

VALIDITY OF THE BOLTZMANN EQUATION BEYOND HARD SPHERES

based on joint work with M. Pulvirenti and C. Saffirio

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OUTLINE

1. INTRODUCTION
2. HIERARCHIES
3. SMOOTH POTENTIALS
4. RESULT

1. INTRODUCTION. THE VALIDITY PROBLEM

Many-body classical system: $i = 1, \dots, N$, $z_i = (x_i, v_i) \in \mathbb{R}^3 \times \mathbb{R}^3$, $\varphi: \mathbb{R}^3 \rightarrow \mathbb{R}$

$$N = 10^{20}$$

$$\begin{cases} \dot{x}_i = v_i \\ \dot{v}_i = - \sum_{j:j \neq i} \nabla \varphi(x_i - x_j) \\ z_i(0) = z_{i,0} \end{cases} \quad (*)$$

$\longleftarrow (z_{i,0})_{i=1}^N$ random variable on $((\mathbb{R}^3 \times \mathbb{R}^3)^N, \mu_0^N)$

\Rightarrow KINETIC THEORY: $f \in \mathcal{P}(\mathbb{R}^3 \times \mathbb{R}^3)$

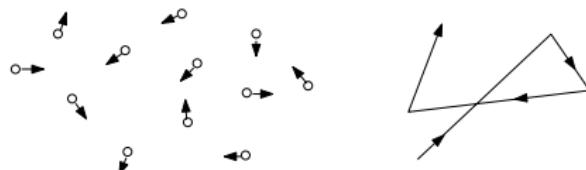
$$\partial_t f + v \cdot \nabla_x f = Q(f, f).$$

Chaos: $f_1^N(t), f_2^N(t)$ first and second marginal of $(*)$:

$$\partial_t f_1^N + v \cdot \nabla_x f_1^N = Q^N(f_2^N) \quad f_2^N \rightarrow f_1^N f_1^N ?$$

- Mean-field (Vlasov)
- Collisions (Boltzmann)

1. FROM NEWTON...



Low density gas

$N = \text{number of particles} ; \quad \varepsilon = \text{collision length}$
 $\text{rate of coll.} \simeq N\varepsilon^2 = 1 ; \quad \text{'volume' density} \simeq N\varepsilon^3 = \varepsilon$
 $\varepsilon \rightarrow 0 \quad : \quad \text{low density limit} \quad (\text{Boltzmann-Grad limit})$

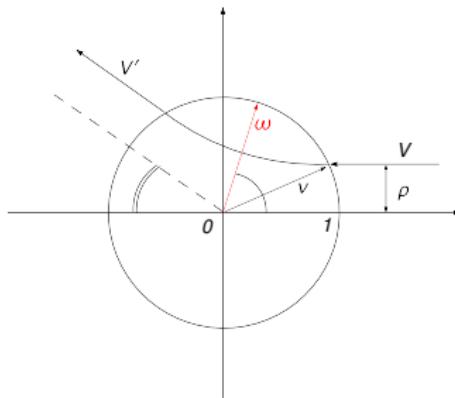
$$i = 1, \dots, N, \quad (x_i, v_i) \in \mathbb{R}^3 \times \mathbb{R}^3, \quad \varphi : \mathbb{R}^3 \rightarrow \mathbb{R}$$

$$\begin{cases} \dot{x}_i = v_i \\ \dot{v}_i = -\frac{1}{\varepsilon} \sum_{j:j \neq i} \nabla \varphi \left(\frac{x_i - x_j}{\varepsilon} \right) \\ (x_i, v_i)(0) = z_{i,0} \end{cases}$$

1. ...TO BOLTZMANN

Grad's conjecture : the first marginal $f_1^N(t) \rightarrow f(t)$ as $\varepsilon \rightarrow 0$

$$(\partial_t + v \cdot \nabla_x) f(x, v, t) = \int_{\mathbb{R}^3} dv_1 \int_{S^2} d\omega B(\omega, V) \\ \times \left\{ f(x, v'_1, t) f(x, v', t) - f(x, v_1, t) f(x, v, t) \right\}$$



$$\begin{cases} v' = v - \omega[\omega \cdot (v - v_1)] \\ v'_1 = v_1 + \omega[\omega \cdot (v - v_1)] \end{cases}$$

$$V = v_1 - v, \quad V' = v'_1 - v'$$

$B(\omega, V)/|V|$ = differential cross-section

$f(x, v, t) dx dv$ = probability of finding a particle in position x with velocity v ,
at time t .

1. VALIDITY THEOREM (1)

Setting

\mathcal{M}_N canonical phase space of N hard spheres in \mathbb{R}^3 (diameter ε)

$$\mathcal{M}_N = \left\{ \underline{z}_N = (z_1, \dots, z_N), z_i = (x_i, v_i) \in \mathbb{R}^3 \times \mathbb{R}^3, |x_i - x_j| > \varepsilon \text{ for } i \neq j \right\}$$

$\underline{z}_N \longrightarrow \underline{z}_N(t)$ = hard-sphere flow (a.e.-defined)

Initial distribution μ_0^N : symmetric density f_0^N s.t.:

- N particles “almost i.i.d.”
- prob. density $f_0 \in \mathcal{P}(\mathbb{R}^3 \times \mathbb{R}^3)$
- $N\varepsilon^2 = 1$
- uniform bounds

Example: “Minimally correlated state”

$$f_0^N := \frac{1}{\mathcal{Z}_N} f_0^{\otimes N}, \quad \|f_0 e^{\mu + \beta(v^2/2)}\|_{L^\infty} < +\infty \quad \mu, \beta > 0, \quad \mathcal{Z}_N = \int d\underline{z}_N f_0^{\otimes N}$$

1. VALIDITY THEOREM (2)

Observables

g_1, g_2, \dots test functions over $\mathbb{R}^3 \times \mathbb{R}^3$, F_1, F_2, \dots observables over \mathcal{M}_N

$F_i(t)(z_1, \dots, z_N) := \varepsilon^2 \sum_{j=1}^N g_i(z_j(t))$ (e.g. number of particles in a cell)

LLN: $F_i(t) \rightarrow \int g_i f(t)$ in the BG limit (*local Poisson*)

Theorem. There exists $t_0 > 0$ such that, if $t \in [0, t_0]$, $j = 1, 2, \dots$

$$\left| \mathbb{E} \left[\prod_{i=1}^j \left(F_i(t) - \int g_i f(t) \right) \right] \right| \longrightarrow 0 \quad \text{as } \varepsilon \rightarrow 0.$$

OP:

- ① $t_0 \rightarrow 2t_0$
- ② $\varphi(x) \sim x^{-k}$, $k > 0$

1. SOME REFERENCES

SHORT TIME, HARD SPHERES [Lanford ('75)

See also: King, Spohn, Illner, Pulvirenti, Uchiyama, Ukai ...]

PERTURBATION OF VACUUM. [Illner, Pulvirenti ('86)]

PERTURBATION OF EQUILIBRIUM. [van Beijeren, Lanford, Lebowitz, Spohn ('80),
Bodineau, Gallagher, Saint-Raymond ('16,'17)]

$M_{N,\beta}$ = Gibbs state (N hard spheres, inv.temp. β)

(i) $M_{N,\beta}(z_1, \dots, z_N) h_0(z_1) \rightarrow$ linear BE (\rightarrow Brownian motion)

(ii) $M_{N,\beta}(z_1, \dots, z_N) \prod_{i=1}^N \left(1 + \frac{1}{N} h_0(z_i)\right) \rightarrow$ linearized BE

QUANTITATIVE CHAOS FAR FROM EQUILIBRIUM. [Pulvirenti, S. ('17)]

2. HIERARCHIES. THE GENERAL STRATEGY

Newton equation \longleftrightarrow Liouville equation

kinetic equation \longleftrightarrow kinetic hierarchy

$$\begin{cases} (\partial_t + \nu \cdot \nabla_x) f = Q(f, f) \\ f(0) = f_0 \in \mathcal{P}(\mathbb{R}^3 \times \mathbb{R}^3) \end{cases} \quad f_0 \longrightarrow f(t) = \mathcal{T}_t f_0$$

$$\pi_0 \in \mathcal{P}(\mathcal{P}(\mathbb{R}^3 \times \mathbb{R}^3)) \quad \pi(t, f) := \pi_0(\mathcal{T}_{-t} f) \quad \text{'Statistical solution'}$$

Moments: $f_j(t) := \int_{\mathcal{P}(\mathbb{R}^6)} f^{\otimes j} d\pi(t, f) = \int_{\mathcal{P}(\mathbb{R}^6)} (\mathcal{T}_t f)^{\otimes j} d\pi_0(f), \quad j = 1, 2, \dots$

$$\Rightarrow (\partial_t + \sum_{i=1}^j \nu_i \cdot \nabla_{x_i}) f_j = \mathcal{C}_{j+1}(f_{j+1}) \quad \text{Boltzmann hierarchy}$$

$$\mathcal{C}_{j+1}(f_{j+1}) = \sum_{i=1}^j Q|_{i,j+1}(f_{j+1})$$

2. KINETIC HIERARCHY

$$\Rightarrow (\partial_t + \sum_{i=1}^j v_i \cdot \nabla_{x_i}) f_j = \mathcal{C}_{j+1}(f_{j+1}) \quad \text{Boltzmann hierarchy}$$

$$\begin{aligned} \mathcal{C}_{j+1}(f_{j+1}) &= \sum_{i=1}^j Q|_{i,j+1}(f_{j+1}) \\ &= \sum_{k=1}^j \int d\omega d\nu_{j+1} B(\omega, \nu_k - \nu_{j+1}) \left[f_{j+1}(\cdots x_k, \nu'_k, \cdots, x_k, \nu'_{j+1}) - f_{j+1}(\cdots x_k, \nu_k, \cdots, x_k, \nu_{j+1}) \right] \end{aligned}$$

Uniqueness: Spohn ('84)

Remark. For any $(f_j)_{j \geq 1}$, $f_j = f_j(z_1, \dots, z_j) \in \mathcal{P}(\mathbb{R}^{6j})$ (i) symmetric and (ii) compatible ($\int d\mu f_{j+1}(z_{j+1}) = f_j$), $\exists!$ Borel π on $\mathcal{P}(\mathbb{R}^6)$ s.t. $f_j = \int_{\mathcal{P}(\mathbb{R}^6)} f^{\otimes j} d\pi(f)$

Propagation of chaos: $\pi_0 = \delta_{f_0} \Rightarrow \pi(t) = \delta_{f(t)}$

2. PARTICLE HIERARCHY

N particles, Hamiltonian H_N

$$\text{Prob. density } f^N \in \mathcal{P}((\mathbb{R}^3 \times \mathbb{R}^3)^N) \quad \partial_t f^N = \{H_N, f^N\} \quad f^N(0) = f_0^N$$

$$\text{Marginals: } f_j^N := \int_{\mathbb{R}^{6(N-j)}} f^N dz_{j+1} \cdots dz_N, \quad j = 1, 2, \dots$$

$$\Rightarrow \left(\partial_t + \sum_{i=1}^j v_i \cdot \nabla_{x_i} - \frac{1}{\varepsilon} \sum_{i,k=1}^j \nabla \varphi \left(\frac{x_i - x_k}{\varepsilon} \right) \cdot \nabla v_i \right) f_j^N = \mathcal{C}_{j+1}^N(f_{j+1}^N) \quad \text{BBGKY}$$

$$\mathcal{C}_{j+1}^N(f_{j+1}^N) = \frac{N-j}{\varepsilon} \sum_{i=1}^j \int_{\mathbb{R}^6} \nabla \varphi \left(\frac{x_i - x_k}{\varepsilon} \right) \cdot \nabla v_i f_{j+1}^N dx_{j+1} dv_{j+1}$$

Uniform bounds for $(f_j^N)_{1 \leq j \leq N}$: Lanford, King ('75)

2. CONVERGENCE

Particle chaos: $f_j^N \rightarrow f_j$ as $N \rightarrow \infty$

$$\left(f_{0,j}^N \rightarrow f_0^{\otimes j} \Rightarrow f_j^N(t) \rightarrow f(t)^{\otimes j} \right)$$

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Remark: Formal comparison BBGKY

$$\begin{aligned} & \left(\partial_t + \sum_{i=1}^j v_i \cdot \nabla_{x_i} - \frac{1}{\varepsilon} \sum_{\substack{i,k=1 \\ i \neq k}}^j \nabla \varphi \left(\frac{x_i - x_k}{\varepsilon} \right) \cdot \nabla_{v_i} \right) f_j^N \\ &= \frac{N-j}{\varepsilon} \sum_{i=1}^j \int dx_{j+1} \int dv_{j+1} \nabla \varphi \left(\frac{x_i - x_{j+1}}{\varepsilon} \right) \cdot \nabla_{v_i} f_{j+1}^N. \end{aligned}$$

vs. Boltzmann hierarchy ? not so enlightening...

2. CONVERGENCE

... unless for hard spheres (Cercignani '72):

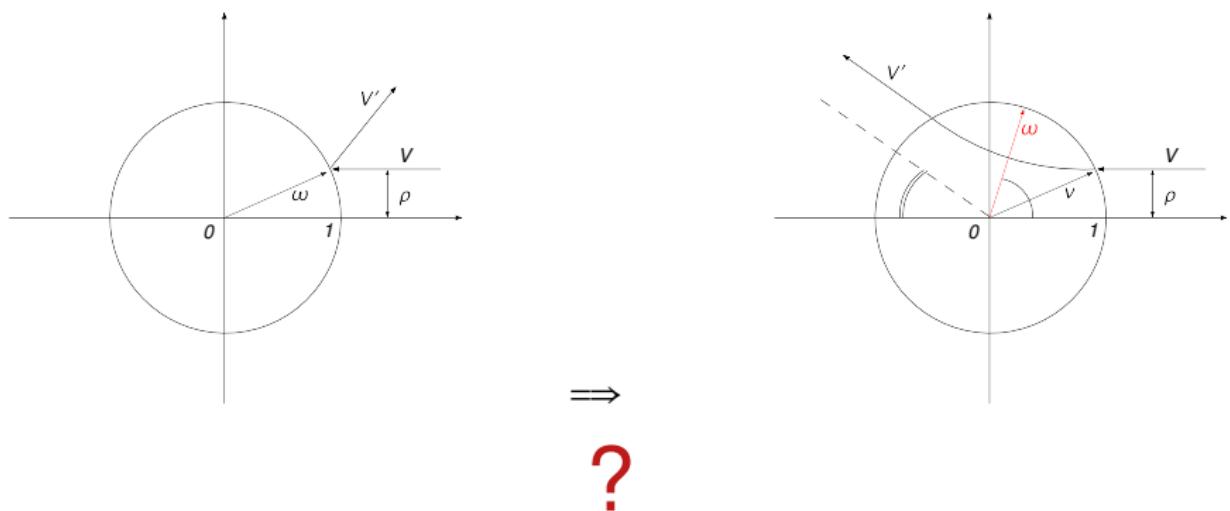
$$(\partial_t + v \cdot \nabla_x) f_1^N(x, v, t) = (N-1) \varepsilon^2 \int_{\mathbb{R}^3} d\nu_1 \int_{S^2} d\omega B(\omega, V) \\ \times \left\{ f_2^N(x - \varepsilon\omega, v'_1, x, v', t) - f_2^N(x + \varepsilon\omega, v_1, x, v, t) \right\}$$

vs.

$$(\partial_t + v \cdot \nabla_x) f(x, v, t) = \int_{\mathbb{R}^3} d\nu_1 \int_{S^2} d\omega B(\omega, V) \\ \times \left\{ f(x, v'_1, t) f(x, v', t) - f(x, v_1, t) f(x, v, t) \right\}$$

$$B(\omega, V) = |\omega \cdot V| \mathbb{1}_{\{\omega \cdot V \leq 0\}}$$

3. SMOOTH POTENTIALS. STATE OF THE ART



- Infinite range: poorly understood [Ayi ('17)]
- Finite range [Gallagher, Saint-Raymond, Texier ('14), Pulvirenti, Saffirio, S. ('14)]

3. BASIC TOOL FOR SHORT RANGE φ

'Reduced marginals': $\tilde{f}_j^N = \int_{S(\underline{x}_j)^{N-j}} dz_{j+1} \cdots dz_N f^N$

$$S(\underline{x}_j) = \{|x - x_k| > \varepsilon \text{ for all } k = 1, \dots, j\}$$

$$\Rightarrow \left(\partial_t + \sum_{i=1}^j v_i \cdot \nabla_{x_i} - \frac{1}{\varepsilon} \sum_{i,k=1}^j \nabla \varphi \left(\frac{x_i - x_k}{\varepsilon} \right) \cdot \nabla_{v_i} \right) \tilde{f}_j^N = \mathcal{C}_{j+1}^\varepsilon \tilde{f}_{j+1}^N + E_j^\varepsilon$$

Grad hierarchy

$$\begin{aligned} \mathcal{C}_{j+1}^\varepsilon \tilde{f}_{j+1}^N(\underline{z}_j, t) &= \varepsilon^2(N-j) \sum_{k=1}^j \int_{S^2 \times \mathbb{R}^3} d\nu d\nu_{j+1} \mathbb{1}_{\{\min_{\ell \neq k} |x_k + \nu \varepsilon - x_\ell| > \varepsilon\}} \\ &\quad \times (v_{j+1} - v_k) \cdot \nu \tilde{f}_{j+1}^N(\underline{z}_j, x_k + \nu \varepsilon, \nu_{j+1}, t). \end{aligned}$$

Error E_j^ε (finite range):

- Couplings to all f_{j+2}, f_{j+3}, \dots
- $E_j^\varepsilon = O(\varepsilon)$
- does not worsen the uniform bounds on $(f_j^N)_{1 \leq j \leq N}$

[King '75 ($\varphi \geq 0$)]

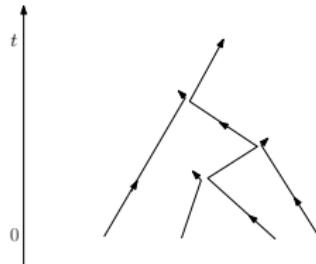
3. DIFFICULTY

Is the Boltzmann equation valid for 'any' compactly supported φ ?

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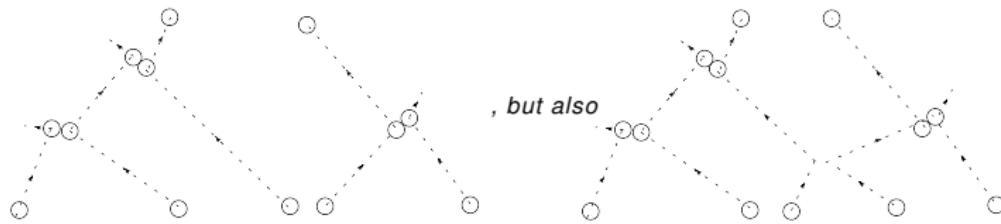
Is the Boltzmann equation valid for 'any' compactly supported φ ?

Caution:
geometrical estimates on recollision sets



Explicit solution of the hierarchy: "weighted average" over backward clusters.

E.g. for two hard spheres with configuration (z_1, z_2) , $z_i = (x_i, v_i)$ at time t :



(Breakdown of chaos: $f_j^N(t) \neq (f_1^N)^{\otimes j}(t)$)

Standard kinetics may fail (Uchiyama model [88], external magnetic field [Bobylev et al '95])

3. COLLISION HISTORIES (1)

Iterated Duhamel:

$$f_j(t) = \sum_{n \geq 0} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \\ \times \mathcal{S}_j(t - t_1) \mathcal{C}_{j+1} \mathcal{S}_{j+1}(t_1 - t_2) \cdots \mathcal{C}_{j+n} \mathcal{S}_{j+n}(t_n) f_{j+n}(0)$$

$$\tilde{f}_j^N(t) = \sum_{n=0}^{N-j} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \\ \times \mathcal{S}_j^\varepsilon(t - t_1) \mathcal{C}_{j+1}^\varepsilon \mathcal{S}_{j+1}^\varepsilon(t_1 - t_2) \cdots \mathcal{C}_{j+n}^\varepsilon \mathcal{S}_{j+n}^\varepsilon(t_n) \tilde{f}_{j+n}^N(0) + O(\varepsilon)$$

$\mathcal{S}_j^\varepsilon(t)$ = flow operator for the j -body dynamics

$\mathcal{S}_j(t)$ = free flow operator

$O(\varepsilon)$ = multiple collisions

Two steps:

- A. Absolute convergence of the series (uniform in ε) ;
- B. Term by term convergence

3. COLLISION HISTORIES (2)

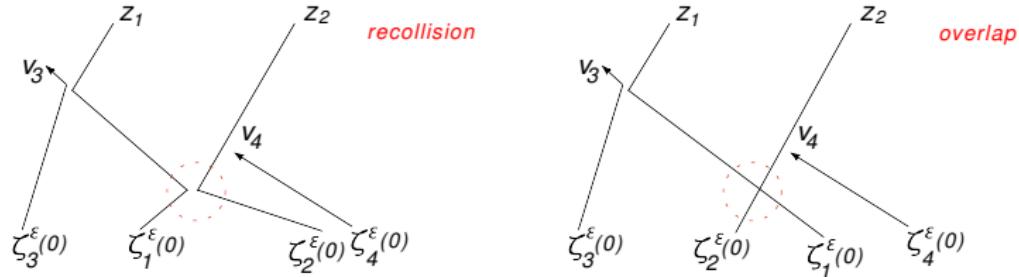
$\underline{\zeta}^\varepsilon(s) = (\zeta_1^\varepsilon(s), \zeta_2^\varepsilon(s), \dots) =$ trajectory of backward clusters

$$\tilde{f}_2^N(z_1, z_2, t) - \tilde{f}_1^N(z_1, t) \tilde{f}_1^N(z_2, t) = \sum_{n \geq 2} \int d\Lambda_n^\varepsilon(\underline{\zeta}^\varepsilon) f_0^{\otimes n}(\underline{\zeta}^\varepsilon(0)) [\chi_{1,2}^{rec} - \chi_{1,2}^{ov}] + O(\varepsilon)$$

" $d\Lambda_n^\varepsilon$ " = (signed) measure over trajectories of n -particle backward clusters

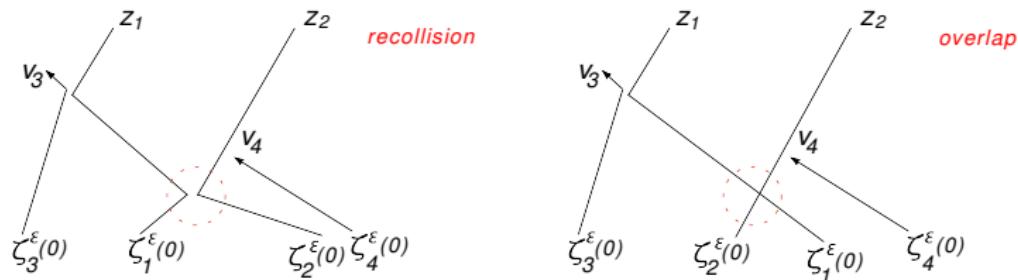
$\chi_{1,2}^{rec} = 1 \iff$ there exists a *recollision* among the clusters 1 and 2.

$\chi_{1,2}^{ov} = 1 \iff$ there exists an *overlap* among the clusters 1 and 2.



3. COLLISION HISTORIES (3)

$$\underline{\zeta}^{\varepsilon}(s) \leftarrow \begin{cases} \underline{z}_j & \text{(starting (time } t \text{) } j\text{-particle configuration)} \\ n & \text{(number of added particles)} \\ t_1, \dots, t_n & \text{(times of creation of added particles)} \\ v_1, \dots, v_n & \text{(impact vector of the added particles)} \\ v_{j+1}, \dots, v_{j+n} & \text{(velocities of added particles)} \end{cases} .$$

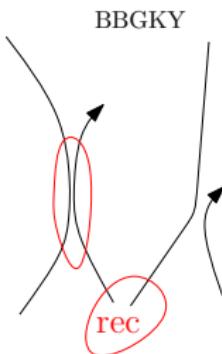


3. COLLISION HISTORIES (3)

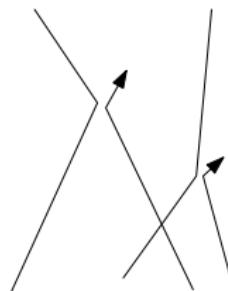
Smooth φ pathologies

1. interaction time

- high-energy
- grazing collisions
- trapping orbits
- ...



Boltzmann

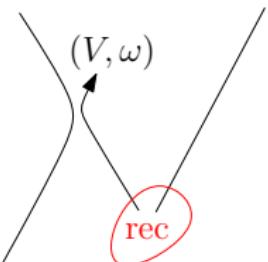


2. cross-section

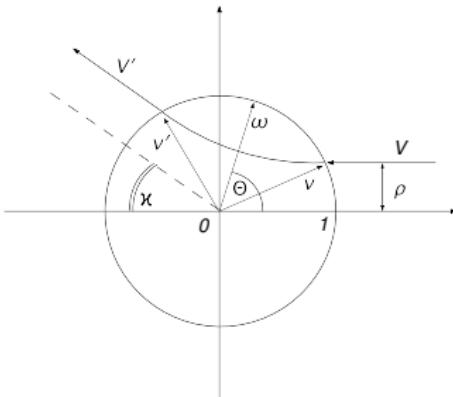
$R > 0$ energy cutoff

$$\int_{S^2} d\hat{V} \int_0^R dV V^2 \int d\omega B(\omega, V) \chi^{rec} = O(R^4 \|\sigma_\varphi\|_\infty \varepsilon^2)$$

σ_φ = differential cross-section. Typically $\|\sigma_\varphi\|_\infty = \infty$



3. EXPLORING SINGULARITIES: $\sigma_\varphi = \frac{\rho}{2|\sin(2\Theta)|} \left| \frac{d\rho}{d\Theta} \right|$



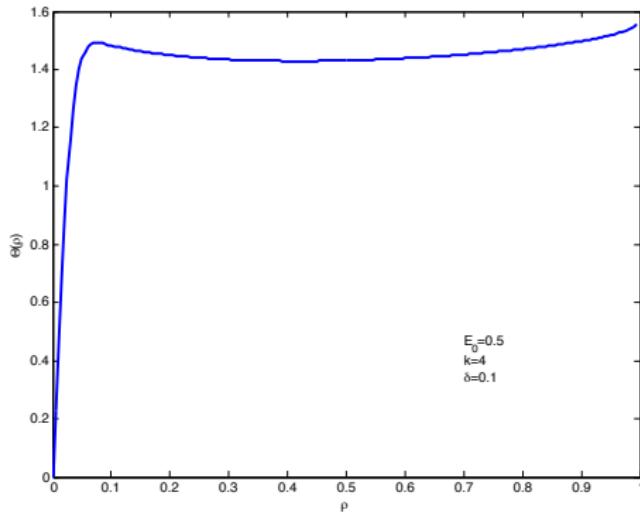
$$\Theta(\rho) = \arcsin \rho + \rho \int_{r_*}^1 dr \frac{1}{r^2 \sqrt{1 - \frac{2\varphi(r)}{V^2} - \frac{\rho^2}{r^2}}} \quad \frac{2\varphi(r)}{V^2} + \frac{\rho^2}{r^2} = \sin^2 \alpha$$

$$\frac{d\Theta}{d\rho} = \frac{1}{\sqrt{1-\rho^2}} \left(1 - \frac{1}{1 - \frac{\varphi'(1^-)}{V^2 \rho^2}} \right) + \int_{\arcsin \rho}^{\pi/2} d\alpha \frac{\sin \alpha}{\left(y - \frac{\rho}{V^2 y^2} \varphi' \left(\frac{\rho}{y} \right) \right)^3} \left[\frac{\rho}{V^2 y^2} \varphi'' \left(\frac{\rho}{y} \right) + \frac{2}{V^2 y} \varphi' \left(\frac{\rho}{y} \right) + \frac{\rho}{V^4 y^4} \left(\varphi' \left(\frac{\rho}{y} \right) \right)^2 \right]$$

$\rho \rightarrow \Theta(\rho)$ monotonic if $|q|\varphi''(|q|) + 2\varphi'(|q|) \geq 0$ [Sone, Aoki]

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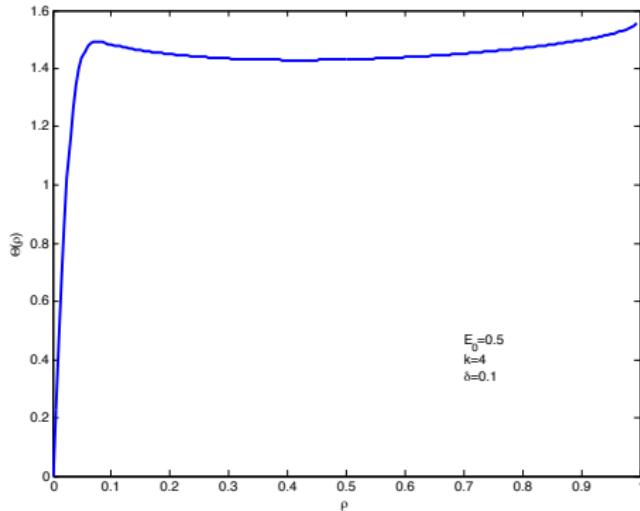
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$$\varphi(q) = \begin{cases} \frac{\delta^{k+2}}{k|q|^k} + \delta - \delta^2(1 + k^{-1}) & 0 < |q| < \delta \\ \delta(1 - |q|) & \delta < |q| < 1 \\ 0 & |q| \geq 1 \end{cases}$$

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Hidden :



$$\varphi(q) = \begin{cases} \frac{\delta^{k+2}}{k|q|^k} + \delta - \delta^2(1 + k^{-1}) & 0 < |q| < \delta \\ \delta(1 - |q|) & \delta < |q| < 1 \\ 0 & |q| \geq 1 \end{cases}$$

Is the Boltzmann equation valid for 'any' compactly supported φ ?

4. RESULT (1)

Hypothesis 1. The two-body potential $\varphi = \varphi(q)$ is radial, with support $|q| < 1$, class $C^2(\mathbb{R}^3 \setminus \{0\})$ and stable ($\sum_{i < k} \varphi(q_i - q_k) \geq -CN$, $C > 0$).

Hypothesis 2. The initial datum for Boltzmann is $f_0 \in C(\mathbb{R}^6)$, $f_0(x, v) \leq Ce^{-(\beta/2)v^2}$, $C, \beta > 0$.

Hypothesis 3. The initial datum for the N -particle system is the symmetric probability density f_0^N , with marginals $f_{0,j}^N \leq e^{\alpha j} e^{-(\beta/2)[\sum_i v_i^2 + \sum_{i,k} \varphi(\frac{x_i - x_k}{\varepsilon})]}$, $\alpha, \beta > 0$.

Hypothesis 4. $f_{0,j}^N \rightarrow f_0^{\otimes j}$ uniformly on compact sets outside the diagonals ($x_i = x_k$).

THEOREM (PULVIRENTI, SAFFIRIO, S.)

Let $\Omega_j = \left\{ \underline{z}_j \text{ t.c. } |x_i - x_k - (v_i - v_k)s| > 0 \text{ } \forall s \geq 0 \right\}$. In the hypotheses 1 – 4, there exists t_0 s.t. for any $t < t_0$, $j > 0$,

$$\lim_{\substack{\varepsilon \rightarrow 0 \\ N\varepsilon^2=1}} f_j^N(t) = f(t)^{\otimes j}$$

uniformly on compact sets in Ω_j .

4. RESULT (2)

Hypothesis 5. φ is non increasing. Moreover, for some $C', L > 0$,

$$\sup_{|x_i - x_k| > \varepsilon} e^{\frac{\beta}{2} \sum_{i=1}^j v_i^2} |f_0^{\otimes j} - f_{0,j}^N| \leq (C')^j \varepsilon \quad (\text{convergence}),$$
$$e^{\frac{\beta}{2} v^2} |f_0(x, v) - f_0(x', v)| \leq L |x - x'| \quad (\text{regularity}).$$

THEOREM (PULVIRENTI, SAFFIRIO, S.)

In the hypotheses 1–5, for any $t < t_0$, $j > 0$, $\underline{z}_j \in \Omega_j$ and ε small enough,

$$|f_j^N(\underline{z}_j, t) - (f(t)^{\otimes j})(\underline{z}_j)| \leq C^j \varepsilon^\gamma,$$

with suitable $C, \gamma > 0$.

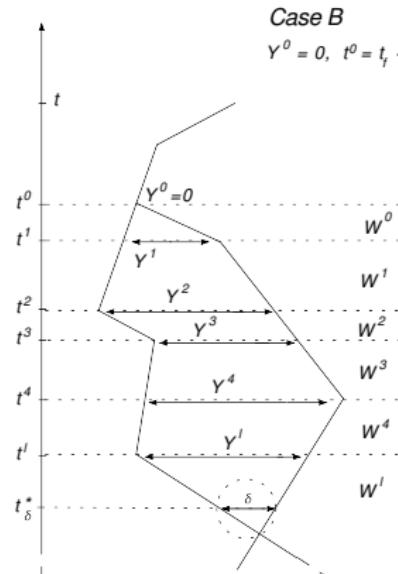
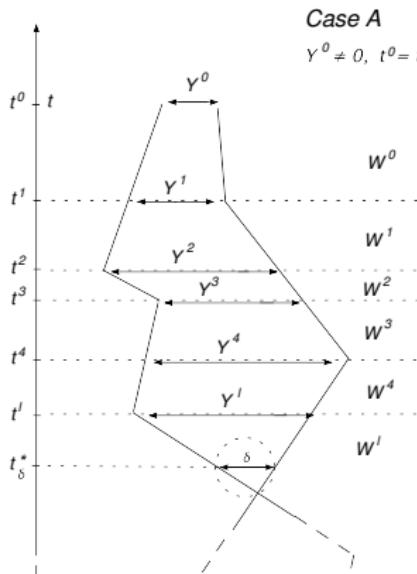
Remark. “ $\underline{z}_j \in \Omega_j$ ” \longleftrightarrow irreversibility.

Improved: ‘one-sided convergence’ [Bodineau, Gallagher, Saint-Raymond, S.’17]

4. PROOF

Boltzmann equation emerging in the form

$$(\partial_t + \nu \cdot \nabla_x) f(x, \nu, t) = \int_{\mathbb{R}^3} d\nu_1 \int_{S_+^2} d\nu (\nu - \nu_1) \cdot \nu \\ \times \left\{ f(x, \nu'_1, t) f(x, \nu', t) - f(x, \nu_1, t) f(x, \nu, t) \right\}$$



Global approach:

- work on the Boltzmann flow ($|Y^l - W^l s| < \delta$)
- integrate over times;
- exploit the global structure of $\underline{\zeta}(s)$;
- keep using ν , not ω .

- unstable interactions
- Vlasov-Boltzmann
- long range

OPEN

- unstable interactions
- Vlasov-Boltzmann
- long range

THANKS!