Large scale limits of particle systems: kinetic theory and applications

Inhomogeneous Random Systems

Institut Henri Poincaré
January 23, 2024

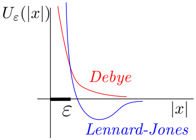
Foundations of kinetic theory: recent progress and open directions

Kinetic Limit

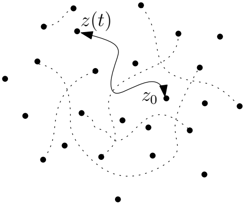
t : time

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

U : molecular potential



N particles (Newton's laws)



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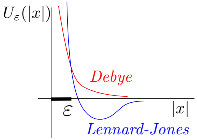

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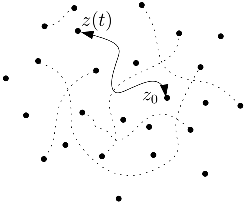


$$f = f(t,z)$$

$$f(t) \underset{t \to \infty}{\longrightarrow} e^{-\frac{v^2}{2}}$$

$$N \longrightarrow \infty$$

chaos propagation

$$\varepsilon \longrightarrow 0$$

$$(\partial_t + v \cdot \nabla_x)\, f \;+\; \underbrace{F(x) \cdot \nabla_v f}_{\text{long-range mean-field}} \;=\; \underbrace{\mathcal{Q}(f,f)}_{\textit{Collisions}}$$

Collisions

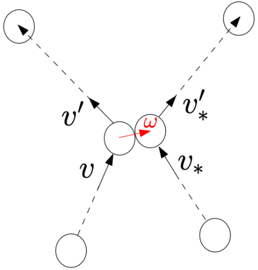
$$\mathcal{Q}_B(f,f)(z) = \int B(v - v_*, \omega)\, [f' f'_* - f f_*]$$

Boltzmann (gas dynamics)

$$\mathcal{Q}_L(f,f)(z) = \nabla_v \int a(v - v_*)\, [f_* \nabla f - f \nabla f_*]$$

Landau (plasma physics)

Hard-Sphere Boltzmann Eq.



$$(v, v_*) \longrightarrow (v', v'_*)$$

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

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

$$f = f(t,x,v) \qquad (x,v) \in \mathbb{T}^d \times \mathbb{R}^d \qquad d \geq 2$$

$$(\partial_t + v \cdot \nabla_x) f = Q(f,f)$$

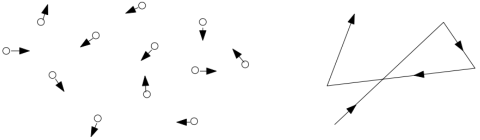
$$Q(f,f)(x,v) = \int_{\mathbb{R}^d} \int_{\mathbb{S}^{d-1}} \left[\omega \cdot (v - v_*)\right]_+ \left\{ f(x,v') f(x,v'_*) - f(x,v) f(x,v_*) \right\} d\omega \, dv_*$$

$$f|_{t=0} = f_0$$

Microscopic H-S system

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

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



SCALING

N = number of spheres ; ε = sphere diameter

rate of coll. $\simeq \mathbb{E}_\varepsilon[N]\varepsilon^{d-1} \to 1$; 'volume' density $\simeq \mathbb{E}_\varepsilon[N]\varepsilon^d \sim \varepsilon$

$\varepsilon \to 0$: low density limit (Boltzmann-Grad limit)

Time zero: density distributions $W^{\varepsilon}_{0,n} : \left(\mathbb{T}^d \times \mathbb{R}^d\right)^n \to \mathbb{R}^+$
(simple choice)

$$\frac{W^{\varepsilon}_{0,n}}{n!} := \frac{1}{\mathcal{Z}^{\varepsilon}} \frac{\mu_{\varepsilon}^{n}}{n!} f_0^{\otimes n} \qquad \text{in} \qquad \Omega^{\varepsilon}_{n}\,, \qquad n = 0, 1, 2 \cdots$$

where $f_0 \in \mathscr{P}(\mathbb{T}^d \times \mathbb{R}^d)$.

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

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

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

HS-BBGKY hierarchy

$\pi^\varepsilon_{\rm emp}(t,\varphi) := \frac{1}{\mu_\varepsilon} \sum_{i=1}^N \varphi(z_i(t))$

$\left(F^\varepsilon_j = F^\varepsilon_j(z_1,\cdots,z_j)\right)_{j\geq 1}$ *correlation functions* on $(\mathbb{T}^d \times \mathbb{R}^d)^j$:

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

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$$\begin{cases} F^\varepsilon_1(t,z_1) := \mathbb{E}_\varepsilon[\mu_\varepsilon^{-1} \sum_{i=1}^N \delta_{z_i(t)}(z_1)] \\ F^\varepsilon_2(t,z_1,z_2) := \mathbb{E}_\varepsilon[\mu_\varepsilon^{-2} \sum_{i_1\neq i_2} \delta_{z_{i_1}(t)}(z_1)\,\delta_{z_{i_2}(t)}(z_2)] \\ \dots \end{cases} ,$$

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

HS-BBGKY hierarchy

$$\pi^{\varepsilon}_{\mathrm{emp}}(t,\varphi) := \frac{1}{\mu_\varepsilon} \sum_{i=1}^{N} \varphi(z_i(t))$$

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

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

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

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

+ b.c. on $\partial\Omega_j^\varepsilon$, $\qquad j = 1,2,\cdots$

Theorem 0. [Lanford (*Lect. Notes Phys.* '75)] (d = 3)

Assume $f_0 \in \mathscr{P}(\mathbb{T}^3 \times \mathbb{R}^3)$, $|f_0| + |\nabla_x f_0| < e^{\alpha - \beta v^2}$, $\alpha \in \mathbb{R}, \beta > 0$.

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

$$\pi^{\varepsilon}_{\mathrm{emp}}(t,\varphi) \longrightarrow \int_{\mathbb{T}^3 \times \mathbb{R}^3} f(t)\varphi$$

$\forall t \in [0, 2T)$ *and* $\varphi \in C^0_b\left(\mathbb{T}^3 \times \mathbb{R}^3\right)$. **(law of large numbers)**

After Lanford

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

LEFT OPEN.

1. Potentials
   [King, Gallagher - Saint-Raymond - Texier, Pulvirenti - Saffirio - S., Ayi]
2. Fluctuations
3. Long times

Fluctuations

Fluctuations

SMALL. * Linearize $Q\big(f,f\big)(x,v) = \iint [\omega \cdot (v - v_*)]_+ \big\{f' f'_* - f f_*\big\}$
as $f \to f + g \rightsquigarrow \mathscr{L}_t$

* Microscopic *fluctuation field*

$$\zeta_t^\varepsilon(\varphi) := \sqrt{\mu_\varepsilon}\Big(\pi^\varepsilon_{\mathrm{emp}}(t,\varphi) - \mathbb{E}_\varepsilon\Big[\pi^\varepsilon_{\mathrm{emp}}(t,\varphi)\Big]\Big)$$

* Conjectured limit: *fluctuating Boltzmann Eq.*
[Ernst - Cohen ('81), Spohn ('81,'83)]

"$d\zeta_t = \mathscr{L}_t(\zeta_t)\, dt + d\eta_t$"

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LARGE.

* Probability of atypical paths:
  $\mathbb{P}_\varepsilon\left[\pi^\varepsilon_{\mathrm{emp}}(t,\varphi) \simeq \int g(t)\varphi \text{ for } t \in [0,T)\right]$

* Conjectured limit: *large deviations functional*
  [Rezakhanlou ('98), Bouchet ('20), Basile et al ('21), Heydecker ('23)]

  "$\mathbb{P}_\varepsilon \sim e^{-\mu_\varepsilon \mathscr{I}_T(g)}$"

Theorem 1.a [Bodineau, Gallagher, Saint-Raymond, S. (*JSP*'20, *Ann.Math.*'23)]

In the assumptions of Theorem 0, the fluctuation field $\left(\zeta_t^\varepsilon\right)_{t\in[0,T)}$ *converges in law to the Gaussian process* $(\zeta_t)_{t\in[0,T)}$ *solving*

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

where:

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

and η_t *is Gaussian noise with zero mean and covariance*

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

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

$$\Delta\varphi(z_1,z_2,\omega) := \varphi(x_1,v_1') + \varphi(x_2,v_2') - \varphi(z_1) - \varphi(z_2)\,.$$

(central limit theorem)

Theorem 1.b [Bodineau, Gallagher, Saint-Raymond, S. (*JSP*'20, *Ann.Math.*'23)]

Moreover $\exists \mathscr{I}_T$ *s.t. the empirical measure satisfies:*

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

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

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

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

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

$$\mathscr{I}_T(g) = \sup_p \Big\{ \int_0^T dt \Big[\int p(t)(\partial_t + v\cdot\nabla_x) g(t) - \mathscr{H}(g(t),p(t)) \Big] \Big\}$$

with

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

Tools

① Liouville equation

$\left(W_n^\varepsilon\right)_{n\geq 0}$

$\Updownarrow$

② BBGKY hierarchy

$\left(F_j^\varepsilon\right)_{j\geq 1}$ (used by Lanford)

$\Updownarrow$

③ Cumulant hierarchy

$\left(f_j^\varepsilon\right)_{j\geq 1}$ (written by Ernst & Cohen)

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

* *capturing information on correlations*
* *concentrated on singular collision sets*

$$I_\varepsilon(t) := \frac{1}{\mu_\varepsilon} \log \, \mathbb{E}_\varepsilon \left[\exp\Big(\mu_\varepsilon \pi^\varepsilon_{\text{emp}}(t,\varphi) \Big) \right]$$

Formally:

$$\begin{aligned} \partial_t I_\varepsilon \quad = \quad & \int \big(\partial_\varphi I_\varepsilon\big)\, v \cdot \nabla_x \varphi \, dz \\ & + \frac{1}{2} \int \big(\partial_\varphi I_\varepsilon\big)^{\otimes 2} \big(e^{\Delta\varphi} - 1\big)\; \delta(x_1 - x_2 + \varepsilon\omega)(\omega \cdot (v_1 - v_2))_+ \, dz_1 \, dz_2 \, d\omega \\ & + \frac{1}{2\mu_\varepsilon} \int \Big(\partial^2_{\varphi^2} I_\varepsilon\Big) \big(e^{\Delta\varphi} - 1\big)\; dz \end{aligned}$$

Proposition. [Bodineau et al]

The functional $I(t) := \lim_{\varepsilon\to 0} I_\varepsilon(t)$ is the solution of the limiting Hamilton-Jacobi equation in a space of regular profiles.

Long times

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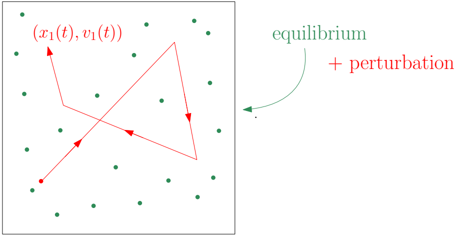
$$Q_{RB}\left(g\right)(x,v) = \int_{\mathbb{R}^3}\int_{\mathbb{S}^2}\left[\omega\cdot(v-v_*)\right]_+ M\left(v_*\right)\left\{g\left(x,v'\right) - g\left(x,v\right)\right\}$$

$$M(v) = (2\pi)^{-3/2}\exp\left(-v^2/2\right)$$



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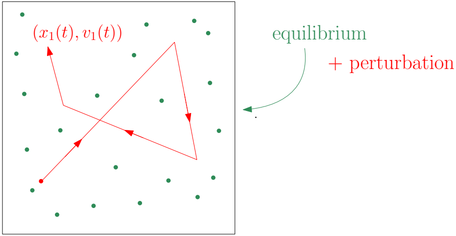

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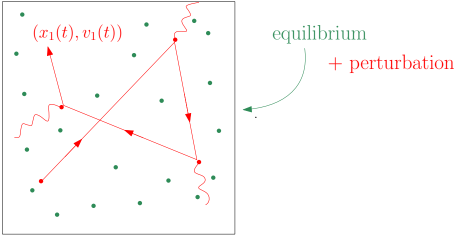

3. **Fluctuation field...**

Theorem 2.a [Bodineau et al (*CPAM*'23, *Ann.Prob.*'24)]

Start from the grand canonical Gibbs measure for hard spheres of diameter ε. Then in the Boltzmann-Grad limit, the fluctuation field $\left(\zeta_t^\varepsilon\right)_{t\in\mathbb{R}^+}$ converges in law to the Ornstein-Uhlenbeck process

$$d\zeta_t = \mathscr{L}_{\text{eq}}(\zeta_t)\,dt + d\eta_t$$

where

$$\mathscr{L}_{\text{eq}}\left(g\right) := -v\cdot\nabla_x g + L_{\text{eq}}\left(g\right) ,$$

$$L_{\text{eq}}(g)(x,v) := \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} [\omega\cdot(v-v_*)]_+ M(v_*)\,\Delta g(x,v,x,v_*,\omega)\,d\omega\,dv_*$$

and η_t as before with $f(t,x,v)$ replaced by $M(v)$.

[Covariance previously for $d=2$: Bodineau - Gallagher - Saint-Raymond ('17)]

Theorem 2.b [Bodineau et al (*Ann.H.Poincaré* '23)]

Assume

$$\mathbb{E}_\varepsilon^{\mathrm{eq}}[N]\,\varepsilon^2 = \alpha_\varepsilon^{-1} = O(\ln\ln\ln\varepsilon^{-1})\,, \quad \alpha_\varepsilon \to 0\,.$$

Then $\forall(\varphi,\psi) \in C^\infty(\mathbb{T}^3;\mathbb{R}^3\times\mathbb{R}),\ \nabla_x\cdot\varphi = 0,$

$$\zeta^\varepsilon_{t/\alpha_\varepsilon}\big(\varphi\cdot v\big) + \zeta^\varepsilon_{t/\alpha_\varepsilon}\Big(\psi\big(\frac{v^2}{5}-1\big)\Big) \Rightarrow \mathscr{U}_t(\varphi) + \Theta_t(\psi)$$

where

$$\begin{cases} \partial_\tau\mathscr{U} = \nu\Delta\mathscr{U} + \sqrt{2\nu}\,P\,\nabla\cdot\dot{\mathbb{W}}_t \\ \partial_\tau\Theta = \kappa\Delta\Theta + \sqrt{2\kappa}\,\nabla\cdot\dot{W}_t\,, \end{cases}$$

with $\nu,\kappa > 0$, $\mathbb{W}_t, W_t$ *white noises,* P *Leray projection.*

(**Fluctuating hydrodynamics** of the perfect gas)

Open Problems

* Nonlinear perturbations

* Homogeneous solutions

* NESS

* Density corrections

* Singular limits for stochastic dynamics (Bird's model)

* Power law interactions

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THANK YOU !