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HAL Id: hal-00641197
https://hal.science/hal-00641197

Submitted on 15 Nov 2011

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Abstract

In this Note we present the main results from the recent work [15], which answers several conjectures raised fifty years ago by Kac [9]. There Kac introduced a many-particle stochastic process (now denoted as Kac's master equation) which, for chaotic data, converges to the spatially homogeneous Boltzmann equation. We answer the three following questions raised in [9]: (1) prove the propagation of chaos for realistic microscopic interactions (i.e. in our results: hard spheres and true Maxwell molecules); (2) relate the time scales of relaxation of the stochastic process and of the limit equation by obtaining rates independent of the number of particles; (3) prove the convergence of the many-particle entropy towards the Boltzmann entropy of the solution to the limit equation (microscopic justification of the H-theorem of Boltzmann in this context). These results crucially rely on a new theory of quantitative uniform in time estimates of propagation of chaos.

Résumé

À propos du Programme de Kac en Théorie Cinétique. Dans cette Note, nous présentons les résultats principaux du travail récent [15], qui répond à plusieurs conjectures proposées il y a une cinquantaine d'années par Kac [9]. Dans ce travail Kac introduit un processus stochastique à grand nombre de particules (aujourd'hui appelé équation maîtresse de Kac) qui converge, pour des données chaotiques, vers l'équation de Boltzmann spatialement homogène. Nous répondons aux trois questions suivantes soulevées dans cet article : (1) prouver la propagation du chaos pour des processus de collision réalistes (dans notre cas : sphères dures et « vraies » molécules maxwelliennes), (2) connecter les vitesses de relaxation du processus stochastique et de l'équation limite en obtenant des taux indépendants du nombre de particules, (3) prouver la convergence de l'entropie en grand nombre de particules vers l'entropie de Boltzmann pour la solution de l'équation limite (justification microscopique du théorème H dans ce contexte). Tous ces résultats font appel de manière cruciale à une nouvelle théorie d'estimations quantitatives et uniformes en temps de propagation du chaos.

Version française abrégée

Le programme de Kac en théorie cinétique consiste à comprendre comment déduire l'équation de Boltzmann spatialement homogène à partir d'un processus stochastique de saut sur l'espace des vitesses à grand

nombre de particules. Le but de ce programme est de comprendre la notion de « chaos moléculaire » dans un cadre plus simple que celui de la dynamique complète des particules, ainsi que de donner une justification microscopique au théorème H (croissance de l'entropie) et au processus de retour vers l'équilibre. Nous renvoyons à la version complète pour l'introduction de l'équation de Boltzmann (1), des processus de saut considérés, ainsi que pour les définitions de la notion de chaos et de la distance de Wasserstein W_1.

Théorème 1 (Résumé des résultats principaux) *On considère $d \geq 2$ et une distribution initiale $f_0 \in P(\mathbb{R}^d) \cap L^\infty$ à support compact ou possédant suffisamment de moments polynômiaux bornés, et que l'on suppose centrée sans perte de généralité. Soit f_t la solution correspondante de l'équation de Boltzmann (1) pour les sphères dures ou les molécules maxwelliennes (sans troncature angulaire), et soit f_t^N la solution du processus de saut à N particules correspondant, avec pour donnée initiale f_0^N : soit (a) la tensorisation de $f_0^{\otimes N}$ de f_0, ou (b) la tensorisée $f_0^{\otimes N}$ conditionnée à la sphère $\mathcal{S}^N$ (définie par (2)).*

(i) **Propagation de chaos quantifiée et uniforme en temps** *: On considère le cas (a) où $f_0^N = f_0^{\otimes N}$. Alors*

$$\forall N \geq 1, \ \forall 1 \leq \ell \leq N, \quad \sup_{t \geq 0} \frac{W_1\left(\Pi_\ell f_t^N, \left(f_t^{\otimes \ell}\right)\right)}{\ell} \leq \alpha(N)$$

avec $\alpha(N) \to 0$ lorsque $N \to \infty$, et où $\Pi_\ell g^N$ désigne la ℓ-marginale d'une probabilité g sur $(\mathbb{R}^d)^N$.

(ii) **Propagation du chaos entropique** *: On considère le cas (b) où f_0^N est conditionnée à $\mathcal{S}^N$. Alors la solution est entropie-chaotique :*

$$\forall t \geq 0, \quad \frac{1}{N} H\left(f_t^N | \gamma^N\right) \to H\left(f_t | \gamma\right), \quad N \to +\infty$$

(voir (3) pour les définitions des fonctionnelles H) avec γ la probabilité gaussienne centrée d'énergie $\mathcal{E}$ égale à l'énergie de f_0 et γ^N la mesure de probabilité uniforme sur $\mathcal{S}^N$. Cela fournit une dérivation microscopique du théorème H dans ce contexte.

(iii) **Taux de relaxation indépendants du nombre de particules** *: On considère le cas (b) où f_0^N est conditionnée à $\mathcal{S}^N$. Alors*

$$\forall N \geq 1, \ \forall 1 \leq \ell \leq N, \ \forall t \geq 0, \quad \frac{W_1\left(\Pi_\ell f_t^N, \Pi_\ell \left(\gamma^N\right)\right)}{\ell} \leq \beta(t) \qquad avec \ \beta(t) \to 0, \ t \to 0.$$

Dans le cas des molécules maxwelliennes, et si la donnée initiale possède une information de Fisher finie (voir (4)), on prouve également $\forall N \geq 1, \ 0 \leq \frac{1}{N} H\left(f_t^N | \gamma^N\right) \leq \beta(t)$ avec $\beta(t) \to 0, \ t \to 0$.

1. Introduction

Motivated by the understanding of irreversibility and "molecular chaos" in the Boltzmann equation [13,1,2] Mark Kac proposed in 1956 [9,10] the simpler and seemingly more tractable question of deriving the *spatially homogeneous* Boltzmann equation from a *many-particle jump process*, and he introduced a rigorous notion of molecular chaos in this context. He proposed the first proof of the *propagation of chaos* along time for a simplified collision process for which series expansions of the solution are available, and he showed how the many-particle limit rigorously follows from it. A key motivation for Kac was the microscopic derivation of the H-theorem (monotonicity of the Boltzmann entropy) in this context which has remained open so far. Kac also raised the natural question of connecting the asymptotic behavior of the many-particle process and that of the limit nonlinear equation. In his mind this program was to be achieved by understanding dissipativity at the level of the linear many-particle jump process and he insisted on the importance of estimating its rate of relaxation. This has motivated beautiful works on this "Kac's spectral gap problem" [3,12,4], but so far this strategy has proved unsuccessful in obtaining relaxation rates which do not degenerate in the many-particle limit, see the interesting discussion in [5].

In this Note we present the main results in [15]. In this paper we develop a quantitative theory of mean-field limit which *strongly relies on detailed knowledge of the limit nonlinear equation, rather than on detailed*

properties of the many-particle Markov process. As the main outcome of this theory we prove uniform in time quantitative propagation of chaos as well as propagation of entropic chaos, and we prove relaxation rates *independent of the number of particles* (measured in Wasserstein distance and relative entropy). All this is done for the two important realistic and achetypal models of collision, namely hard spheres and true (without cutoff) Maxwell molecules. This provides a first complete answer to the questions raised by Kac, however our answer is an "inverse" answer in the sense that our methodology is "top-down" from the limit equation to the many-particle system rather than "bottom-up" as was proposed by Kac.

1.1. *The Boltzmann equation*

The *spatially homogeneous Boltzmann equation* reads

$$\frac{\partial f}{\partial t}(t, v) = Q(f, f)(t, v), \qquad v \in \mathbb{R}^d, \quad t \geq 0, \tag{1}$$

where $d \geq 2$ is the dimension and Q is defined by

$$Q(g, f)(v) = \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{S}^{d-1}} B(|v - v_*|, \cos \theta) \left(g_*' f' + g' f_*' - g_* f - g f_* \right) dv_* \, d\sigma,$$

where we have used the shorthands $f = f(v)$, $f' = f(v')$, $g_* = g(v_*)$ and $g_*' = g(v_*')$. Moreover, v' and v_*' are parametrized by

$$v' = \frac{v + v_*}{2} + \frac{|v - v_*|}{2} \sigma, \qquad v_*' = \frac{v + v_*}{2} - \frac{|v - v_*|}{2} \sigma, \qquad \sigma \in \mathbb{S}^{d-1}.$$

Finally, $\theta \in [0, \pi]$ is the deviation angle between $v' - v_*'$ and $v - v_*$ defined by $\cos \theta = \sigma \cdot \hat{u}$, $u = v - v_*$, $\hat{u} = u/|u|$, and B is the Boltzmann collision kernel determined by physics (related to the cross-section $\Sigma(v - v_*, \sigma)$ by the formula $B = |v - v_*| \Sigma$).

Boltzmann's collision operator has the fundamental properties of conserving mass, momentum and energy

$$\frac{d}{dt} \int_{\mathbb{R}^d} f \, \phi(v) \, dv = \int_{\mathbb{R}^d} Q(f, f) \, \phi(v) \, dv = 0, \quad \phi(v) = 1, v, |v|^2,$$

and satisfying the so-called Boltzmann's H theorem which writes (at the formal level)

$$-\frac{d}{dt} H(f) := -\frac{d}{dt} \int_{\mathbb{R}^d} f \log f \, dv = -\frac{d}{dt} H(f|\gamma) := -\frac{d}{dt} \int_{\mathbb{R}^d} f \log \frac{f}{\gamma} \, dv = -\int_{\mathbb{R}^d} Q(f, f) \log(f) \, dv \geq 0$$

where γ is the gaussian with same mass, momentum and energy as f. Note that the H functional is the *opposite* of the physical entropy.

We shall consider the folllowing important physical cases for B (see [15] for more details)

$$B = \Gamma(|v - v_*|) \, b(\cos \theta) \qquad \text{with } \Gamma, b \geq 0 \qquad \text{given by one of the following formulas:}$$

(1) **(HS) Hard Spheres collision kernel**: $B(|v - v_*|, \cos \theta) = \Gamma(|v - v_*|) = C \, |v - v_*|$ for some $C > 0$.
(2) **(tMM) True Maxwell Molecules collision kernel**:
   $B(|v - v_*|, \cos \theta) = b(\cos \theta) \sim_{\theta \sim 0} C \, \theta^{-5/2}$ for some $C > 0$.
(3) **(GMM) Grad's cutoff Maxwell Molecules kernel**: $B(|v - v_*|, \cos \theta) = 1$.

1.2. *Kac's program*

Kac's jump process runs as follows: consider N particles with velocities $v_1, \ldots, v_N \in \mathbb{R}^d$. Compute random times for each pair of particles (v_i, v_j) following an exponential law with parameter $\Gamma(|v_i - v_j|)$, take the

smallest, and perform a collision $(v_i, v_j) \to (v_i^*, v_j^*)$ given by a random choice of a direction parameter whose law is related to $b(\cos\theta)$, then recommence. This process can be considered on $\mathbb{R}^{dN}$, however it leaves invariant some submanifolds of $\mathbb{R}^{dN}$ (depending on the number of conserved quantities during collision) and can be restricted to them. In the original simplified model of Kac $d = 1$ (scalar velocities), the direction parameter is θ with collision rule

$$v_i^* = v_i \cos\theta + v_j \sin\theta, \qquad v_j^* = -v_i \sin\theta + v_j \sin\theta$$

and the collision process can be restricted to $\mathbb{S}^{N-1}(\sqrt{\mathcal{E}N})$ the sphere with radius $\sqrt{\mathcal{E}N}$, for any given value of the *energy* $\mathcal{E}$. For the more realistic hard spheres of Maxwell molecules models, $d = 3$, the direction parameter is $\sigma \in \mathbb{S}^2$ with collision rule

$$v_i^* = \frac{v_i + v_j}{2} + \frac{|v_i - v_j|}{2}\,\sigma, \qquad v_j^* = \frac{v_i + v_j}{2} - \frac{|v_i - v_j|}{2}\,\sigma \qquad \text{with} \quad \sigma \cdot \frac{(v_i - v_j)}{|v_i - v_j|} = \cos\theta$$

and the collision process can be restricted to the sphere

$$\mathcal{S}^N := \mathbb{S}^{dN-1}\left(\sqrt{N\mathcal{E}}\right) \cap \{v_1 + \ldots + v_N = 0\}. \tag{2}$$

Kac formulated the notion of *propagation of chaos* that we shall now explain. Consider a sequence $(f^N)_{N \geq 1}$ of probabilities on $\mathbb{R}^{dN}$: the sequence is said *f-chaotic* if $f^N \sim f^{\otimes N}$ when $N \to \infty$ for some given one-particle probability f on $\mathbb{R}^d$. The meaning of this convergence is the following: convergence in the weak measure topology for any marginal depending on a finite number of variables. This is a *low correlation* assumption. It was clear since Boltzmann that in the case when the joint probability density f^N of the N-particle system is tensorized *during some time interval* into N copies $f^{\otimes N}$ of a 1-particle probability density, then the latter would satisfy the limit nonlinear Boltzmann equation during this time interval. In general interactions between particles prevent any possibility of propagation of the "tensorization" property, however if the weaker property of chaoticity can be propagated along time in the correct scaling limit it is sufficient for deriving the limit equation. Kac hence proved the propagation of chaos (with no rate) on the simplified collision rule above (with $B = 1$). His beautiful combinatorial argument is based on an infinite series "tree" representation of the solution according to the collision history of particles, and a Leibniz derivation-like formula for the iterated N-particle operator acting on tensor products.

He then raises several questions that we schematize as follows:

(i) The first one is concerned with the restriction of the models as compared to realistic collision processes: **can one prove propagation of chaos for the hard spheres collision process?**

(ii) Following closely the spirit of the previous question it seems to us very natural to ask whether **one can prove propagation of chaos for the true Maxwell molecules collision process**? This is related with *long-range interactions* and *fractional derivative operators*.

(iii) Kac **conjectures the propagation of the convergence of the N-particle H-functional towards the limit H-functional of the solution to the limit equation along time in the mean-field limit**. Since the latter always decays for a many-particle jump process, in his words "*If the above steps could be made rigorous we would have a thoroughly satisfactory justification of Boltzmann's H-theorem.*"

(iv) He finally discusses the relaxation times, with the goal of deriving relaxation times of the limit equation from the many-particle system. This imposes to have estimates *independent of the number of particles* on this relaxation times: **can one prove relaxation times** *independent of the number of particles* **in Wasserstein distance and/or relative entropy?**

This paper is concerned with solving the four questions outlined above.

2. Main results

2.1. *A few words on previous results*

For Boltzmann collision processes, Kac [9] has proved the propagation of chaos in the case of his baby one-dimensional model. It was generalized by McKean [14] to the Boltzmann collision operator for "Maxwell molecules with cutoff", i.e. the case **(GMM)** above (see also [19] for a partial result for non-cutoff Maxwell molecules). Grünbaum [8] then proposed in a very compact and abstract paper another method for dealing with hard spheres, based on the Trotter-Kato formula for semigroups and a clever functional framework. Unfortunately this paper was incomplete for several reasons (see the discussion in [15]). A completely different approach was undertaken by Sznitman in the eighties [17,18] and he gave a full proof of propagation of chaos for hard spheres by a probabilistic (non-constructive) approach. Let us also emphasize several quantitative results on a finite time interval by Graham, Méléard and Fournier for Maxwell molecules models [11,6,7], and the works on the so-called "Kac's spectral gap problem" [3,12,4,5].

2.2. *Main results*

Theorem 2.1 (Summary of the main results) *Consider some initial distribution $f_0 \in P(\mathbb{R}^d) \cap L^\infty$ with compact support or polynomial moment bounds, taken to be centered without loss of generality. Consider the corresponding solution f_t to the spatially homogeneous Boltzmann equation for hard spheres of Maxwell molecules, and the solution f_t^N of the corresponding Kac's jump process starting either (a) from the tensorization $f_0^{\otimes N}$ of f_0 or (b) the latter conditionned to $\mathcal{S}^N$ (defined in (2)).*

The results in [15] can be classified into three main statements:

(i) **Quantitative uniform in time propagation of chaos (with any number of marginals)***:*

$$\forall\, N \geq 1,\ \forall\, 1 \leq \ell \leq N, \quad \sup_{t \geq 0} \frac{W_1\left(\Pi_\ell f_t^N, \left(f_t^{\otimes \ell}\right)\right)}{\ell} \leq \alpha(N)$$

for some $\alpha(N) \to 0$ as $N \to \infty$, where $\Pi_\ell g^N$ stands for the ℓ-marginal of an N-particle distribution g^N, and where W_1 is the Wasserstein distance between probabilities on $\mathbb{R}^{d\ell}$:

$$W_1(p_1, p_2) := \sup_{[\varphi]_{\mathrm{Lip}(\mathbb{R}^{d\ell})} \leq 1} \int_{\mathbb{R}^{d\ell}} \varphi\,(dp_1 - dp_2) \qquad \text{where } [\cdot]_{\mathrm{Lip}} \text{ denotes the Lipschitz semi-norm.}$$

In the case (a) $f_0^N = f_0^{\otimes N}$ one has moreover explicit power law rate (for Maxwell molecules) or logarithmic rate (for hard spheres) estimates on α.

(ii) **Propagation of entropic chaos***: Consider the case (b) where the initial datum of the many-particle system is restricted to $\mathcal{S}^N$. Then if the initial datum is entropy-chaotic in the sense*

$$\frac{1}{N}\, H\left(f_0^N | \gamma^N\right) \to H\left(f_0 | \gamma\right), \quad N \to +\infty$$

$$\text{with} \quad H\left(f_0^N | \gamma^N\right) := \int_{\mathcal{S}^N} \frac{df_0^N}{d\gamma^N} \log \frac{df_0^N}{d\gamma^N}\, \gamma^N(dV) \quad \text{and} \quad H\left(f_0 | \gamma\right) := \int_{\mathbb{R}^d} f_0 \log \frac{f_0}{\gamma}\, dv \tag{3}$$

and where γ is the gaussian equilibrium with energy $\mathcal{E}$ and γ^N is the uniform probability measure on $\mathcal{S}^N$, then the solution is also entropy-chaotic for any later time:

$$\forall\, t \geq 0, \quad \frac{1}{N}\, H\left(f_t^N | \gamma^N\right) \to H\left(f_t | \gamma\right), \quad N \to +\infty.$$

Since our f_0^N is entropy-chaotic, this proves the derivation of the H-theorem in this context.

(iii) **Quantitative estimates on relaxation times, independent of the number of particles**: *Consider the case (b) where the initial datum of the many-particle system is restricted to $\mathcal{S}^N$. Then*

$$\forall\, N \geq 1, \ \forall\, 1 \leq \ell \leq N, \ \forall\, t \geq 0, \quad \frac{W_1\left(\Pi_\ell f_t^N, \Pi_\ell\left(\gamma^N\right)\right)}{\ell} \leq \beta(t) \qquad \text{with } \beta(t) \to 0, \ t \to 0.$$

Moreover in the case of Maxwell molecules, and assuming moreover that the Fisher information of the initial datum f_0 is finite:

$$\int\limits_{\mathbb{R}^d} \frac{|\nabla_v f_0|^2}{f_0}\, dv < +\infty, \tag{4}$$

the following estimate also holds: $\forall\, N \geq 1, \quad 0 \leq \frac{1}{N} H\left(f_t^N | \gamma^N\right) \leq \beta(t) \quad \text{with } \beta(t) \to 0, \ t \to 0.$

3. A few words on the methods and proofs

Let us briefly explain some ideas underlying the result Theorem 2.1-(i). The other results are then obtained on the basis of this key estimate, combined with the other latest results obtained in this field.

– We aim at reducing the problem to a stability analysis when approximating a linear semigroup. To this purpose a key idea is to compare the linear N-particle dual evolution in $C_b(\mathbb{R}^{dN})$ with the (linear!) *push-forward* evolution associated with the limit equation.

– This push-forward semigroup is defined as follows: if S_t^{NL} denotes the nonlinear semigroup of (1), this push-forward semigroup is defined on $P(P(\mathbb{R}^d))$ by $T_t^\infty[\Phi](f) = \Phi(S_t^{NL}(f))$.

– In order to make this comparison between semigroups, we use the empirical measure $\mu_V^N = (\sum_{i=1}^N \delta_{v_i})/N$ in order to embed the dynamics in $P(\mathbb{R}^{dN})$ into a dynamics in $P(P(\mathbb{R}^d))$.

– One then considers the following term to be estimated

$$\left| \left\langle \left(S_t^N(f_0^N) - \left(S_t^{NL}(f_0)\right)^{\otimes N} \right), \varphi \otimes 1^{\otimes N - \ell} \right\rangle \right|$$

for some test function φ only depending on ℓ variables.

– The approximation of these marginals by empirical measure estimates yields a first error term on the N-particle semigroup

$$\left| \left\langle S_t^N(f_0^N), \varphi \otimes 1^{\otimes N-\ell} \right\rangle - \left\langle S_t^N(f_0^N), R_\varphi^\ell \circ \mu_V^N \right\rangle \right| \qquad \text{with} \quad R_\varphi^\ell(f) := \int\limits_{\mathcal{R}^{d\ell}} \varphi\, f^{\otimes \ell}(dv_1 \ldots dv_\ell)$$

which is controlled by combinatorial arguments, and then a second error term

$$\left| \left\langle f_0^N, (T_t^\infty R_\varphi^\ell) \circ \mu_V^N) \right\rangle - \left\langle (S_t^{NL}(f_0))^{\otimes \ell}, \varphi \right\rangle \right|$$

which is controlled thanks a stability for measure solutions of the limit equation.

– Finally there remains the most important term where the two dynamics are effectively compared

$$\left| \left\langle f_0^N, T_t^N(R_\varphi^\ell \circ \mu_V^N) \right\rangle - \left\langle f_0^N, (T_t^\infty R_\varphi^\ell) \circ \mu_V^N) \right\rangle \right|.$$

This term is controlled by using (1) a quantitative argument à la Trotter-Kato in order to express the difference of semigroups in terms of the difference of their generators G^N and G^∞, (2) a *consistency estimate* between those generators, (3) a *stability estimate* on the limit equation.

– There is a *loss of derivative* in the consistency estimate in the sense of differentiable functions acting on $P(\mathbb{R}^d)$, which lead us to develop a differential calculus on this space adapted to our purpose.

– The stability estimate means, once translated on the original nonlinear semigroup S_t^{NL} of (1), a propagation of a bound $C^{1+\theta}(P(\mathbb{R}^d))$ on S_t^{NL}. The role played by such stability estimates is a key novelty of our study. Proving them for Boltzmann is also one of the most technical aspects of [15].

– There are many possible choices of distances on the space of probabilities (total variation but also many non-equivalent weak measure distances), and it is a crucial point that our method is flexible enough to allow for many such different choices adapted to the equations it is applied to.

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