsilon \quad (\text{BG limit}: f_{\Omega_1} F_1^\varepsilon \to 1).$

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The particle state approximates f.

$$\begin{split} \text{Empirical measure} &: \pi^{\varepsilon}_{\text{emp}}(\varphi) = \varepsilon^{d-1} \sum_{i=1}^{N} \varphi(z^{\varepsilon}_{i}) \\ & \pi^{\varepsilon}_{\text{emp}}(\varphi) \longrightarrow \int_{\Omega_{1}} f \varphi \quad \forall \varphi \in C^{0}_{b}(\Omega_{1}) \text{ in probability.} \end{split}$$

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This is the statement that we aim to propagate dynamically. However, this is **not** possible...

Moment generating function :

$$\mathbb{E}_{\varepsilon}\left[\exp\left(\pi_{\mathrm{emp}}^{\varepsilon}(\varphi)\right)\right] = 1 + \sum_{j \geq 1} \frac{1}{j!} \int_{\Omega_j} \rho_j^{\varepsilon} \left(e^{\varepsilon^{d-1}\varphi} - 1\right)^{\otimes j}$$

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Cumulant generating function :

$$\log \mathbb{E}_{\varepsilon} \left[\exp \left(\varepsilon^{-(d-1)} \pi_{\exp}^{\varepsilon}(\varphi) \right) \right] = \sum_{j \ge 1} \frac{\varepsilon^{-j(d-1)}}{j!} \int_{\Omega_j} f_j^{\varepsilon} \left(e^{\varphi} - 1 \right)^{\otimes j}$$

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Inverse formula: $F_j^{\varepsilon}(Z_j) = \sum_{k=1}^j \sum_{\sigma \in \mathscr{P}_j^k} \prod_{i=1}^k f_{|\sigma_i|}^{\varepsilon} (Z_{\sigma_i})$ $Z_j = (z_1, \dots, z_j), \quad Z_A = (z_\ell)_{\ell \in A}, \quad \sigma = (\sigma_1, \dots, \sigma_k),$ \mathscr{P}_j^k the set of partitions of $\{1, \dots, j\}$ in k parts.

"Maximally chaotic state" (MCS) :

 $\frac{1}{n!} W_n^{\varepsilon}(z_1, \cdots, z_n) := \frac{1}{\mathcal{I}_{\varepsilon}} \frac{\varepsilon^{-n(d-1)}}{n!} f^{\otimes n}(z_1, \cdots, z_n) \psi_n^{\varepsilon}(x_1, \cdots, x_n) , \qquad n \ge 0$

 $\mathcal{Z}_{\varepsilon}$: partition function

 $f: \Omega_1 \rightarrow \mathbb{R}^+$: smooth macroscopic density

$$\psi_n^{\varepsilon}(x_1, \cdots, x_n) = \prod_{i < j} \exp\left(-\beta U\left(\frac{x_i - x_j}{\varepsilon}\right)\right), \qquad \beta > 0$$

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Exercises

Set
$$U = U_{\text{h.c.}}(x) = \begin{cases} \infty & |x| < 1 \\ 0 & |x| \ge 1 \end{cases}$$

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Exercises

Set $U = U_{\text{h.c.}}(x) = \begin{cases} \infty & |x| < 1 \\ 0 & |x| \ge 1 \end{cases}$.

(Q1) Show that the second cumulant $f_2^{\varepsilon} \to 0$ in L^1 , in the BG limit. (Q2) Is the convergence true in L^{∞} ? Find a pointwise estimate for f_2^{ε} . (Q3) Find an L^1 estimate on f_j^{ε} , $j \ge 2$. **Definition.** The *fluctuation field* ζ^{ε} is

$$\zeta^{\varepsilon}(\varphi) = \frac{1}{\varepsilon} \left(\pi^{\varepsilon}_{\mathrm{emp}}(\varphi) - \mathbb{E}_{\varepsilon} \left[\pi^{\varepsilon}_{\mathrm{emp}}(\varphi) \right] \right)$$

Exercises

(Q1') Compute the covariance of the fluctuation field in terms of the first cumulants $f_1^{\varepsilon}, f_2^{\varepsilon}$

(Q2') Deduce that, for the hard-core MCS, ζ^{ε} converges to white noise.

(Q3') For which other potentials is this still true?

Newton's flow on Ω : $T_t^{\varepsilon} (T_t^{(n,\varepsilon)})_n$ Potential : $U_{\varepsilon}(x) = U(\frac{x}{\varepsilon})$ Initial state : $\mathcal{W}_0^{\varepsilon}$ Time-evolved state : $\mathcal{W}^{\varepsilon}(t) = \mathcal{W}_0^{\varepsilon} \circ T_{-t}^{\varepsilon}$ Density functions : $\{W_n^{\varepsilon}(t)\}_{n\geq 0}, \quad W_n^{\varepsilon} = W_n^{\varepsilon}(t, z_1, \cdots, z_n)$

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Liouville Equation :
$$(\partial_t + \sum_i v_i \cdot \nabla_{x_i} - \sum_{i \neq j} \nabla U_{\varepsilon}(x_i - x_j) \cdot \nabla_{v_i}) W_n^{\varepsilon} = 0$$

 $W_n^{\varepsilon}|_{t=0} = W_{0,n}^{\varepsilon}$ $n = 0, 1, 2 \cdots$

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BBGKY Hierarchy :

$$\left(\partial_t + \sum_i v_i \cdot \nabla_{x_i} - \sum_{i \neq j} \nabla U_{\varepsilon}(x_i - x_j) \cdot \nabla_{v_i}\right) \rho_j^{\varepsilon} = \sum_i \int \nabla U_{\varepsilon}(x_i - x_{j+1}) \cdot \nabla_{v_i} \rho_{j+1}^{\varepsilon} dz_{j+1}$$

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Cumulant Hierarchy : ··· [Ernst - Cohen '81]

1.2. A warm-up problem

N = 1 Lorentz gas at low density



$$\begin{split} &z=(x,v)\in \mathbb{T}^d\times \mathbb{S}^{d-1}, \ d\geq 2\\ &t\to z^\varepsilon(t): \text{free flow}+\text{elastic reflection}\\ &\text{Hard core scatterers, radius }\varepsilon>0\\ &\text{randomly distributed}\\ &\text{Density of scatterers}: \varepsilon^{-(d-1)} \end{split}$$

Initial data: probability distribution of scatterer centers $\left\{\frac{1}{n!}W_n^{\varepsilon}(c_1,\cdots,c_n)\right\}$
N = 1 Lorentz gas at low density



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Hyp. (i) $\exists A, c > 0$ such that $F_j^{\varepsilon} \leq Ac^j$ (ii) $\exists r \in C(\mathbb{T}^d)$ such that $\lim_{\varepsilon \to 0} F_j^{\varepsilon} = r^{\otimes j}$ outside diagonals

N = 1 Lorentz gas at low density



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Theorem. [Gallavotti '69, Spohn '78] $z^{\varepsilon}(t) \Rightarrow z(t)$ z(t) Markov jump process with forward equation $(\partial_t + v \cdot \nabla_x) f = r(x) \int_{\mathbb{S}^{d-1}} [v \cdot \omega]_+ \{f(x, v - 2[v \cdot \omega]\omega) - f(x, v)\} d\omega$

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$$\begin{split} P\left(dt_1d\omega_1\cdots dt_kd\omega_k\right) &= \frac{1}{Z}\prod_i r(x(t_i))[v(t_i^+)\cdot\omega_i]_+dt_1d\omega_1\cdots dt_kd\omega_k\\ \text{on path space }\Lambda_t &= \cup_{k\geq 0}\Lambda_{t,k}, \Lambda_{t,k} = \{(t_1,\omega_1,\cdots,t_k,\omega_k), 0 < t_1 < \cdots t_k < t, \omega_i \in \mathbb{S}^{d-1}\}. \end{split}$$

Recall

$$\begin{split} P(dt_1 d\omega_1 \cdots dt_k d\omega_k) &= \frac{1}{Z} \prod_i r(x(t_i)) [\nu(t_i^+) \cdot \omega_i]_+ dt_1 d\omega_1 \cdots dt_k d\omega_k \\ \Lambda_{t,k} &= \left\{ (t_1, \omega_1, \cdots, t_k, \omega_k), \ 0 < t_1 < \cdots < t_k < t, \omega_i \in \mathbb{S}^{d-1} \right\} \\ P^{\varepsilon} &= ? \end{split}$$

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Step 1 : **bad set** $\mathcal{N}_k \subset \Lambda_{t,k}$

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$$\underbrace{\underline{\text{Step 1}}}_{\mathcal{N}_k} : \underbrace{\text{bad set}}_{\mathcal{N}_k} \in \mathcal{N}_k \subset \Lambda_{t,k}$$
$$\mathcal{N}_k = \left\{ \exists i \in \{1, \cdots, k\}, t_i \mid x(t_i) \text{ is crossed twice} \right\}$$

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$$\mathcal{N}_k \subset \Lambda_{t,k}$$

 $\mathcal{N}_k = \{ \exists i \in \{1, \dots, k\}, t_i \mid x(t_i) \text{ is crossed twice } \}$

Lemma. $P(\mathcal{N}_k) = 0.$

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$$\begin{split} P\left(dt_1d\omega_1\cdots dt_kd\omega_k\right) &= \frac{1}{Z}\prod_i r(x(t_i))[\nu(t_i^+)\cdot\omega_i]_+dt_1d\omega_1\cdots dt_kd\omega_k\\ \Lambda_{t,k} &= \left\{(t_1,\omega_1,\cdots,t_k,\omega_k), \ 0 < t_1 < \cdots < t_k < t, \omega_i \in \mathbb{S}^{d-1}\right\}\\ P^{\varepsilon} &= ? \end{split}$$

$$\underbrace{\frac{\text{Step 1}}{\text{Step 1}}: \text{bad set} \quad \mathcal{N}_k \subset \Lambda_{t,k}}_{\mathcal{N}_k} = \left\{ \exists i \in \{1, \cdots, k\}, t_i \mid x(t_i) \text{ is crossed twice} \right\}$$

Lemma. $P(\mathcal{N}_k) = 0.$

Good set : $\mathscr{A} \subset \Lambda_{t,k} \setminus \mathscr{N}_k$ compact

Recall

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$$\underbrace{\underline{\text{Step 1}}}_{k} : \underbrace{\text{bad set}}_{\mathcal{N}_k} \subset \Lambda_{t,k}$$
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Lemma. $P(\mathcal{N}_k) = 0.$

 $\begin{array}{l} \textit{Good set}: \ \mathscr{A} \subset \Lambda_{t,k} \setminus \mathscr{N}_k \ \text{ compact} \\ \Rightarrow \ \text{for } \varepsilon \ \text{small, each scatterer is hit at most once in } \mathscr{A}. \end{array}$

Step 2 : parametrization

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Gallavotti '69: "The proof is based on several simple changes of variables..."

$$c_1, c_2, \dots \longrightarrow t_1, \omega_1, t_2, \omega_2, \dots$$
 $((x^0, v^0) \text{ fixed})$

scatterers \rightarrow paths

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scatterers \rightarrow paths

Lemma. $dc_i = \varepsilon^{d-1} [v^{\varepsilon}(t_i^-) \cdot \omega_i]_- dt_i d\omega_i$

For simplicity :
$$d = 2$$
, $\frac{W_n^{\varepsilon}}{n!} = \frac{1}{\mathcal{Z}_{\varepsilon}} e^{-\varepsilon^{-1}} \frac{\varepsilon^{-n}}{n!}$, $\mathcal{Z}_{\varepsilon} \simeq 1$, $n \ge 0$.

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$$P^{\varepsilon}(\mathscr{A}) = \frac{e^{-\varepsilon^{-1}}}{\mathcal{I}_{\varepsilon}} \varepsilon^{-k} \int dc_1 \cdots dc_k \, \mathbf{1}_{\mathscr{A}} \sum_{m \ge 0} \frac{\varepsilon^{-m}}{m!} \int dc'_1 \cdots dc'_m \, \left(1 - \mathbf{1}_{\mathscr{T}^{\varepsilon}(c_1, \cdots, c_k)}\right).$$



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$$= \frac{e^{-2t}}{\mathcal{I}_{\varepsilon}} \int_{\Lambda_{t,k}} dt_1 d\omega_1 \cdots dt_k d\omega_k \prod_i [v(t_i^-) \cdot \omega_i]_{-} \mathbf{1}_{\mathscr{A}} \to P(\mathscr{A}) \text{ as } \varepsilon \to 0.$$

Question.

Replace
$$U = U_{\text{h.c.}}(x) = \begin{cases} \infty & |x| < 1 \\ 0 & |x| \ge 1 \end{cases}$$

with
$$U = U_k(x) = \frac{1}{|x|^k}$$
, $k > 0$.

Is the theorem still valid?

2. Hard sphere dynamics

2.1. Hard sphere gas: law of large numbers





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



scaling

N = number of spheres ; $\varepsilon =$ sphere diameter rate of coll. $\simeq \mathbb{E}_{\varepsilon}[N]\varepsilon^{d-1} \rightarrow 1$; 'volume' density $\simeq \mathbb{E}_{\varepsilon}[N]\varepsilon^{d} \sim \varepsilon$ $\varepsilon \rightarrow 0$: low density limit (Boltzmann-Grad limit)

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Proposition. [Alexander '75, Vaserstein '79] The hard sphere flow $T_t^{(n,\varepsilon)}$ exists for all times t, almost everywhere in Ω_n^{ε} with respect to the Lebesgue measure. It admits the standard flow properties.





$$(v, v_*) \longrightarrow (v', v'_*)$$
$$v' = v - \omega[\omega \cdot (v - v_*)]$$
$$v'_* = v_* + \omega[\omega \cdot (v - v_*)]$$

 $v, v_* \sim \text{i.i.d.}$

$$\begin{split} f &= f(t, x, v) \qquad (x, v) \in \mathbb{T}^d \times \mathbb{R}^d \qquad d \ge 2 \\ (\partial_t + v \cdot \nabla_x) f &= Q(f, f) \\ Q(f, f)(x, v) &= \int_{\mathbb{R}^d} \int_{\mathbb{S}^{d-1}} \left[\omega \cdot (v - v_*) \right]_+ \left\{ f(x, v') f(x, v'_*) - f(x, v) f(x, v_*) \right\} d\omega dv_* \\ f|_{t=0} &= f_0 \end{split}$$

Properties : $\frac{d}{dt}\int (1, v, v^2)f(t, x, v)dxdv = 0$, $\frac{d}{dt}\int f\log f dxdv \le 0$.

Let the initial probability distribution of hard spheres $\left\{\frac{W_{0,n}^{\varepsilon}}{n!}\right\}$ over $\bigcup_n (\mathbb{T}^3 \times \mathbb{R}^3)^n (W_{0,n}^{\varepsilon} \text{ supported in } \Omega_n^{\varepsilon})$ satisfy the two assumptions:

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(ii) $\exists f_0 \in C^1(\mathbb{T}^3 \times \mathbb{R}^3)$, $\int f_0 = 1$, such that $\lim_{\varepsilon \to 0} F_{0,j}^{\varepsilon} = f_0^{\otimes j}$, uniformly on compact sets outside the diagonals $\{x_i = x_k, i \neq k\}$.

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$$\pi^{\varepsilon}_{\mathrm{emp}}(t,\varphi) = \varepsilon^2 \sum_{i=1}^{N} \varphi(z^{\varepsilon}_i(t)) \longrightarrow \int_{\mathbb{T}^3 \times \mathbb{R}^3} f(t)\varphi$$

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Note. Lanford used the hard-sphere BBGKY hierarchy (written by Cercignani in '72).
Remark. Topology encodes irreversibility.

 $\mathcal{B}^{j\pm}_{\varepsilon}(t) = \left\{ (z_1, \cdots, z_j) \in \Omega^{\varepsilon}_j, \qquad \exists s \in [0, t], \exists i, j, \qquad |x_i - x_j \pm s(v_i - v_j)| \le \varepsilon \right\}$

• $F_{i}^{\varepsilon}(0)$ converges on $\mathscr{B}_{\varepsilon}^{j+}(t)$

collisions towards the future collisions towards the past

• $F_i^{\varepsilon}(t)$ does **not** converge on $\mathscr{B}_{\varepsilon}^{j-}(t)$

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$$f_0 \in C^1(\mathbb{T}^3 \times \mathbb{R}^3)$$
, $\int f_0 = 1$, $|f_0| < e^{\alpha' - \beta' \nu^2}$, $\alpha', \beta' > 0$.

Proposition. The hard sphere MCS

$$\frac{W_{0,n}^{\varepsilon}}{n!} = \frac{1}{\mathcal{Z}_{\varepsilon}} \frac{\varepsilon^{-2n}}{n!} f_0^{\otimes n} \mathbf{1}_{\Omega_n^{\varepsilon}}, \qquad n \ge 0$$
(HSMCS)

satisfies the hypotheses.

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For simplicity, we will assume the initial state is the HSMCS from now on.

$$Z_N^0 = (z_1^0, \cdots, z_N^0) \to Z_N^\varepsilon(t) = (z_1^\varepsilon(t), \cdots, z_N^\varepsilon(t)) \,, \qquad t \in [0, T]$$

well defined (almost surely) for arbitrary T.

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Definition. [Sinai '72]

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Definition. [Sinai '72]

(i) Two particles are neighbours if they collided during the time interval [0, T].

$$Z^0_N = (z^0_1, \cdots, z^0_N) \to Z^\varepsilon_N(t) = (z^\varepsilon_1(t), \cdots, z^\varepsilon_N(t)) \,, \qquad t \in [0, T]$$

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(i) Two particles are neighbours if they collided during the time interval [0, T].

(ii) A *dynamical cluster* is any maximal connected component of the neighbour relation (i).

(iii) A *cluster path* $\lambda = \lambda([0, T])$ is the trajectory in [0, T] of dynamical cluster (ii).

 \mathcal{P}_A = partitions of A

$$\left(Z_N^0 \longrightarrow \left(Z_N^{\varepsilon}(t)\right)_{t \in [0,T]}\right) \implies \{\lambda_1, \lambda_2, \cdots\} \in \mathcal{P}_{\left(Z_N^{\varepsilon}(t)\right)_{t \in [0,T]}}$$



cluster path decomposition



cluster path decomposition

Empirical measure on cluster paths : $\pi_{emp}^{\varepsilon}(\lambda) = \varepsilon^2 \sum_i \delta_{\lambda_i([0,T])}(\lambda)$

Step 1 : we can define a *bad set* as for the Lorentz gas.

A good cluster path is a path λ of size $|\lambda| = \ell$ with exactly $\ell - 1$ collisions.



Step 2 : parametrization

$$\begin{split} & \left(z_1^0, \cdots, z_{\ell}^0\right) \longrightarrow \lambda = \left(\mathcal{T}_{\ell}, x_{\rm cm}, V_{\ell}^0, t_1, \omega_1, \cdots, t_{\ell-1}, \omega_{\ell-1}\right) \\ & \text{particles} \longrightarrow \text{cluster paths} \\ & \text{cluster path space} : \Lambda_T = \bigcup_{\ell \in \mathbb{N}} \left\{\mathcal{T}_{\ell}\right\} \times \mathbb{T}^3 \times \mathbb{R}^{3\ell} \times [0, T]^{\ell-1} \times \mathbb{S}^{2(\ell-1)} \end{split}$$



- Ingredients describing the cluster path $\lambda = (z_1(t), \dots, z_{\ell}(t))_{t \in [0,T]}$ of size ℓ :
- a tree graph \mathcal{T}_{ℓ} on ℓ vertices



- the center of mass at time zero $x_{\rm cm}$
- the collection of velocities V_{ℓ}^0
- impact times and angles $(t_i, \omega_i) \in [0, T] \times \mathbb{S}^2$ (ignoring recollisions)

$$dZ_{\ell}^{0} = d\lambda \, \varepsilon^{2(\ell-1)} \prod_{e = \{\alpha, \beta\} \in E(\mathcal{T}_{\ell})} \left[\omega_{e} \cdot \left(v_{\alpha}(t_{e}) - v_{\beta}(t_{e}) \right) \right]_{+}$$

$$\mathbb{E}_{\varepsilon}\left[\pi_{\mathrm{emp}}^{\varepsilon}(\lambda)\right] = \frac{1}{\tilde{\mathcal{I}}_{\varepsilon}} \sum_{k \ge 0} \frac{\varepsilon^{-2k}}{k!} \int d\nu(\lambda_0) \cdots d\nu(\lambda_k) \,\delta_{\lambda_0}(\lambda) \prod_{\substack{i,j=0\\i \neq j}}^{k} \mathbf{1}_{\lambda_i \neq \lambda_j}$$

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$$d\nu(\lambda) = d\lambda \frac{1}{\ell!} f_0^{\otimes \ell} \prod_{e = \{\alpha, \beta\} \in E(\mathcal{T}_\ell)} \left[\omega_e \cdot \left(v_\alpha(t_e) - v_\beta(t_e) \right) \right]_+$$

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$$\mathbf{1}_{\lambda_i \neq \lambda_k} = \mathbf{1}_{\{\lambda_i, \lambda_k \text{ disconnected }\}}$$



 $\lambda_i \not\sim \lambda_k$



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"Boltzmann factor" : $\psi_{k+1}^{\varepsilon}(\lambda_0, \cdots, \lambda_n) = \prod_{i,j} \mathbf{1}_{\lambda_i \nsim \lambda_j} = \prod_{i,j} \left(1 - \mathbf{1}_{\lambda_i \sim \lambda_j} \right)$

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cluster tubes $\mathcal{T}^{\varepsilon}(\lambda)$



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cluster tubes $\mathcal{T}^{\varepsilon}(\lambda)$



Question. How many effective terms in ψ_k^{ε} ?

H: smooth test function on the space of cluster paths.

(Rescaled) Cumulant gen. func. :

$$\mathscr{I}^{\varepsilon}(T,H) = \varepsilon^2 \log \mathbb{E}_{\varepsilon} \left[e^{\varepsilon^{-2} \pi_{emp}^{\varepsilon}(H)} \right] = \varepsilon^2 \log \mathbb{E}_{\varepsilon} \left[e^{\sum_i H(\lambda_i([0,T]))} \right]$$
(CGF)

 $\mathsf{Remark}: \mathbb{E}_{\mathcal{E}}\left[\pi^{\mathcal{E}}_{\mathrm{emp}}(\lambda)\right] = \partial_{u}\mathscr{I}^{\mathcal{E}}(T, uH)\Big|_{u=0}.$

 $\text{Remind}: \mathscr{I}^{\varepsilon}(T,H) = \varepsilon^2 \sum_{j \ge 1} \frac{\varepsilon^{-2j}}{j!} \int_{\Omega_j} \tilde{f}^{\varepsilon}_j \left(e^H - 1 \right)^{\otimes j} \qquad (\tilde{f}^{\varepsilon}_j \text{ cumulant of } \pi^{\varepsilon}_{\text{emp}}(\lambda))$

Proposition. [Bodineau - Gallagher - Saint-Raymond - S. '22] There exists T > 0 and a constant *C* (depending only on f_0 , $||H||_{\infty}$) such that

$$\|\tilde{f}_{j}^{\varepsilon}\|_{1} \leq (CT)^{j} \ j^{j-2} \varepsilon^{2(j-1)}$$

for ε small enough and all $j \ge 1$, and the expansion of the CGF converges absolutely.

Further consequences.

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Theorem. The emp. meas. on cluster paths in [0, t] converges:

$$\forall \delta > 0 , \qquad \mathbb{P}_{\varepsilon} \left(\left| \pi^{\varepsilon}_{\mathrm{emp}}(H) - \int_{\Lambda_{t}} d\Upsilon(t,\lambda) H(\lambda) \right| > \delta \right) \xrightarrow[\varepsilon \to 0]{} 0 , \qquad t \in [0,T)$$

 $\forall H \text{ smooth on } \Lambda_t$, where $\Upsilon(t)$ solves the Boltzmann-cluster equation:

$$\begin{cases} \int dY(t,\lambda)H(\lambda) = \int dY(0,\lambda)H(\lambda) \\ + \frac{1}{2} \int d\tau \, d\omega \, dY(\tau,\lambda) \, dY(\tau,\lambda_*) \sum_{\substack{i \in \lambda \\ j \in \lambda_*}} \left[(v_i(\tau) - v_j(\tau)) \cdot \omega \right]_+ \delta_{x_i(\tau)}(x_j(\tau)) \\ \times \left\{ H \left[[\lambda \wedge \lambda_*]^{i,j,\tau,\omega} \right] - H(\lambda) - H(\lambda_*) \right\} \\ Y|_{t=0} = f_0(x_{\rm cm}, v_1^0) \, \delta_{\ell=1}, \quad Y|_{t < t_i, \ell > 1} = 0 \end{cases}$$

where $[\lambda \wedge \lambda_*]^{i,j,\tau,\omega}$ is the merging of the clusters due to a binary collision between particles *i* and *j* at time τ with scattering angle ω .

Lemma.

Define

$$f(t,z) := \int d\Upsilon(t,\lambda) \,\ell \,\delta_z \,(z_1(t))$$

For times short enough, f solves the Boltzmann eq. with initial datum f_0 .

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Corollary.

Let

$$R(t,x,v) := \int f(t,x,v_*) \left[\omega \cdot (v-v_*) \right]_+ d\omega dv_*$$

be the free-flight time rate. For times short enough, the Boltzmann-cluster distribution is given by $(t > \max_i t_i)$

$$\Upsilon(t,\lambda) = \frac{1}{\ell!} \prod_{i=1}^{\ell} e^{-\int_0^t R(s,z_i(s))ds} f_0(z_i(0)) \prod_{e=\{\alpha,\beta\} \in E(\mathcal{T}_\ell)} \left[\omega_e \cdot \left(\nu_\alpha(t_e) - \nu_\beta(t_e) \right) \right]_+$$

 $\left(\text{ for the 2D Lorentz gas } e^{-2t} f_0(z_1(0)) \prod_{j=1}^k \left[\omega_j \cdot v_1(t_j) \right] \right)$

Toy model (Kac):

- no space dependence $[\omega \cdot (v v_*)]_+ \longrightarrow |S^2|^{-1}$

$$n(t,k) = \int d\Upsilon(t,\lambda) \, \ell \, \delta_{\ell=k} = \frac{k^{k-2}}{(k-1)!} \, t^{k-1} \, e^{-kt} \simeq \frac{\left(ete^{-t}\right)^k}{\sqrt{2\pi} t \, k^{3/2}}$$

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Hard spheres:



Fig. 5 Sizes of all clusters for a single realization of the system (logarithmic scale).



Fig. 6 Cluster size distribution before, at and after the gelation time (log-log scale). The solid lines show the power law with exponent $-\frac{5}{2}$.

3. Long time results

Long time results

Dispersing cloud in R^d. [Illner - Pulvirenti '89, Denlinger '18] Equation as in Theorem 0.

[Deng - Hani - Ma preprint]

Tracer particle. [van Beijeren - Lanford - Lebowitz - Spohn '80, Bodineau - Gallagher - Saint-Raymond '16]

 $\begin{aligned} &Q_{RB}\left(g\right)(x,v) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \left[\omega \cdot (v - v_*)\right]_+ M(v_*) \left\{g\left(x,v'\right) - g\left(x,v\right)\right\} \\ &M(v) = (2\pi)^{-3/2} \exp\left(-v^2/2\right) \end{aligned}$



Fluctuation field. [Bodineau - Gallagher - Saint-Raymond - S. '24]