

KINETIC LIMIT AND DYNAMICAL CLUSTER EXPANSION

Sergio Simonella

Sapienza University

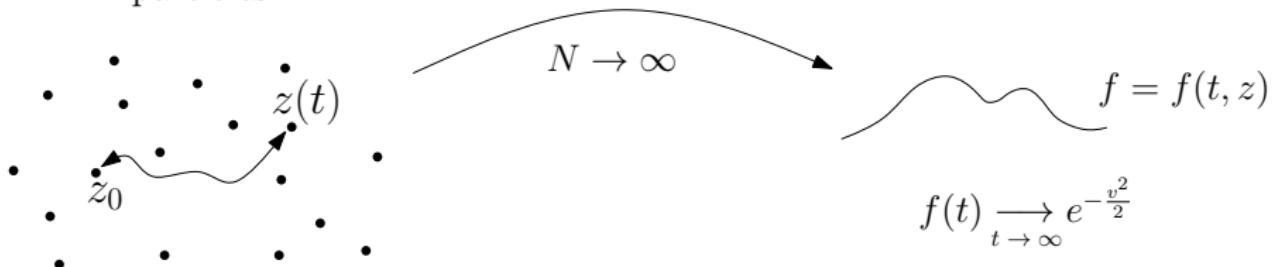
T. Bodineau (IHES), I. Gallagher (ENS), L. Saint-Raymond (IHES)

The problem of Boltzmann

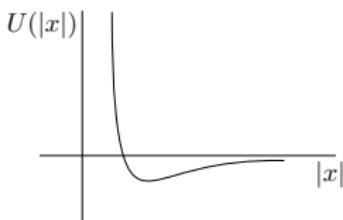
t : time

$z = (x, v)$: pos., vel.

N particles



molecular potential :



- $t = 0$: statistical assumption
- scaling limit

Microscopic dynamics

$$\mathcal{H} : (\mathbb{T}^d \times \mathbb{R}^d)^N \rightarrow \mathbb{R}, \quad N \in \mathbb{N}, \quad d \geq 2$$

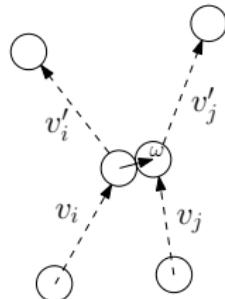
$$\mathcal{H} = \frac{1}{2} m v_1^2 + \sum_{i \geq 2} \frac{1}{2} M v_i^2 + \sum_{i < j} U_{\text{h.c.}}^\varepsilon(x_i - x_j)$$

$z_1 = (x_1, v_1)$ tracer particle, mass $m > 0$

$(z_i)_{i \geq 2} = (x_i, v_i)_{i \geq 2}$ fluid particles, mass $M > 0$

$\varepsilon > 0$: small interaction distance

$$U_{\text{h.c.}}^\varepsilon(x) = \begin{cases} \infty & |x| < \varepsilon \\ 0 & |x| \geq \varepsilon \end{cases}$$



$$(v_i, v_j) \longrightarrow (v'_i, v'_j)$$

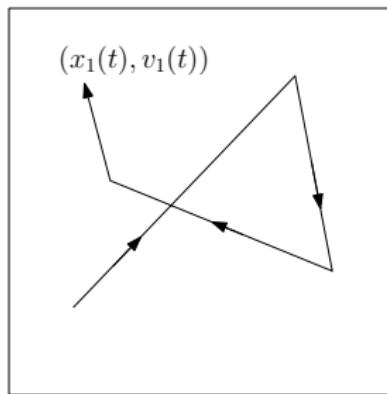
$$v'_i = v_i - \frac{2m_j}{m_i+m_j} \omega [\omega \cdot (v_i - v_j)]$$
$$v'_j = v_j + \frac{2m_i}{m_i+m_j} \omega [\omega \cdot (v_i - v_j)]$$

$$\omega = (x_j - x_i)/\varepsilon$$

$$\mathcal{H} = \frac{1}{2} m v_1^2 + \sum_{i \geq 2} \frac{1}{2} M v_i^2 + \sum_{i < j} U_{\text{h.c.}}^\varepsilon(x_i - x_j)$$

fluid density $\simeq N\varepsilon^d \ll 1$

$\varepsilon \rightarrow 0$, $N\varepsilon^{d-1} \sim 1$ (Boltzmann-Grad limit)



Problem. Given a “good” configuration

$$\frac{1}{N} \sum_i \delta_{(x_i^0, v_i^0)}(x, v) \simeq f_0(x, v)$$

is it true that $(x_i^0, v_i^0)_i \longrightarrow (x_i(t), v_i(t))_i$ “ \simeq ” $f(t)$?

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Time zero: density distributions $W_{0,n}^\varepsilon : (\mathbb{T}^d \times \mathbb{R}^d)^n \rightarrow \mathbb{R}^+$
(simple choice)

$$\frac{W_{0,n}^\varepsilon}{n!} := \frac{1}{\mathcal{Z}^\varepsilon} \frac{\mu_\varepsilon^n}{n!} f_0^{\otimes n} \prod_{i < j} \mathbf{1}_{|x_i - x_j| \geq \varepsilon}, \quad n = 0, 1, 2 \dots$$

where $f_0 \in \mathcal{P}(\mathbb{T}^d \times \mathbb{R}^d)$ (equilibrium $f_0 = M_\beta := (2\pi/\beta)^{-d/2} e^{-\beta v^2/2}$).

$$\mu_\varepsilon \simeq \mathbb{E}_\varepsilon [N] \rightarrow \infty$$

$$\mu_\varepsilon \varepsilon^d \ll 1$$

$$\mu_\varepsilon = \varepsilon^{-d+1} \quad (\text{Boltzmann-Grad limit})$$

Hard sphere gas ($m = M = 1$, f_0 smooth, $f_0 \leq \rho M_\beta$, $\rho, \beta > 0$)

Traditional method: **BBGKY**

[Lanford '75]

There exists a time $T_L > 0$ such that, in the Boltzmann-Grad limit,

$$\pi_{\text{emp}}^\varepsilon(t, z) := \frac{1}{\mu_\varepsilon} \sum_{i=1}^N \delta_{z_i(t)}(z) \longrightarrow f(t, z) , \quad z = (x, v) , \quad t \in [0, T_L)$$

weakly in probability, where f solves

$$\begin{cases} (\partial_t + v \cdot \nabla_x) f = \int_{\mathbb{R}^d} \int_{\mathbb{S}^{d-1}} [\omega \cdot (v - v_*)]_+ \{f(x, v') f(x, v'_*) - f(x, v) f(x, v_*)\} d\omega dv_* \\ f|_{t=0} = f_0 \end{cases}$$

BOLTZMANN VALIDITY [Lanford ('75)]

[Spohn, Cercignani - Illner - Pulvirenti, Cercignani - Gerasimenko - Petrina, Uchiyama, Ukai...
(more recently) Matthies - Theil (- Stone), Gapyak - Gerasimenko, Winter, Ampatzoglou - Pavlović, Dolmaire, Le Bihan...]

SMOOTH POTENTIALS [King, Gallagher - Saint-Raymond - Texier, Pulvirenti - Saffirio - S., Ayi]

FLUCTUATIONS [Spohn, Pulvirenti - S., Bodineau - Gallagher - Saint-Raymond - S.]

PERTURB. VACUUM [Illner - Pulvirenti, Denlinger]

PERTURB. EQUILIBRIA [van Beijeren - Lanford - Lebowitz - Spohn, Bodineau - Gallagher - Saint-Raymond (- S.)]

BBGKY-method

$\left(F_j^\varepsilon = F_j^\varepsilon(z_1, \dots, z_j) \right)_{j \geq 1}$ correlation functions on $(\mathbb{T}^d \times \mathbb{R}^d)^j$:

$$\mathbb{E}_\varepsilon \left[\exp \left(\pi_{\text{emp}}^\varepsilon(t, \varphi) \right) \right] = 1 + \sum_{j \geq 1} \frac{\mu_\varepsilon^j}{j!} \int F_j^\varepsilon(t) \left(e^{\mu_\varepsilon^{-1} \varphi} - 1 \right)^{\otimes j} dz_1 \cdots dz_j$$

$$\begin{cases} F_1^\varepsilon(t, z_1) := \mathbb{E}_\varepsilon \left[\mu_\varepsilon^{-1} \sum_{i=1}^N \delta_{z_i(t)}(z_1) \right] \\ F_2^\varepsilon(t, z_1, z_2) := \mathbb{E}_\varepsilon \left[\mu_\varepsilon^{-2} \sum_{i_1 \neq i_2} \delta_{z_{i_1}(t)}(z_1) \delta_{z_{i_2}(t)}(z_2) \right] \\ \dots \end{cases}$$

$$\int F_j^\varepsilon(t) dz_1 \cdots dz_j = \mu_\varepsilon^{-j} \mathbb{E}_\varepsilon [N(N-1) \cdots (N-j+1)]$$

$$D_t^{(j)} F_j^\varepsilon = \sum_{i=1}^j \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} \omega \cdot (v_{j+1} - v_i) F_{j+1}^\varepsilon(\cdot, x_i + \varepsilon \omega, v_{j+1}) d\omega dv_{j+1}$$

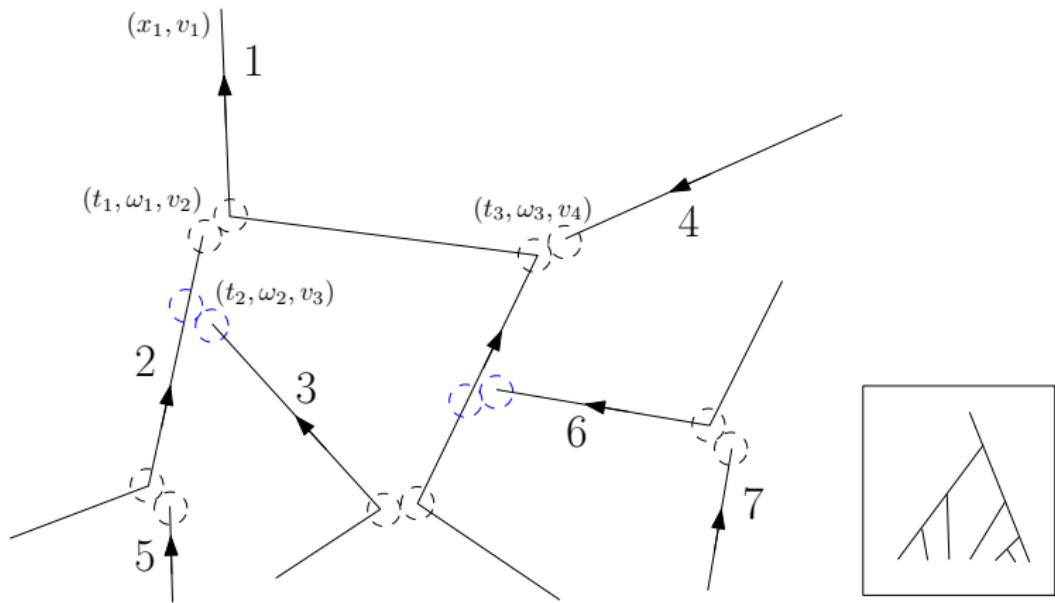
$D_t^{(j)}$ = (interacting) transport operator of j hard spheres.

Prove that $F_j^\varepsilon(t) \rightarrow f^{\otimes j}(t)$ (*chaos propagation*)

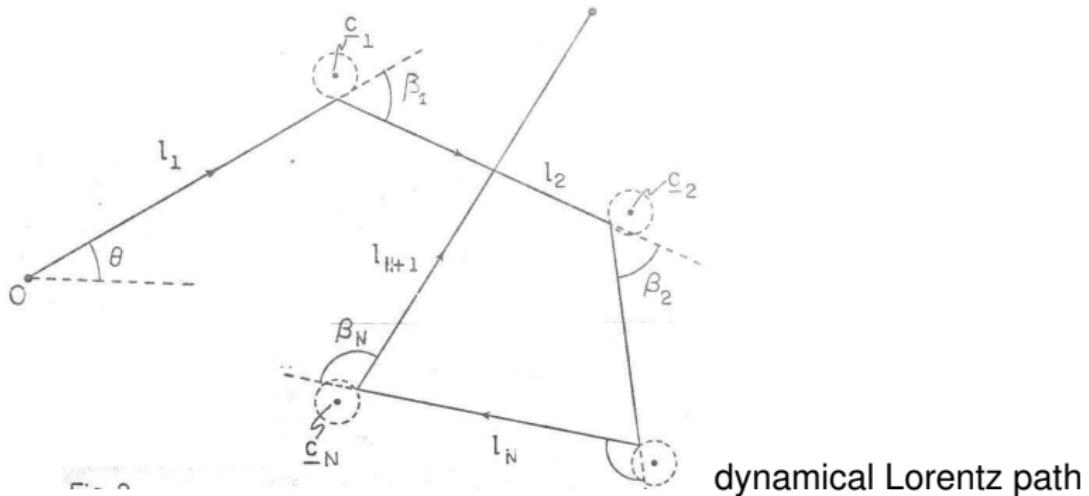
BBGKY

$$(z_1^0, \dots, z_N^0) \longrightarrow (x_1, v_1), (t_1, \omega_1, v_2), (t_2, \omega_2, v_3) \dots$$

particles \longrightarrow backward flow ("pseudo – trajectories")



Lorentz gas ($m/M = 0$)



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

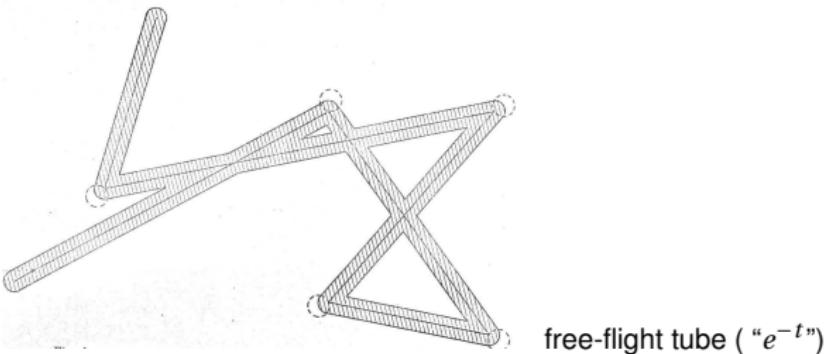
1. Parametrization of paths

$$c_1, c_2, \dots \longrightarrow l_1, \beta_1, l_2, \beta_2, \dots \quad ((x_1^0, v_1^0) \text{ fixed})$$

particles \longrightarrow trajectories

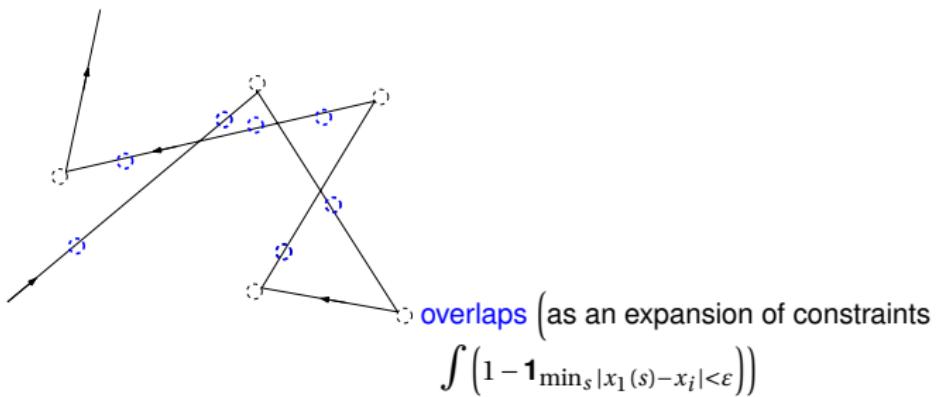
(\rightarrow coupling: linear Boltzmann process)

Lorentz gas



2. Collision rate

$$e^{-\mu_\varepsilon} \sum_{k \geq 0} \frac{\mu_\varepsilon^k}{k!} (1 - |\text{Tube}|)^k = \sum_{k \geq 0} \frac{1}{k!} (-1)^k \mu_\varepsilon^k |\text{Tube}|^k = e^{-\mu_\varepsilon |\text{Tube}|} \gtrsim e^{-\mu_\varepsilon \varepsilon t} \quad (d = 2, \text{ Poisson})$$



Hard sphere gas ($m = M = 1$)

Same plan:

- * *real* trajectories
- * *forward* in time
- * full *information* on the microscopic dynamics

$$Z_N^0 := (z_1^0, \dots, z_N^0) \rightarrow Z_N(t), \quad t \in [0, T]$$

Fix $T > 0$.

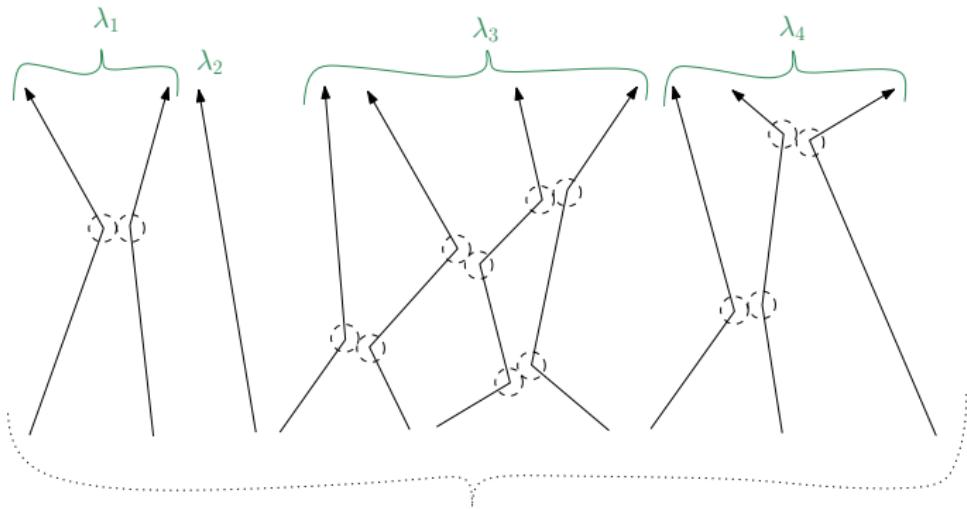
Definition.

- (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).

[Sinai '72]

$\mathcal{P}_A = \text{partitions of } A$

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



$$Z_N^0 := (z_1^0, \dots, z_N^0)$$

cluster path decomposition

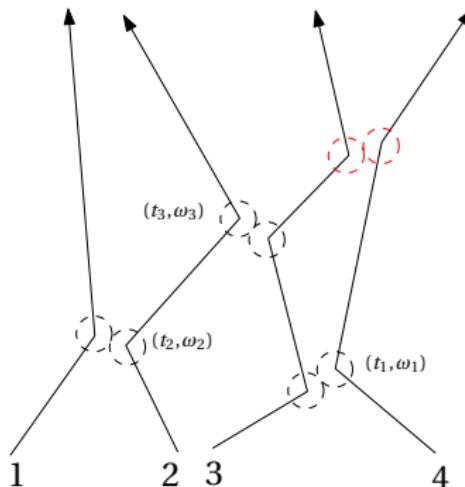
$$\pi_{\text{emp}}^\varepsilon(\lambda) := \frac{1}{\mu_\varepsilon} \sum_i \delta_{\lambda_i([0, T])}(\lambda)$$

1. Parametrization of cluster paths:

$$(z_1^0, \dots, z_\ell^0) \longrightarrow \Lambda := (\mathcal{T}_\ell, x_{\text{cm}}, V_\ell^0, t_1, \omega_1, \dots, t_{\ell-1}, \omega_{\ell-1})$$

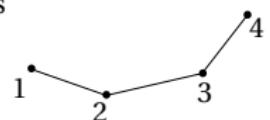
particles \longrightarrow trajectories (cluster path)

(\rightarrow coupling : Boltzmann cluster process)



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



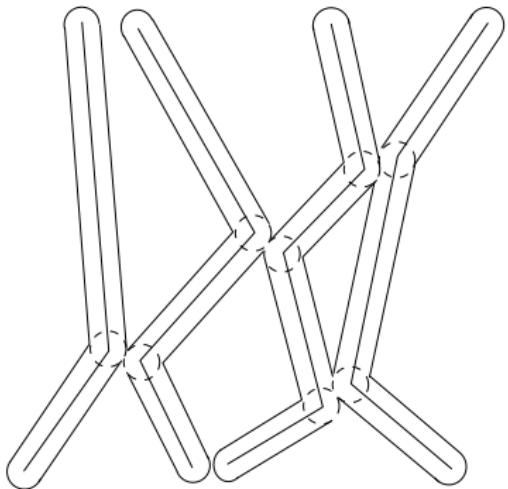
- the center of mass at time zero x_{cm}
- the collection of velocities V_ℓ^0
- impact times and angles $(t_i, \omega_i) \in [0, T] \times \mathbb{S}^{d-1}$
(ignoring **recollisions**)

$$dZ_\ell^0 = d\Lambda \mu_\varepsilon^{-(\ell-1)} \prod_{e=\{\alpha, \beta\} \in E(\mathcal{T}_\ell)} [\omega_e \cdot (v_\alpha(t_e) - v_\beta(t_e))]_+$$

$$(z_1^0, \dots, z_\ell^0) \longrightarrow \Lambda := (\mathcal{T}_\ell, x_{\text{cm}}, V_\ell^0, t_1, \omega_1, \dots, t_{\ell-1}, \omega_{\ell-1})$$

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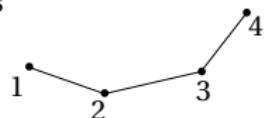
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(ignoring recollisions)

Problem 2: collision rate \longrightarrow background

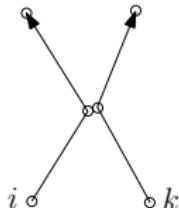
Solution: cluster expansion [Penrose, Ruelle ('63).....]

2. Collision rate

$$\mathbf{1}_{i \not\sim k} = 1 - \mathbf{1}_{i \sim k}$$

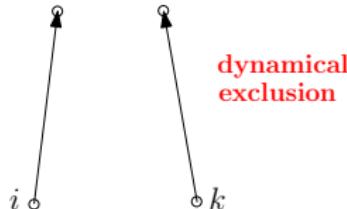
C

$“| \text{collision} | \approx O(\varepsilon^{d-1})”$



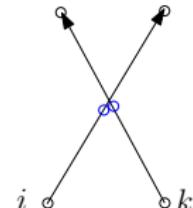
D

$“| i \not\sim k | = |\text{independence}| - O(\varepsilon^{d-1})”$



O

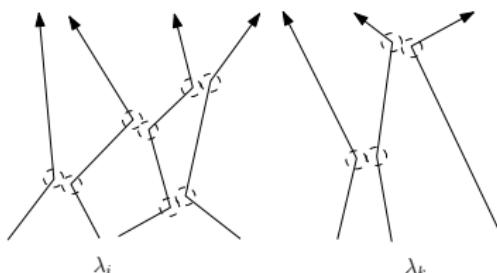
$“| i \sim k | = |\text{overlap}| = O(\varepsilon^{d-1})”$



connection (O) - disconnection (D) relation

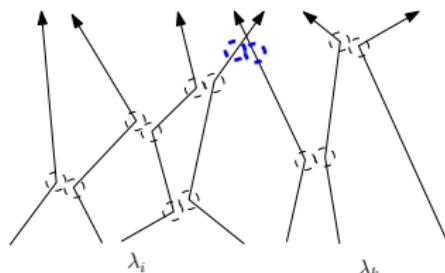
D

$$\lambda_i \not\sim \lambda_k$$



O

$$\lambda_i \sim \lambda_k$$



overlaps (as an expansion of constraints $\int (1 - \mathbf{1}_{\lambda_i \sim \lambda_k})$)

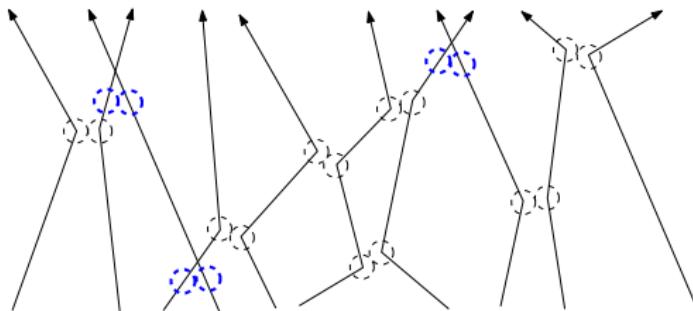
Cluster path distribution

$$\mathbb{E}_\varepsilon \left[\pi_{\text{emp}}^\varepsilon(\lambda) \right] = v(\lambda) \sum_{k \geq 0} \frac{\mu_\varepsilon^k}{k!} \int d\nu(\lambda_1) \cdots d\nu(\lambda_k) \varphi^\varepsilon(\lambda, \lambda_1, \dots, \lambda_k)$$

where

- $d\nu(\lambda) := d\Lambda \frac{1}{\ell!} f_0^{\otimes \ell} \prod_{e=\{\alpha, \beta\} \in E(\mathcal{T}_\ell)} [\omega_e \cdot (v_\alpha(t_e) - v_\beta(t_e))]_+$
- $\varphi^\varepsilon(\lambda, \lambda_1, \dots, \lambda_k) = \text{Ursell function on cluster paths}$

$$\varphi^\varepsilon(\lambda, \lambda_1, \dots, \lambda_k) \simeq (-1)^k \mathbf{1}_{\{\lambda, \lambda_1, \dots, \lambda_k\} \text{ connected under } \sim}$$



aggregates of clusters

$$\Lambda^\varepsilon(T, H) := \frac{1}{\mu_\varepsilon} \log \mathbb{E}_\varepsilon \left[e^{\mu_\varepsilon \pi_{\text{emp}}^\varepsilon(H)} \right] = \frac{1}{\mu_\varepsilon} \log \mathbb{E}_\varepsilon \left[e^{\sum_i H(\lambda_i([0, T]))} \right]$$

Notice $\mathbb{E}_\varepsilon \left[\pi_{\text{emp}}^\varepsilon(\lambda) \right] = \partial_u \Lambda^\varepsilon(T, uH) \Big|_{u=0}$. We write it as

$$\Lambda^\varepsilon(T, H) = \frac{1}{\mu_\varepsilon} \log \frac{\mathcal{Z}_T^\varepsilon(e^H)}{\mathcal{Z}^\varepsilon}$$

$$\mathcal{Z}_T^\varepsilon(e^H) := \sum_{n \geq 0} \frac{\mu_\varepsilon^n}{n!} \int d\nu(\lambda_1) \cdots d\nu(\lambda_n) e^{\sum_{i=1}^n H(\lambda_i)} \prod_{j \neq k} \mathbf{1}_{\lambda_j \succ \lambda_k}$$

Proposition. [Bodineau, Gallagher, Saint-Raymond, S. '22]

There exists a time $T > 0$ and a constant C (depending only on $f_0, \|H\|_\infty$) such that uniformly in the Boltzmann-Grad scaling ($\mu_\varepsilon = \varepsilon^{-(d-1)}$) and for $k \geq 1$

$$\int d\nu(\lambda_1) \cdots d\nu(\lambda_k) e^{\sum_{i=1}^k |H(\lambda_i)|} |\varphi^\varepsilon(\lambda_1, \dots, \lambda_k)| \leq \mu_\varepsilon^{-(k-1)} k! C^k (T + \varepsilon)^{k-1}$$

for any smooth test function H on the space of cluster paths. The cluster expansion of the partition function converges absolutely for ε small:

$$\frac{1}{\mu_\varepsilon} \log \mathcal{Z}_T^\varepsilon(e^H) = \sum_{k \geq 1} \frac{\mu_\varepsilon^{k-1}}{k!} \int d\nu(\lambda_1) \cdots d\nu(\lambda_k) e^{\sum_{i=1}^k H(\lambda_i)} \varphi^\varepsilon(\lambda_1, \dots, \lambda_k)$$

Space of limiting cluster paths:

$$\mathcal{C} := \bigcup_{\ell \in \mathbb{N}} \{\mathcal{T}_\ell\} \times \mathbb{T}^d \times \mathbb{R}^{d\ell} \times [0, T]^{\ell-1} \times \mathbb{S}^{(d-1)(\ell-1)}$$

$$\lambda \longmapsto \Lambda = \left(\mathcal{T}_\ell, x_{\text{cm}}, V_N^0, t_1, \omega_1, \dots, t_{\ell-1}, \omega_{\ell-1} \right)$$

Theorem. [Bodineau, Gallagher, Saint-Raymond, S. '22]

In the Boltzmann-Grad limit, the emp. meas. on cluster paths in $[0, t]$ converges:

$$\forall \delta > 0, \quad \mathbb{P}_\varepsilon \left(\left| \pi_{\text{emp}}^\varepsilon(H) - \int_{\mathcal{C}} dY(t, \lambda) H(\lambda) \right| > \delta \right) \xrightarrow[\varepsilon \rightarrow 0]{} 0, \quad t \in [0, T)$$

$\forall H$ smooth on \mathcal{C} , where $Y(t)$ solves the **Boltzmann-cluster equation**:

$$\begin{cases} \int dY(t, \lambda) H(\lambda) = \int dY(0, \lambda) H(\lambda) \\ \quad + \frac{1}{2} \int d\tau d\omega dY(\tau, \lambda) dY(\tau, \lambda_*) \sum_{\substack{i \in \lambda \\ j \in \lambda_*}} \left[(\nu_i(\tau) - \nu_j(\tau)) \cdot \omega \right]_+ \delta_{x_i(\tau)}(x_j(\tau)) \\ \quad \times \left\{ H([\lambda \wedge \lambda_*]^{i,j,\tau,\omega}) - H(\lambda) - H(\lambda_*) \right\} \\ Y|_{t=0} = f_0(x_{\text{cm}}, \nu_1^0) \delta_{\ell=1}, \quad Y|_{t < t_i, \ell > 1} = 0 \end{cases}$$

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

Lemma.

For times short enough,

$$f(t, z) = \int dY(t, \Lambda) \ell \delta_z(z_1(t))$$

solves the Boltzmann eq. with initial datum f_0 .

Corollary.

Let

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

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

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

(For the Lorentz gas $e^{-t} f_0(z_1(0)) \prod_{j=1}^k [\omega_j \cdot v_1(t_j)]_+$)

Toy model (Kac):

- no space dependence
- $[\omega \cdot (\nu - \nu_*)]_+ \longrightarrow |\mathbb{S}^{d-1}|^{-1}$

$$n(t, k) := \int dY(t, \Lambda) \ell \delta_{\ell=k} = \frac{k^{k-2}}{(k-1)!} t^{k-1} e^{-kt} \simeq \frac{(ete^{-t})^k}{\sqrt{2\pi} t k^{3/2}}$$

Hard spheres:

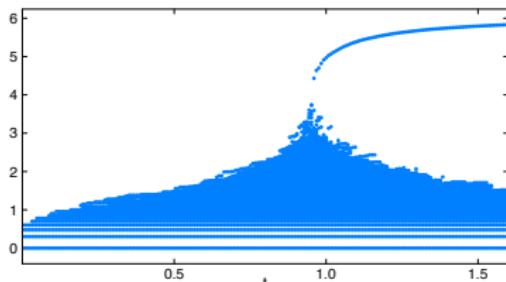


Fig. 5 Sizes of all clusters for a single realization of the system (logarithmic scale).

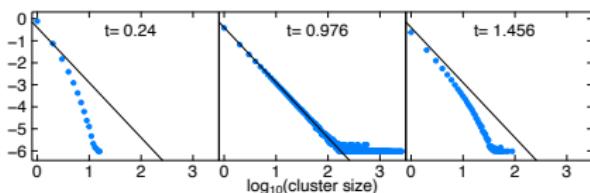


Fig. 6 Cluster size distribution before, at and after the gelation time (log-log scale). The solid lines show the power law with exponent $-\frac{5}{2}$.

Atypical paths

Proposition. [Bodineau et al]

The limiting functional

$$I(t) := \lim_{\varepsilon \rightarrow 0} \mu_\varepsilon^{-1} \log \mathbb{E}_\varepsilon \left[\gamma^{\otimes N}(z_1(t), \dots, z_N(t)) \exp \left(- \sum_{i=1}^N \int_0^t g(s, z_i(s)) ds \right) \right]$$

is the solution of the [Hamilton-Jacobi](#) equation

$$\partial_t I = \frac{1}{2} \int \frac{\partial I}{\partial \gamma}(z_1) \frac{\partial I}{\partial \gamma}(z_2) (\gamma(z'_1)\gamma(z'_2) - \gamma(z_1)\gamma(z_2)) d\mu(z_1, z_2, \omega)$$

in the space

$$\begin{aligned} \mathcal{A} := & \left\{ (g, \gamma) \in C^0([0, T] \times \mathbb{T}^d \times \mathbb{R}^d; \mathbb{C}) \times C^0(\mathbb{T}^d \times \mathbb{R}^d; \mathbb{C}) \mid \right. \\ & \left. |\gamma(z)| \leq e^{\frac{1}{2}(\alpha + \frac{\beta}{4}|v|^2)}, \quad \sup_{s \in [0, T]} |g(s, z)| \leq \frac{1}{2T} \left(\alpha + \frac{\beta}{4}|v|^2 \right) \right\}. \end{aligned}$$

Theorem 2. (a) [Bodineau et al]

The fluctuation field $(\zeta_t^\varepsilon)_{t \in [0, T]}$ converges in law to the Gaussian process $(\zeta_t)_{t \in [0, T]}$ solving

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

where:

$$\mathcal{L}_t(g) := -v \cdot \nabla_x g + Q(f, g) + Q(g, f)$$

and η_t is Gaussian noise with zero mean and covariance

$$\mathbb{E} \left[\int dt dz_1 \varphi(z_1) \eta_t(z_1) \int ds dz_2 \psi(z_2) \eta_s(z_2) \right] = \frac{1}{2} \int dt d\mu f(t, z_1) f(t, z_2) \Delta\varphi \Delta\psi$$

$$d\mu = d\mu(z_1, z_2, \omega) = \delta(x_1 - x_2) (\omega \cdot (v_1 - v_2))_+ dz_1 dz_2 d\omega,$$

$$\Delta\varphi(z_1, z_2, \omega) := \varphi(x_1, v'_1) + \varphi(x_2, v'_2) - \varphi(z_1) - \varphi(z_2).$$

(central limit theorem)

The “fluctuating Boltzmann equation” from [Ernst - Cohen ('81); Spohn ('81)].

Theorem 2. (b) [Bodineau et al]

Moreover $\exists \mathcal{J}_T$ s. t. the empirical measure satisfies:

(i) for closed sets \mathbf{C} of the Skorokhod space $D([0, T], \mathcal{M})$

$$\limsup_{\varepsilon \rightarrow 0} \mu_\varepsilon^{-1} \log \mathbb{P}_\varepsilon(\mathbf{C}) \leq - \inf_{g \in \mathbf{C}} \mathcal{J}_T(g),$$

(ii) for open sets \mathbf{O} of the Skorokhod space $D([0, T], \mathcal{M})$

$$\liminf_{\varepsilon \rightarrow 0} \mu_\varepsilon^{-1} \log \mathbb{P}_\varepsilon(\mathbf{O}) \geq - \inf_{g \in \mathbf{O} \cap \mathbf{R}} \mathcal{J}_T(g),$$

for a nontrivial subset \mathbf{R} of $D([0, T], \mathcal{M})$,
and

$$\mathcal{J}_T(g) = \sup_p \left\{ \int_0^T dt \left[\int p(t) (\partial_t + \nu \cdot \nabla_x) g(t) - \mathcal{H}(g(t), p(t)) \right] \right\}$$

with

$$\mathcal{H}(g, p) := \frac{1}{2} \int g(z_1) g(z_2) (e^{\Delta p} - 1) d\mu(z_1, z_2, \omega).$$

Same of : [Rezakhanlou ('98), Basile - Benedetto - Bertini ('20,'21), Bouchet ('20,'21)]

Gradient flow? [Adams - Dirr - Peletier - Zimmer ('11), Mielke - Peletier - Renger ('14),
Peletier - Rossi - Savaré - Tse ('20)]

Related open problems

- * Beyond critical time
(cluster structures, Hamilton-Jacobi, large deviations)
- * Dynamical phase transition [Patterson, Wagner, Heydecker]
- * Theory of dense gases [Winter]
- * Boundary conditions [Dolmaire, Le Bihan]
- * Stationary solutions