Quantitative uniform propagation of chaos for Maxwell molecules

Joaquín Fontbona
(joint work with Roberto Cortez)

Center for Mathematical Modeling, University of Chile

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1. The spatially homogeneous Boltzmann equation

Boltzmann equation

Boltzmann equation on $\mathbb{R}^3$ (1872)

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

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- Very difficult!
- Following Kac ('56), we consider spatially homogeneous version: $f = f_t(v)$.

Spatially homogeneous Boltzmann equation

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$$\partial_t f_t(v) = Q(f_t, f_t)(v)$$
$$:= \frac{1}{2}\int_{\mathbb{R}^3} dv_* \int_{\mathbb{S}^2} d\sigma B(|v - v_*|, \theta)\left[f_t(v')f_t(v'_*) - f_t(v)f_t(v_*)\right],$$

- $v' = v'(v, v_*, \sigma) := \frac{v+v_*}{2} + \frac{|v-v_*|}{2}\sigma$.
- $v'_* = v'_*(v, v_*, \sigma) := \frac{v+v_*}{2} - \frac{|v-v_*|}{2}\sigma$.
- θ: deviation angle, defined by $\cos\theta = \frac{v-v_*}{|v-v*|} \cdot \sigma$.
- $B(|v - v_*|, \theta)$: collision kernel, depends on physics of the model.

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In the sequel, "Boltzmann equation" always means its **spatially homogeneous version**

Elementary properties :

- Preserves mass:

$$\int f_t(v)dv = \text{Constant} = 1$$

- Preserves momentum:

$$\int v f_t(v)dv = \text{Constant}$$

- Preserves kinetic energy:

$$\int |v|^2 f_t(v)dv = \text{Constant}$$

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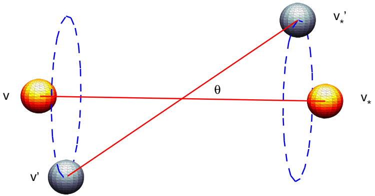

Exact conservation of momentum and energy:

$$v + v_* = v' + v'_*,$$
$$|v|^2 + |v_*|^2 = |v'|^2 + |v'_*|^2.$$

Collision kernel

- We will work with the Maxwell molecules case:

$$B(|v-v_*|,\theta)\sin\theta = \beta(\theta),$$

with $\beta(\theta) \overset{0}{\sim} \theta^{-3/2}$, then

$$\int_0^{\pi/2} \beta(\theta)d\theta = \infty \qquad \text{(prevalence of grazing collisions).}$$

- Sometimes one uses a cutoff version of β, so $\int_0^{\pi/2} \beta(\theta)d\theta < \infty$ in those cases.

2. Propagation of chaos

Kac's program ('56)

Goal

- Mathematical validation of the Boltzmann equation from **"molecular chaos"** : to obtain its solution as limit of random, jump N-particles systems as $N \to \infty$.

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....by 2017:

- relaxation of the equation (Maxwell) "understood" (PDE results)
- Kac's program in spatially homogeneous case: Mischler & Mouhot '13 for Maxwell and hard spheres cases by **"top-down"** approach. Also,**bounds are hard to make explicit**.

Particle system

- $N \in \mathbb{N}$: number of particles.
- Particle system is a Markov jump process on $(\mathbb{R}^3)^N$, denoted

$$\mathbf{V}_t = (V_t^1, \ldots, V_t^N)$$

with (exchangeable) generator $\mathcal{A}^N$ given by:

$$\mathcal{A}^N \Phi(\mathbf{v}) = \frac{1}{2(N-1)} \sum_{i \neq j} \int_{\mathbb{S}^2} d\sigma [\Phi(\mathbf{a}_{ij}(\mathbf{v}, \sigma)) - \Phi(\mathbf{v})] B(\theta),$$

where $\mathbf{a}_{ij}(\mathbf{v}, \sigma) \in (\mathbb{R}^3)^N$ is vector $\mathbf{v} = (v^1, \ldots, v^N) \in (\mathbb{R}^3)^N$

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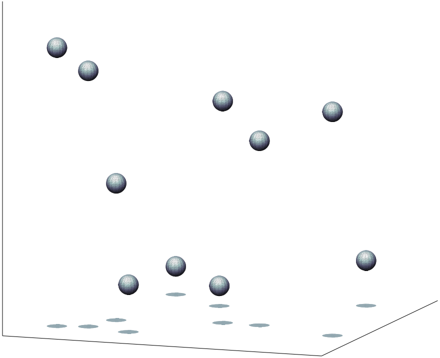
Notational dependence on N will be omitted!!!

Particle system dynamics (cutoff case)



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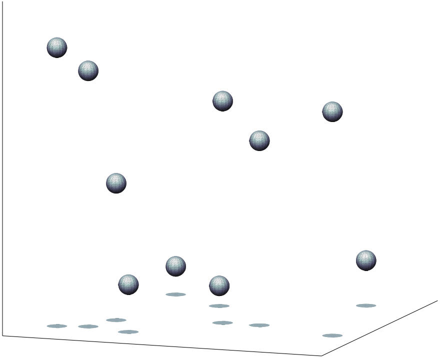

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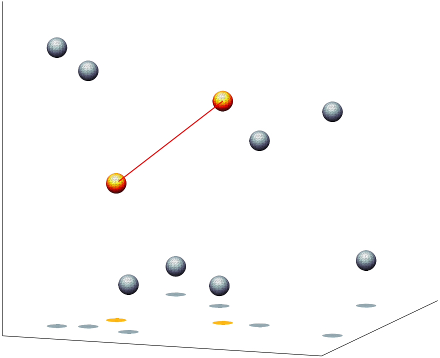

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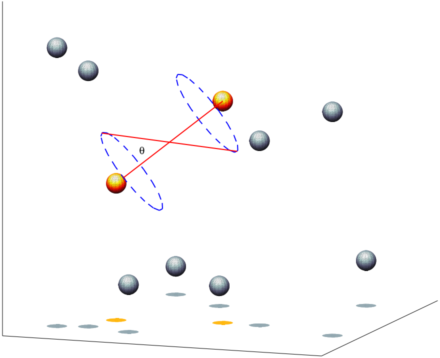

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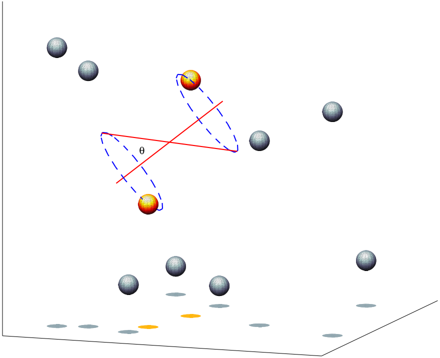

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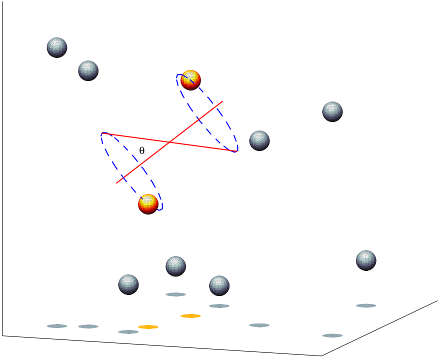

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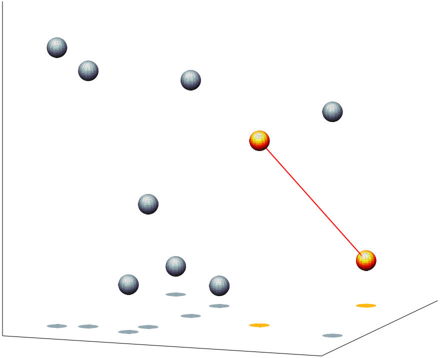

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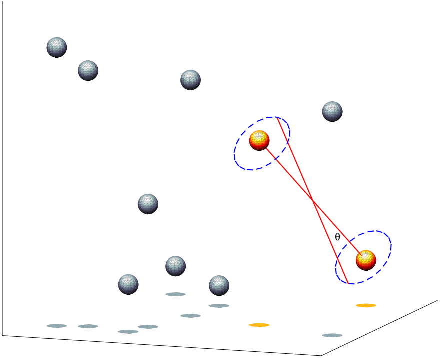

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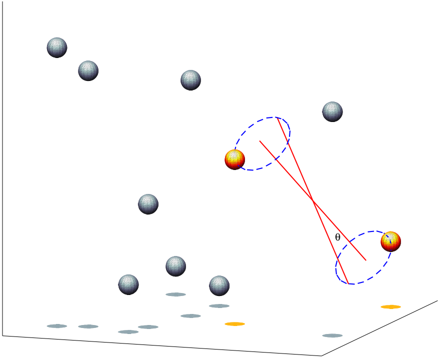

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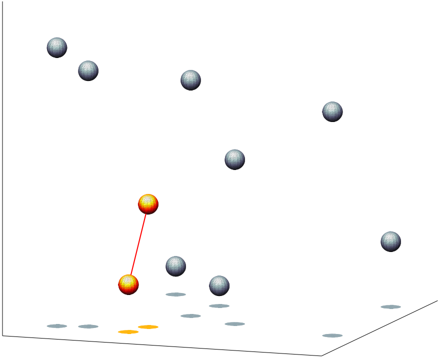

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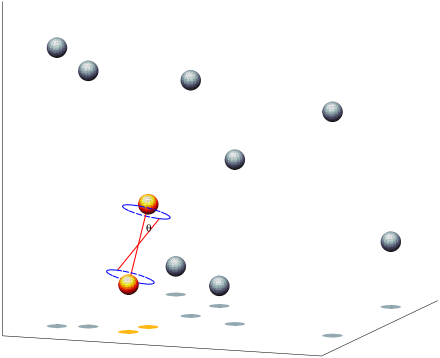

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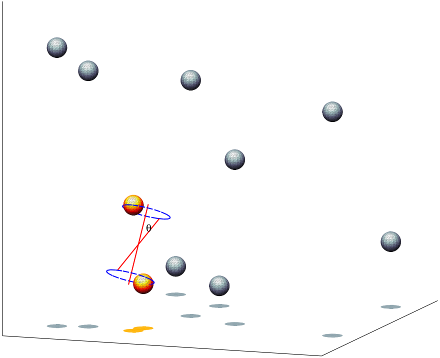

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as $N \to \infty$.

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Our goal

Quantify this convergence in the Maxwell molecules case, with explicit rates .

Known results or approaches (Maxwell case)

Technique	Authors	Rate
Weak convergence, expansions	Kac (1d), McKean, Grünbaum, ~ 60–70's	no rate
Trajectorial coupling with "nonlinear process" (Mostly cut-off)	Tanaka ~ 80, Sznitmann ~ 90, Graham & Méléard '97	$\frac{e^t}{N}$
semigroup, PDE stability	Mischler & Mouhot '13	$\frac{1}{N^{\varepsilon}}$ in $\mathcal{W}_1$
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"Nanbu" case:

- only one particle updates upon collision (non-physical).
- Rate in N corresponds to **empirical measure of i.i.d. sample** (Fournier& Guillin '14).

3. Main result and outline of the proof

Wasserstein distance and optimal coupling

We need

Definition

Let μ, ν be probability measures on $(\mathbb{R}^3)^k$. Define:

Coupling: a random pair $(\mathbf{X}, \mathbf{Y}) = \big((X^1, \dots, X^k), (Y^1, \dots, Y^k)\big)$ with Law$(X) = \mu$ and Law$(Y) = \nu$.

p-Wasserstein distance: minimal expected L^p-distance between couplings:

$$\mathcal{W}_p(\mu, \nu) = \left(\inf_{\mathbf{X}, \mathbf{Y}} \mathbb{E} \frac{1}{k} \sum_{i=1}^{k} |X^i - Y^i|^p \right)^{1/p}$$

Optimal coupling: random pair $(\mathbf{X}, \mathbf{Y})$ achieving the infimum (always exists).

Main result

Theorem (Cortez & F. '15 submitted)

If f_0 has finite moments of all orders, and $\mathbf{V}_0 \sim f_0^{\otimes N}$,

$$\sup_{t\geq 0} \mathbb{E}\left(\mathcal{W}_2^2\left(\frac{1}{N}\sum_{i=1}^N \delta_{V_t^i}\right), f_t\right) \leq \frac{C_\epsilon}{N^{\frac{1}{3}-\epsilon}}$$

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- Also valid if $\mathbf{V}_0$ is only exchangeable (additional term $\mathcal{W}_2^2(\text{Law}(\mathbf{V}_0), f_0^{\otimes N})$).
- **Similar result obtained in '15 for Landau equation through related ideas (but different techniques) by Fournier&Guillin**

Main result

Steps of the proof

1) Extend to Boltzmann setting new coupling argument (F.&Cortez, AAP '16) for 1d (Kac-type) particles systems with true binary collisions, rely also on estimates of Fournier& Mischler'16 for the Nambu case
This will yield (non-uniform) quantitative estimate for $\mathcal{W}_2^2$:

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2) Combine with recent uniform in N (polynomial) stabilization result for the N- particle system of M. Rousset ('14).

4. Coupling construction

The particle system and coupling construction

Consider (for fixed N):

Poisson point measure $\mathcal{N}$ on $\mathbb{R}_+ \times \mathbb{R}_+ \times [0, 2\pi) \times \mathcal{G}$

$$\mathcal{N}(\underbrace{dt, dz}_{\text{rate } N/2 \,\times\, \infty,} , \underbrace{d\phi}_{\text{uniform in } [0,2\pi),} , \underbrace{d\xi, d\zeta}_{\text{uniform in } \mathcal{G}})$$

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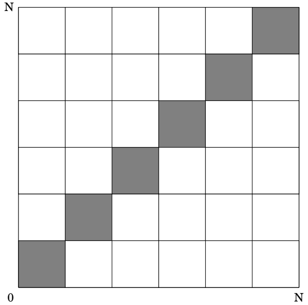
- $t \geq 0$: collision times
- $z \geq 0$: parametrization of θ
- $\phi \in [0, 2\pi)$: angle in circles
- $\mathbf{i}(\xi) = \lfloor \xi \rfloor + 1$ for $\xi \in [0, N)$.
- $\mathcal{G} = \{(\xi, \zeta) \in [0, N)^2 : \mathbf{i}(\xi) \neq \mathbf{i}(\zeta)\}$.
- $\mathbf{i}(\xi), \mathbf{i}(\zeta)$: indexes of colliding particles.



The particle system and coupling construction

- Consider for each $i = 1, \ldots, N$,

$$\mathcal{N}^i(dt, dz, d\phi, d\xi) := \overbrace{\mathcal{N}(dt, dz, d\phi, [i-1, i), d\xi)}^{i \text{ chooses another particle to interact with}} + \underbrace{\mathcal{N}(dt, dz, d\phi, d\xi, [i-1, i))}_{\text{someone else chooses } i \text{ to interact with}}$$

- Define $(V^1, \ldots, V^N)$ by

$$dV_t^i = \int_0^\infty \int_0^{2\pi} \int_0^N c(V_{t-}^i, V_{t-}^{\mathbf{i}(\xi)}, z, \phi) \mathcal{N}^i(dt, dz, d\phi, d\xi),$$

where $c(v, v_*, z, \phi) := v'(v, v_*, \theta, \phi) - v$.

- Under $\mathcal{N}^i$, $V_{t-}^{\mathbf{i}(\xi)}$ is an ξ-sample from the (random) measure

$$\frac{1}{N-1} \sum_{j \neq i} \delta_{V_{t-}^j}.$$

The particle system and coupling construction

Nonlinear processes

- Remark: if $V_{t^-}^{\mathbf{i}(\xi)}$ above is replaced by an ξ-realization $Y_t^i(\xi)$ of the law f_t, the resulting SDE of the form:

$$dU_t^i = \int_0^\infty \int_0^{2\pi} \int_0^N c(U_{t-}^i, Y_t^i(\xi), z, \phi) \mathcal{N}^i(dt, dz, d\phi, d\xi),$$

corresponds to a **nonlinear process** (cf. Tanaka).

- Also known as **Boltzmann process**, it is a jump process U on $\mathbb{R}^3$, such that Law$(U_t) = f_t$.

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$$dU^i_t = \int_0^\infty \int_0^{2\pi} \int_0^N c(U^i_{t-}, Y^i_t(\xi), z, \phi)\mathcal{N}^i(dt, dz, d\phi, d\xi),$$

  corresponds to a **nonlinear process** (cf. Tanaka).
- Also known as **Boltzmann process**, it is a jump process U on $\mathbb{R}^3$, such that Law$(U_t) = f_t$.
- Heuristic: it represents the trajectory of a fixed particle immersed in an infinite population of "virtual particles".
- Classical propagation of chaos argument: to couple particles with independent nonlinear processes $\tilde{U}^1, ..., \tilde{U}^N$

The particle system and coupling construction

Key idea

Define a system of nonlinear processes $\mathbf{U}_t = (U_t^1, \ldots, U_t^N)$ in such a way that $Y_t^i(\xi)$ is optimally coupled to $V_{t^-}^{\mathbf{i}(\xi)}$ for each i.

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- **Effective binary collisions (our case):** coupling argument introduced in Cortez & F. '16 AAP for 1d Kac's model and variants. Some measurability issues must be taken care of...

The particle system and coupling construction

Lemma (Coupling Lemma (Cortez & F. '16))

There exists a (measurable) mapping $(t, \mathbf{x}, \xi) \mapsto \Pi_t^i(\mathbf{x}, \xi)$ *such that for each* $\mathbf{x} = (x^1, \ldots, x^N) \in (\mathbb{R}^3)^N$ *the pair*

$$(x^{\mathbf{i}(\xi)}, \Pi_t^i(\mathbf{x}, \xi))$$

is an optimal coupling (for $\mathcal{W}_2^2$*) between* $\frac{1}{N-1} \sum_{j \neq i} \delta_{x^j}$ *and* f_t *when* ξ *is chosen uniformly in* $[0, N) \backslash [i-1, i)$.

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In addition to choosing "virtual velocities" to interact with, here we also need to choose "circles" and couple their choices too...

The particle system and coupling construction

Lemma (Optimal coupling of circles, Cortez &F. '16)

$\exists$ measurable function $\varphi : \mathbb{R}^3 \times \mathbb{R}^3 \times [0, 2\pi) \to [0, 2\pi)$ such that $\forall v, v_*, u, u_* \in \mathbb{R}^3$, $\forall \theta, \vartheta \in [0, 2\pi)$, the angle $\varphi = \varphi(v - v_*, u - u_*, \phi)$ is such that

$$(v'(v, v_*, \theta, \phi), u'(u, u_*, \vartheta, \varphi))$$

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Moreover, if $b, \tilde{b} \in \mathbb{R}^3$ *denote their centers,* $r, \tilde{r} \geq 0$ *their radii, and* $d, \tilde{d} \in \mathbb{S}^2$ *their orthogonal unitary vectors, the optimal cost is*

$$\underbrace{|b - \tilde{b}|^2}_{\text{traslation}} + \underbrace{(r - \tilde{r})^2}_{\text{dilation}} + \underbrace{r\tilde{r}(1 - |d \cdot \tilde{d}|)}_{\text{inclination}}$$

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("Tanaka trick", sharp version)

The particle system and coupling construction

SDEs for $\mathbf{V} = (V^1, \ldots, V^N)$ **and** $\mathbf{U} = (U^1, \ldots, U^N)$ become:

$$dV_t^i = \int_0^\infty \int_0^{2\pi} \int_0^N c(V_{t-}^i, V_{t-}^{\mathbf{i}(\xi)}, \theta, \phi) \mathcal{N}^i(dt, dz, d\phi, d\xi),$$
$$dU_t^i = \int_0^\infty \int_0^{2\pi} \int_0^N c(U_{t-}^i, \Pi_t^i(\mathbf{V}_{t-}, \xi), \theta, \varphi_t^i) \mathcal{N}^i(dt, dz, d\phi, d\xi).$$

with

- $\Pi_t^i(\mathbf{V}_{t-}, \xi)$ as in Coupling Lemma above and
- $\varphi_t^i := \varphi(V_{t-}^i - V_{t-}^{\mathbf{i}(\xi)}, U_{t-}^i - \Pi_t^i(\mathbf{V}_{t-}, \xi), \phi)$ couples the angles "ϕ" "optimally".

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By construction, processes $(U^1, \dots, U^N)$ are exchangeable but not independent (they have some simultaneous jumps).

5. Time-dependent estimate

Proof of the time-dependent bound

1) Itô calculus and Gronwall's Lemma yield

$$\mathbb{E}|V_t^i - U_t^i|^2 \leq C(1+t)^2 \mathbb{E}\mathcal{W}_2^2\left(\frac{1}{N-1}\sum_{j\neq i}\delta_{U_t^j}, f_t\right)$$

and

$$\begin{aligned}\mathbb{E}\mathcal{W}_2^2\left(\frac{1}{N}\sum_{j}\delta_{V_t^j}, f_t\right) \leq & C(1+t)^2 \mathbb{E}\mathcal{W}_2^2\left(\frac{1}{N-1}\sum_{j\neq i}\delta_{U_t^j}, f_t\right) \\ & + C\mathbb{E}\mathcal{W}_2^2\left(\frac{1}{N}\sum_{j}\delta_{U_t^j}, f_t\right)\end{aligned}$$

2) Need to bound two expectations on the left by $CN^{-\frac{1}{3}}$.

Proof of the time-dependent bound

3) As in F.& Cortez AAP'16, we prove : for each $k \leq N$,

$$\frac{1}{2}\mathbb{E}\mathcal{W}_2^2\left(\frac{1}{N}\sum_j \delta_{U_t^j}, f_t\right) \leq \mathcal{W}_2^2\left(\mathsf{Law}|_k(\mathbf{U}_t), f_t^{\otimes k}\right) + \varepsilon_k(f_t) + \frac{k}{N}\int |v|^2 f_0(dv)$$

where

$$\varepsilon_k(f_t) := \mathbb{E}\mathcal{W}_2^2\left(\frac{1}{k}\sum_j \delta_{\tilde{U}_t^j}, f_t\right) \leq \frac{C(f_0)}{k^{1/2}}$$

for $\tilde{U}_t^1, \ldots \tilde{U}_t^k$ i.i.d. $\sim f_t$ (Fournier& Guillin '14).

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4) Prove Decoupling Lemma: $\mathcal{W}_2^2\left(\text{Law}|_k(\mathbf{U}_t), f_t^{\otimes k}\right) \leq C\frac{k}{N}$.
(Change jumps of particles $j > k$ with particle i by indep. ones)

Proof of the time-dependent bound

Hence, for each $k \leq N$,

$$\frac{1}{2}\mathbb{E}\mathcal{W}_2^2\left(\frac{1}{N}\sum_j \delta_{U_t^j}, f_t\right) \leq C\frac{k}{N} + \frac{C'}{k^{1/2}}$$

Choosing $k = \lfloor N^{2/3} \rfloor$ yields the required order $N^{-1/3}$.

6. Uniform relaxation and time independent bound

Uniform in N relaxation of particles

Call $\mathcal{U}^N$ the uniform distribution on the **Boltzmann sphere**

$$\mathcal{S}^N = \left\{ \mathbf{v} \in (\mathbb{R}^3)^N : \frac{1}{N}\sum_{i=1}^N v^i = 0, \frac{1}{N}\sum_{i=1}^N |v^i|^2 = 1 \right\},$$

which are invariant for the $N-$particles dynamics.

Theorem (M.Rousset '14)

Let $\mathbf{V}_0$ be exchangeable, concentrated in $\mathcal{S}^N$. Then, $\forall \delta > 0, q > 1$

$$\partial_t^+ \mathcal{W}_{2,\text{sym}}(\text{Law}(\mathbf{V}_t), \mathcal{U}^N) \leq -c_{\delta,q}(t) \mathcal{W}_{2,\text{sym}}(\text{Law}(\mathbf{V}_t), \mathcal{U}^N)^{1+1/\delta},$$

where $c_{\delta,q}(t) = k_{\delta,q}\mathbb{E}(|V_t^1|^{2q(1+\delta)})^{-1/2q\delta}$ for some $k_{\delta,q} > 0$ not depending on N and

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where $c_{\delta,q}(t) = k_{\delta,q}\mathbb{E}(|V_t^1|^{2q(1+\delta)})^{-1/2q\delta}$ *for some* $k_{\delta,q} > 0$ *not depending on* N *and*
$\mathcal{W}^2_{2,\text{sym}}(\mu,\nu) = \inf_{\mathbf{X},\mathbf{Y}} \mathbb{E}\mathcal{W}_2^2\left(\frac{1}{N}\sum_j \delta_{X^j}, \frac{1}{N}\sum_j \delta_{Y^j}\right)$.

Proof of the uniform in time bound

1) Prove preservation of $p-$moments for arbitrary $p > 4$ by particle the system (follows from a "Povzner lemma")

Proof of the uniform in time bound

1) Prove preservation of $p-$moments for arbitrary $p > 4$ by particle the system (follows from a "Povzner lemma")
2) This improves Rousset's Thm. to : for all $0 < \delta < p - 2$,

$$\mathcal{W}^2_{2,\text{sym}}(\text{Law}(\mathbf{V}_t), \mathcal{U}^N) \leq C_{p,\delta}(1+t)^{-\delta},$$

where $C_{p,\delta}$ depends only on p, δ and $\sup_N \mathbb{E}|V_0^1|^p$.
3) For $\mathbf{V}_0$ exchangeable, concentrated in $\mathcal{S}^N$, this and $\mathcal{W}_2^2(\mathcal{U}^N, (\mathcal{N}(0, I_3))^{\otimes N}) \leq CN^{-1/2}$ yield

$$\mathbb{E}\mathcal{W}_2^2(\bar{\mathbf{V}}_t, f_t) \leq C_{p,\delta}(1+t)^{-\delta} + CN^{-1/2} \leq CN^{-1/3}$$

for $t \geq \bar{t}(N, \epsilon)$. For $t \leq \bar{t}(N, \epsilon)$, use our first bound.
4) General exchangeable $\mathbf{V}_0$: reduce to previous case by "standarizing" the particle system.

Thank you!

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