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From hard spheres dynamics to the Stokes–Fourier equations: An L^2 analysis of the Boltzmann–Grad limit

De la dynamique des sphères dures aux équations de Stokes–Fourier : Une analyse L^2 de la limite de Boltzmann–Grad

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ABSTRACT

We derive the Stokes–Fourier equations in dimension 2 as the limiting dynamics of a system of N hard spheres of diameter ε when $N \to \infty$, $\varepsilon \to 0$, $N\varepsilon = \alpha \to \infty$, using the linearized Boltzmann equation as an intermediate step. Our proof is based on the strategy of Lanford [6], and on the pruning procedure developed in [3] to improve the convergence time. The main novelty here is that uniform a priori estimates come from a L^2 bound on the initial data, the time propagation of which involves a fine symmetry argument and a systematic study of recollisions.

RÉSUMÉ

Les équations de Stokes–Fourier sont obtenues, en dimension 2, comme dynamique limite d'un système de N sphères dures de diamètre ε quand $N \to \infty$, $\varepsilon \to 0$, $N\varepsilon = \alpha \to \infty$, en utilisant l'équation de Boltzmann linéarisée comme étape intermédiaire. Notre preuve est basée sur la stratégie de Lanford [6] et sur la procédure de troncature développée dans [3] pour améliorer le temps de convergence. La principale nouveauté ici est que les estimations a priori uniformes viennent d'une borne L^2 sur la donnée initiale, dont la propagation en temps repose sur un argument fin de symétrie et une étude systématique des recollisions.

Version française abrégée

On s'intéresse à la limite de faible densité pour un gaz de sphères dures de dimension 2 décrit par (1). Si, au temps initial, les particules sont indépendantes et identiquement distribuées, le théorème de Lanford montre que le chaos est

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propagé asymptotiquement quand $N \to \infty$, et que la distribution à une particule est proche de la solution de l'équation de Boltzmann non linéaire (2). Néanmoins, ce résultat n'est valable qu'en temps court, typiquement comme $O(1/\alpha)$, où α est l'inverse du libre parcours moyen. Une idée naturelle pour améliorer ce temps est de considérer de petites fluctuations autour de la mesure invariante (3). On considère ici une fluctuation symétrique d'ordre $1/N$.

Théorème 0.1 *([4]). Soit f_N^0 la donnée initiale définie par (5). On note $f_N(t)$ la distribution à N particules à l'instant t (transportée de f_N^0 par le flot de (1)). Alors*

- *la distribution à une particule $f_N^{(1)}(t,x,v)$ est proche de la solution de l'équation de Boltzmann linéarisée (4), au sens où elle vérifie l'estimation (7) dans la limite $N \to \infty$, $\varepsilon \to 0$, $N\varepsilon = \alpha$;*
- *la distribution à une particule $f_N^{(1)}(\alpha\tau,x,v)$ (remise à l'échelle en temps) converge vers la solution des équations de Stokes–Fourier (8) dans la limite $N \to \infty$, $\varepsilon \to 0$, $N\varepsilon = \alpha \to \infty$ avec $\alpha \ll \sqrt{\log\log\log N}$.*

La stratégie de la preuve suit les idées de [6,5,3]. La principale différence vient du fait que l'espace fonctionnel adapté à la donnée initiale considérée est de type L^2. En utilisant un argument de symétrie, on montre un développement du type (15) pour les marginales. Un contrôle fin des recollisions permet alors d'obtenir la continuité des opérateurs de collision et de contrôler la croissance des arbres de collision.

1. Introduction and main results

We consider a gas consisting of N hard spheres of diameter ε in a two-dimensional periodic box $\mathbf{T}^2$, with positions and velocities $(x_i, v_i)_{1\le i\le N} \in (\mathbf{T}^2 \times \mathbf{R}^2)^N$, the dynamics of which is

$$\frac{dx_i}{dt} = v_i\,, \quad \frac{dv_i}{dt} = 0 \quad \text{as long as } |x_i(t) - x_j(t)| > \varepsilon \quad \text{for } 1 \le i \ne j \le N\,, \tag{1}$$

with specular reflection after a collision. We are interested here in describing the macroscopic behavior in the low-density limit, i.e. as $N \to \infty$, $\varepsilon \to 0$, $N\varepsilon = \alpha$ with $\alpha = O(1)$ or converging very slowly to ∞.

If at initial time the particles are "independent" and identically distributed, it has been known since the work of Lanford [6] that chaos is propagated (asymptotically for $N >> 1$) and that the one-particle distribution is well approximated by the solution to the nonlinear Boltzmann equation:

$$\begin{aligned}(\partial_t + v\cdot\nabla_x) f(t,x,v) &= \alpha \int \Big(f(t,x,v^*)f(t,x,v_1^*) - f(t,x,v)f(t,x,v_1)\Big)\Big((v_1 - v)\cdot\nu\Big)_+ d\nu dv_1\,,\\ \text{with } v^* := v - (v - v_1)\cdot\nu\,\nu, &\quad v_1^* := v_1 + (v - v_1)\cdot\nu\,\nu\,.\end{aligned} \tag{2}$$

However, this convergence result holds only for very short times, typically like $O(1/\alpha)$. This is due to the fact that, forgetting about signs, the equation essentially looks like $\partial_t Y = \alpha Y^2$. Nevertheless, because of compensations between gain and loss terms, the Boltzmann equation admits global equilibria of the type $M_\beta(v) := \frac{\beta}{2\pi}\exp(-\beta\frac{|v|^2}{2})$, which are actually the limiting form (in the low density limit) of the invariant Gibbs measures for the N particle system:

$$M_{N,\beta}(x_1,v_1,\dots,x_N,v_N) := \frac{1}{\mathcal{Z}_N}\mathbf{1}_{\mathcal{D}_N}(x_1,\dots,x_N)\left(\frac{\beta}{2\pi}\right)^N \exp(-\beta\sum_{i=1}^N |v_i|^2)\,, \tag{3}$$

where $\mathcal{D}_N := \big\{(x_1,\dots,x_N) \in \mathbf{T}^{2N} \,/\, |x_i - x_j| > \varepsilon\,, \forall i \ne j\big\}$, and $\mathcal{Z}_N$ is the partition function.

A natural way to improve the lifespan of solutions is to consider small fluctuations around such an equilibrium. In [3], the motion of a tagged particle was analyzed, and the initial data was a perturbation of order 1 of the stationary state, namely a perturbation of this single tagged particle. The Boltzmann–Grad limit led to the linear Boltzmann equation. Contrary to that equation, the linearized Boltzmann equation

$$(\partial_t + v\cdot\nabla_x) g_\alpha = -\alpha \int M_\beta(v_1)\Big(g_\alpha(v) + g_\alpha(v_1) - g_\alpha(v^*) - g_\alpha(v_1^*)\Big)\Big((v_1 - v)\cdot\nu\Big)_+ d\nu dv_1 \tag{4}$$

describes the response of the whole system to a perturbation. Physically, if the distribution of a tagged particle is initially modified, the linearized equation records the impact of this particle on the rest of the system, which will modify by an order $1/N$ the distribution of each of the $N-1$ particles in the background. Thus one has to keep track of corrections of order $1/N$, as opposed to [3], where only the corrections of order 1 were relevant. We rephrase this problem in a symmetric way by considering the following initial data: writing $z_i := (x_i, v_i)$ and $Z_N := (z_1,\dots,z_N)$, we assume there is a function $g_{\alpha,0}$ such that $g_{\alpha,0}$ belongs to $L^\infty \cap \mathrm{Lip}$ and

$$f_{N,0}(Z_N) = M_{N,\beta}(Z_N)\sum_{i=1}^N g_{\alpha,0}(z_i) \qquad \text{with} \quad \int M_\beta g_{\alpha,0}(z)\,dz = 0\,. \tag{5}$$

The perturbation is now of order N and we are interested in the evolution of the first marginal. Using that $g_{\alpha,0}$ is mean free, and the bound $\mathcal{Z}_N^{-1} \le \exp(C\alpha^2)$ (valid in dimension 2 only), we then get

$$f_{N,0}(Z_N) \le N\|g_{\alpha,0}\|_\infty M_{N,\beta}(Z_N), \qquad \int \frac{f_{N,0}^2}{M_{N,\beta}}(Z_N)\,\mathrm{d}Z_N \le N\exp(C\alpha^2)\int M_\beta g_{\alpha,0}^2(z)\,\mathrm{d}z\,. \tag{6}$$

We shall take advantage of the invariance of the Gibbs measure $M_{N,\beta}$ to obtain a priori estimates that hold for all times, and enable us to prove the following result.

Theorem 1.1 *([4]). Consider the initial distribution f_N^0 defined in (5). The one-particle distribution $f_N^{(1)}(t,z)$ is close to $M_\beta(v)g_\alpha(t,z)$, where $g_\alpha(t,z)$ is the solution of the linearized Boltzmann equation (4) with initial data $g_{\alpha,0}(z)$. More precisely, there exist a continuous function ω with $\omega(0)=0$ and a non-negative constant C such that for all $t>0$ and all $\alpha>1$, in the limit $N\to\infty$, $N\varepsilon\alpha^{-1}=1$, one has*

$$\left\| f_N^{(1)}(t,z) - M_\beta(v)g_\alpha(t,z)\right\|_{L^1(\mathbf{T}^2\times\mathbf{R}^2)} \le \omega\left(\frac{t^3\,\mathrm{e}^{C\alpha^2}}{\log\log N}\right). \tag{7}$$

Note that a convergence to the linearized Boltzmann equation was first obtained in [2], but only for short times. Once Theorem 1.1 is known, it is possible to take the limit $\alpha\to\infty$ while conserving a small error on the right-hand side of (7). Rescaling time as $t=\alpha\tau$ and taking limits as $\alpha\to\infty$, we get the following diffusive approximation by the Stokes–Fourier dynamics.

Corollary 1.2 *([4]). Consider N hard spheres on the space $\mathbf{T}^2\times\mathbf{R}^2$, initially distributed according to f_N^0 defined in (5). Assume that the initial data is well prepared in the sense that g_0, the limit in $L^2(M_\beta \mathrm{d}x\mathrm{d}v)$ of $g_{\alpha,0}$ when $\alpha\to\infty$, satisfies*

$$g_0(x,v) = u_0(x)\cdot v + \frac{|v|^2-4}{2}\theta_0(x) \quad \text{with} \quad u_0,\theta_0 \text{ in } L^\infty, \quad \nabla_x\cdot u_0 = 0\,.$$

Then as $N\to\infty$, $N\varepsilon=\alpha\to\infty$ slower than $\sqrt{\log\log\log N}$, the distribution $f_N^{(1)}(\alpha\tau,x,v)$ remains close in L^1-norm to $M_\beta g$ where $g(\tau,x,v) := u(\tau,x)\cdot v + \frac{|v|^2-4}{2}\theta(\tau,x)$ and (u,θ) satisfies the Stokes–Fourier equations with initial data (u_0,θ_0):

$$\partial_\tau u - \nu_\beta\Delta_x u = 0\,, \quad \nabla_x\cdot u = 0\,, \quad \partial_\tau\theta - \kappa_\beta\Delta_x\theta = 0 \tag{8}$$

with

$$\nu_\beta := \int \phi\mathcal{L}_\beta^{-1}\phi M_\beta(v)\,\mathrm{d}v \quad \text{with} \quad \phi(v) = (v\otimes v - \frac{|v|^2}{2}Id)\,,$$
$$\kappa_\beta := \frac{1}{2}\int \psi\mathcal{L}_\beta^{-1}\psi M_\beta(v)\,\mathrm{d}v \quad \text{with} \quad \psi(v) = v\left(\frac{|v|^2}{2}-2\right).$$

Remark 1. For general not well prepared initial data, the asymptotics is also well known (see [1]). It is a superposition of

- the mean motion described by the Stokes–Fourier equation;
- fast oscillations governed by the acoustic operator on time scale $O(\alpha^{-1})$;
- an initial relaxation layer of size $O(\alpha^{-2})$ if the initial profile is not a fluctuation of a local infinitesimal Maxwellian.

2. General strategy

The proof of Theorem 1.1 is built on the strategy of Lanford [6] and the improvements in [5]. The Liouville equation can be rewritten as the BBGKY hierarchy that describes the evolution of the marginals

$$\forall s\le N, \qquad \partial_t f_N^{(s)} + \sum_{i=1}^s v_i\cdot\nabla_{x_i} f_N^{(s)} = \alpha C_{s,s+1} f_N^{(s+1)} \text{ on } \mathcal{D}_s\times\mathbf{R}^{2s}\,, \tag{9}$$

where the collision operator is defined by

$$\begin{aligned}\big(C_{s,s+1}f_N^{(s+1)}\big)(Z_s) := \frac{(N-s)\varepsilon}{\alpha}\Big(\sum_{i=1}^s\int f_N^{(s+1)}(\dots,x_i,v_i^*,\dots,x_i+\varepsilon\nu,v_{s+1}^*)\Big((v_{s+1}-v_i)\cdot\nu\Big)_+\mathrm{d}\nu\,\mathrm{d}v_{s+1}\\ -\sum_{i=1}^s\int f_N^{(s+1)}(\dots,x_i,v_i,\dots,x_i+\varepsilon\nu,v_{s+1})\Big((v_{s+1}-v_i)\cdot\nu\Big)_-\mathrm{d}\nu\,\mathrm{d}v_{s+1}\Big).\end{aligned}$$

Understanding the limiting behavior of (9) in the Boltzmann–Grad scaling $N\varepsilon = \alpha$ reduces to proving the convergence of the BBGKY hierarchy to the limiting Boltzmann hierarchy.

The first step to prove the convergence is to rewrite the evolution of the first marginal $f_N^{(1)}$ by the iterated Duhamel formula

$$f_N^{(1)}(t) = \sum_{n=0}^{N-1} Q_{1,n+1}(t) f_{N,0}^{(n+1)}, \tag{10}$$

where $Q_{1,n+1}$ encodes n collisions and $\mathbf{S}_k$ is the transport operator with exclusion for k particles

$$Q_{1,n+1}(t) := \alpha^n \int_0^t \int_0^{t_2} \dots \int_0^{t_{n-1}} \mathbf{S}_1(t-t_2) C_{1,2} \mathbf{S}_2(t_2 - t_3) C_{2,3} \dots \mathbf{S}_{1+n}(t_{1+n}) \, \mathrm{d}t_2 \dots \mathrm{d}t_n \,. \tag{11}$$

This operator can be interpreted as a sum over trees in which each *collision* corresponds to a creation of a new particle. The main difference between the BBGKY hierarchy and the limiting Boltzmann hierarchy is that the free transport on $\mathbf{T}^{2s}$ does not coincide with the transport $\mathbf{S}$ on $\mathcal{D}_s$. We will use the word *recollision* when two particles encounter in flow $\mathbf{S}$.

To prove the convergence of the series (10) in the Boltzmann–Grad scaling $N\alpha^{-1}\varepsilon = 1$, the L^∞-functional setting was used in [6]. The collision operator is bounded in weighted L^∞ spaces (with exponential decay in v) denoted by $\tilde{L}^\infty$:

$$\left\| \int_0^t \mathrm{d}t_1 \mathbf{S}_s(t-t_1) C_{s,s+1} \mathbf{S}_{s+1}(t_1) h_{s+1} \right\|_{\tilde{L}^\infty} \leq Cst \|h_{s+1}\|_{\tilde{L}^\infty} \,. \tag{12}$$

For general initial data, a Cauchy–Kowalewski argument can be implemented to obtain the convergence of the series expansion for short times [6,5]. Thus, only the first terms of the series are relevant in the limit behavior of (10). They are interpreted as collision trees with a small number of collisions and they converge termwise. Indeed, one can show by a geometric argument that recollisions occur for a small set of initial configurations and outside this set, the transport $\mathbf{S}$ with exclusion coincides with the free transport.

The main difficulty to generalize this approach to a longer time range is a control of the large collision trees. This was achieved in [3], for a perturbation of the stationary measure such that the initial data satisfies $f_N^0 \leq CM_{N,\beta}$. Under this assumption, the convergence time can be extended, since we have uniform, global in time a priori $\tilde{L}^\infty$ estimates for all marginals thanks to the maximum principle: for all t, $f_N^{(s)}(t) \leq CM_{N,\beta}^{(s)}$. The analysis distinguishes between collision trees with super-exponential growth and collision trees with sub-exponential growth:

- for collision trees with sub-exponential growth, the geometric argument can be applied directly to control the difference between the BBGKY and the Boltzmann dynamics;
- the main novelty in [3] is to prove that the contribution of super-exponential trees is negligible. This is done thanks to a pruning procedure, splitting the macroscopic time interval $[0,t]$ in small intervals of size h, and stopping the backwards expansion of collision trees on the first interval k, for which the branching process shoots up (meaning that the tree has more than 2^k branching points). Note that this can be done because we know a priori that $f_N^{(s)}(t-kh) \leq CM_{N,\beta}^{(s)}$.

The a priori estimate (6) is much worse than in [3]: $f_{N,0} \leq CNM_{N,\beta}$ and the divergence in N prevents us from applying the L^∞ strategy explained above; the difficult part of the proof is the control of the large collision trees. The idea is to exploit the better L^2 estimate (6) and to bound the collision operators $C_{s,s+1}$ in L^2. More precisely, the L^2 estimate will be crucial for trees with at most one recollision and the L^∞ estimate will be used for trees with more than one recollision.

3. L^2-estimates: control of super exponential trees with at most one recollision

The operator $C_{s,s+1}$ is ill-defined in L^2 (as it acts on hypersurfaces) and it has to be combined with the transport operator to recover the missing dimension (see [5] Section 5). Geometrically the integral $\int_0^t \mathrm{d}t_1 \mathbf{S}_s(t-t_1) C_{s,s+1}^- \mathbf{S}_{s+1}(t_1) h_{s+1}$ can be interpreted as a configuration Z_s evolving backward to which a particle is added with velocity v_{s+1} and deflection angle ν_{s+1}. Consider the corresponding mapping

$$(Z_s, \nu_{s+1}, v_{s+1}, \tau) \mapsto Z_{s+1} = \mathbf{\Psi}_{s+1}(\tau, X_s, V_s, x_i + \varepsilon\nu_{s+1}, v_{s+1}), \tag{13}$$

where $\mathbf{\Psi}_{s+1}$ denotes the transport with exclusion. This mapping preserves the measure, but it is not a bijection due to possible recollisions arising in the flow. If no recollision occurs, then the transport $\mathbf{S}$ coincides with the free transport $\mathbf{S}^0$ and, using the change of variables (13), one can prove that for weighted L^2 norms denoted by $\tilde{L}^2$

$$\left\| \int_0^t \mathrm{d}\tau C_{s,s+1} \mathbf{S}_{s+1}^0(-\tau) h_{s+1} \right\|_{\tilde{L}^2} \leq C \sqrt{\frac{st}{\varepsilon}} \|h_{s+1}\|_{\tilde{L}^2} \,. \tag{14}$$

In the case of $C^+_{s,s+1}$, a change of variables involving the scattering operator leads to the same bound. If a single recollision occurs, the mapping (13) is quasi-bijective and a bound similar to (14) still holds. For configurations leading to multiple recollisions, a different strategy based on L^∞ estimates will be explained in Section 4. At first sight, the L^2-norm (14) of $C_{s,s+1}$ is worse than the L^∞-norm (12), as it diverges as $\varepsilon^{-1/2}$. Thus is cannot be used directly to control $f_N^{(s)}$. To overcome this problem, the key idea is to use the exchangeability to decompose the marginals in terms of symmetric functions $g_N^{(i)} \in \tilde{L}^2$

$$f_N^{(s)}(t, Z_s) = M_\beta^{\otimes s} \sum_{i=1}^{s} \sum_{\sigma \in \mathfrak{S}_s^i} g_N^{(i)}(t, Z_\sigma) \quad \text{with} \quad \|g_N^{(i)}\|^2_{\tilde{L}^2} \le \frac{CN \exp(C\alpha^2)}{C_N^i} \|g_{\alpha,0}\|^2_{\tilde{L}^2}, \tag{15}$$

where $\mathfrak{S}_s^i$ denotes the set of all parts of $\{1, \dots, s\}$ with i elements. Intuitively, the structure of the initial data (5) should be preserved in the leading term of the distribution:

$$f_N(t, Z_N) \simeq M_{N,\beta}(Z_N) \sum_{i=1}^{N} g^{(1)}(t, z_i) \quad \text{with} \quad \int M_\beta \, g^{(1)}(t, z) \, dz = 0 .$$

However the dynamics induce weak correlations between the particles and thus corrections to the measure. The decomposition (15) encodes the fact that the higher-order correlations decrease in L^2-norm according to the number of particles. This is a step towards proving local equilibrium, but these estimates are not strong enough to deduce directly the propagation of chaos. The measure decomposition (15) is proved by combining the a priori estimate (6) and the exchangeability of the variables.

To evaluate the operator $Q_{1,s+1}$ on a function of the form $M_\beta^{\otimes s} g_N^{(i)}(t, Z_\sigma)$ (with $i \le s < N/2$), the idea is to iterate $i-1$ times the L^2-bound (14) as $s+1-i$ coordinates of this function are distributed according to the stationary state and can be analyzed in a simpler way. Thus the idea is to balance the divergence in $\sqrt{\varepsilon^{i-1}}$ by the norm of $g_N^{(i)}$ (15), which vanishes as $\frac{1}{\sqrt{N^{i-1}}}$. Compared to the L^∞ framework, extra care is required to bound the L^2 contribution of the large trees.

4. L^∞-estimates: control of super exponential trees with more than one recollision

Consider a collision tree with s particles and total energy bounded by $R \sim |\log \varepsilon|$. When particle $s+1$ is added to the collision tree, then a small set of velocities may lead to a recollision with one of the other particles in the tree. If all the particles are far apart, the occurrence of a recollision before a time τ has a cost of order $\tau\,\varepsilon$. However, as particles might get closer to each other, the cost of a recollision is slightly larger and cannot compensate the divergence in $N = \varepsilon^{-1}$ of the L^∞ estimate of $f_N(t)$. Thus the cost of a second recollision has to be estimated. If the dynamics has at least two recollisions, then one can identify at most four collision operators encoding these recollisions and for which the constraints on the set of parameters (collision times, impact parameter and velocity of the additional particles) lead to a cost $O(\varepsilon)$. Note that this estimate is optimal when the two recollisions follow each other.

This additional smallness balances the divergence of the L^∞ norm and allows us to use L^∞ bounds as in [3] to control the super exponential trees with at least two recollisions.

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