Derivation of Hydrodynamic Limits from either the Liouville Equation or Kinetic Models: Study of an Example

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dedicated to Seiji Ukai on his 60th birthday

Abstract

Hydrodynamic limits can be derived, either formally from the N body Liouville equation, or from the Boltzmann equation. In the latter case, some mathematical proofs of these derivations have been proposed in the last 20 years. However, both derivations may rely on different scaling assumptions and could lead to different equations of state. We first discuss this issue on the derivation of the compressible Euler equation from either the N-body Liouville equation or the Boltzmann equation. Then we study two examples where complete mathematical proofs have been given: the periodic Lorentz gas, and a Knudsen gas with non classical gas-surface interaction (modeling the impingement of gas molecules on a rough surface).

1. Introduction

The general problem of deriving the physical properties of macroscopic bodies from the microscopic dynamics of its elementary constituents (molecules, ions, atoms...) has been the driving force leading to the foundation of statistical mechanics. More precisely, it seems that this very basic and general question received a mathematical formulation only after the pioneering achievements of Maxwell and Boltzmann in the kinetic theory of gases.

Yet, the status of the kinetic theory of gases in the derivation of the macroscopic limits from microscopic first principle dynamics is ambiguous. Indeed, the Boltzmann equation can be derived rigorously from the classical dynamics of a large number of hard spheres of vanishingly small radius. Also, the classical models of fluid mechanics can be derived, more or less rigorously from the Boltzmann equation. However, to this date, there is no direct derivation of the Euler or Navier-Stokes equations from the classical N body problem, and the existing attempts at formal derivations of these models sometimes lead to local equilibrium states and equations of states that may be noticeably different from the ones obtained from the Boltzmann equation.

In the present paper, we propose a few examples of this situation. In section 2, we show how a formal derivation of the compressible Euler equation from the N-body Liouville equation may lead to different equations of state than the perfect gas pressure law which one gets in the derivation from the Boltzmann equation. In sections 3 and 4, we discuss two examples of particle systems the macroscopic behavior of which is described by a diffusion equation that can be derived either directly from the particle system or from a kinetic model describing its mesoscopic dynamics. However, even though both the original particle system or the kinetic model lead to the same type of macroscopic equation, namely a diffusion equation, the diffusion coefficients obtained from both derivations happen to be different. Thus, kinetic models sometimes may fail to capture the correct macroscopic dynamics of particles systems.

Nevertheless, even if the mathematical theory of gas dynamics remains the source of some of the most challenging open problems in mathematics, we have gained some partial understanding of this question of macroscopic limits. Undoubtedly, the progress made in the last 25 years in the mathematical theory of the Boltzmann equation paved the way to the theory of hydrodynamic limits as it now stands. Seiji Ukai contributed greatly to this progress, by giving the first proof of global existence and uniqueness of a solution to the Cauchy problem for the Boltzmann equation [U]. Therefore, we offer this little essay to our friend and colleague in recognition of the influence that his scientific achievements have had on some of the topics touched here.

2. The Euler Limit

Consider a gas made of N like particles of mass m the motion of which is described by Newton's law of Mechanics expressed in the form of the Hamilton equations for the Hamiltonian function given by

$$H_N \equiv \tfrac{1}{2}m\sum_{i=1}^{N}|v_i|^2 + m^2\sum_{1\le i<j\le N}\Phi(|x_i-x_j|)\,, \tag{2.1}$$

where $\Phi : \mathbf{R}_+^* \to \mathbf{R}_+^*$ is a smooth nonincreasing function (so that the interparticle force is indeed repulsive).

First pick a length scale σ for the apparent radius of the particles. One way of doing this is by first prescribing a velocity scale c (that one can think of as the mean thermal speed of the gas) and define σ by the formula $2m\Phi(\sigma) = c^2$. With this apparent radius so defined, the potential is rescaled as follows:

$$m\Phi(r) = U\left(\frac{r}{\sigma}\right)\,, \qquad r > 0\,, \tag{2.2}$$

where $U : \mathbf{R}_+^* \to \mathbf{R}_+^*$.

Next think of all these particles as moving in the whole space $\mathbf{R}^3$, with a reference volume $\mathcal{V}$ which sets the macroscopic length scale to $\mathcal{V}^{1/3}$. Intuitively, the mean free path of these particles should be a length scale that is inversely proportional to the number of particles per unit volume times the cross section of each individual particle; this suggests the formula

$$\text{mean free path } = \frac{\mathcal{V}}{N\pi\sigma^2}\,. \tag{2.3}$$

Another natural notion is that of "packed volume" occupied by the gas (i.e. the sum of the volumes occupied by each molecule viewed as a hard sphere of radius σ):

$$\text{packed volume } = N\tfrac{4}{3}\pi\sigma^3\,. \tag{2.4}$$

Thus we can define a dimensionless number R by the formula

$$R = \frac{\text{packed volume}}{\mathcal{V}} = \frac{4}{3}\frac{\sigma}{\text{mean free path}}\,. \tag{2.5}$$

We study macroscopic limits of the system of particles above by keeping the volume $\mathcal{V}$ fixed, letting $N \to \infty$ and $\sigma \to 0$. However these assumptions are compatible with $R \to R_*$ with either $R_* = 0$ or $R_* \in]0,1[$.

Consider now the Liouville equation for $F_N \equiv F_N(t, x_1, v_1, \dots, x_N, v_N)$ (the N particle distribution function):

$$\partial_t F_N + \sum_{1\le i\le N} v_i \cdot \nabla_{x_i} F_N = \tfrac{1}{2} \sum_{1\le i\le N} \left(\sum_{1\le j\ne i\le N} \frac{1}{\sigma} U' \left(\frac{|x_i - x_j|}{\sigma} \right) \frac{x_i - x_j}{|x_i - x_j|} \right) \cdot \nabla_{v_i} F_N \quad (2.6)$$

with an initial data

$$F_N(0, x_1, v_1, \dots, x_N, v_N) = F_N^{in}(x_1, v_1, \dots, x_N, v_N) \quad (2.7)$$

which is symmetrical in all the particle coordinates in phase space. In other words, it is assumed that, for any permutation τ of $\{1, \dots, N\}$,

$$F_N^{in}(x_1, v_1, \dots, x_N, v_N) = F_N^{in}(x_{\tau(1)}, v_{\tau(1)}, \dots, x_{\tau(N)}, v_{\tau(N)}) \,. \quad (2.8)$$

It is easily seen that this symmetry is preserved by the Hamiltonian flow so that for all $t > 0$ and all $x_1, v_1, \dots, x_N, v_N$,

$$F_N(t, x_1, v_1, \dots, x_N, v_N) = F_N(t, x_{\tau(1)}, v_{\tau(1)}, \dots, x_{\tau(N)}, v_{\tau(N)}) \,. \quad (2.9)$$

Next introduce the marginals of the density F_N:

$$F_N^k(x_1, v_1, \dots, x_k, v_k) =$$
$$\int F_N^k(x_1, v_1, \dots, x_k, v_k, x_{k+1}, v_{k+1}, \dots, x_N, v_N) dx_{k+1} dv_{k+1} \dots dx_N dv_N \,; \quad (2.10)$$

The formal derivation of the Euler equation outlined below requires only partial information concerning the marginals of the N-particle distribution F_N. In particular, we try to delineate the minimal set of assumptions needed for this derivation.

First, the equation for the first marginal, can be obtained from (2.6) by integration in all variables but t, x_1 and v_1:

$$\partial_t F_N^1 + v_1 \cdot \nabla_{x_1} F_N^1 = \tfrac{1}{2}(N-1) \nabla_{v_1} \cdot \int \frac{1}{\sigma} U' \left(\frac{|x_1 - x_2|}{\sigma} \right) \frac{x_1 - x_2}{|x_1 - x_2|} F_N^2(t, x_1, v_1, x_2, v_2) dx_2 dv_2 \,. \quad (2.11)$$

In order to obtain local conservation laws for macroscopic quantities, one multiplies (2.11) successively by 1, v_1 and $\frac{1}{2}|v_1|^2$, and integrate in v_1, which leads to local conservation laws for the moments of F_N^1 of order less than or equal to 2.

At this point the importance of the scaling appears and, following the beautiful analysis due to Morrey [Mo], one introduces a "fast " variable $\xi = (x_2 - x_1)/\sigma$ and define a new 2-point distribution function by the formula

$$G_N^2(t, x_1, v_1, \xi, v_2) = F_N^2(t, x_1, v_1, x_1 + \sigma\xi, v_2)\,. \tag{2.12}$$

In terms of G_N^2, the local conservation laws of mass, momentum and energy are

$$\partial_t \int F_N^1 dv_1 + \nabla_{x_1} \cdot \int v_1 F_N^1 dv_1 = 0\,, \tag{2.13}$$

$$\begin{aligned}\partial_t \int v_1 F_N^1 dv + \nabla_{x_1} \cdot \int v_1 \otimes v_1 F_N^1 dv_1 = \\ -\tfrac{1}{2}(N-1)\sigma^3 \iiint \frac{1}{\sigma} U'(|\xi|)\frac{\xi}{|\xi|} G_N^2(t, x_1, v_1, \xi, v_2) d\xi dv_2 dv_1\,,\end{aligned} \tag{2.14}$$

$$\begin{aligned}\partial_t \int \tfrac{1}{2}|v_1|^2 F_N^1 dv + \nabla_{x_1} \cdot \int v_1 \tfrac{1}{2}|v_1|^2 F_N^1 dv_1 = \\ -\tfrac{1}{2}(N-1)\sigma^3 \iiint \frac{1}{\sigma} U'(|\xi|)\frac{\xi}{|\xi|} \cdot v_1 G_N^2(t, x_1, v_1, \xi, v_2) d\xi dv_2 dv_1\,.\end{aligned} \tag{2.15}$$

Consider first the right hand side of (2.14). By the symmetry (2.9),

$$\begin{aligned}G_N^2(t, x_1, v_1, \xi, v_2) = F_N^2(x_1, v_1, x_1 + \sigma\xi, v_2) &= F_N^2(x_1 + \sigma\xi, v_2, x_1, v_1) \\ &= G_N^2(t, x_1 + \sigma\xi, v_2, -\xi, v_1)\end{aligned} \tag{2.16}$$

Thus

$$\begin{aligned}&\iiint \frac{1}{\sigma} U'\left(|\xi|\right) \frac{\xi}{|\xi|} G_N^2(t, x_1, v_1, \xi, v_2) d\xi dv_2 dv_1 \\ &= \iiint -\frac{1}{\sigma} U'\left(|\xi|\right) \frac{\xi}{|\xi|} G_N^2(t, x_1 - \sigma\xi, v_2, \xi, v_1) d\xi dv_2 dv_1 \\ &= \iiint -\frac{1}{\sigma} U'\left(|\xi|\right) \frac{\xi}{|\xi|} G_N^2(t, x_1 - \sigma\xi, v_1, \xi, v_2) d\xi dv_2 dv_1 \\ &= \tfrac{1}{2} \iiint U'\left(|\xi|\right) \frac{\xi}{|\xi|} \left[\frac{G_N^2(t, x_1, v_1, \xi, v_2) - G_N^2(t, x_1 - \sigma\xi, v_1, \xi, v_2)}{\sigma}\right] d\xi dv_2 dv_1\,.\end{aligned} \tag{2.17}$$

If the families F_N^1 and G_N^2 satisfy the following condition

$$\begin{aligned}(1 + |v_1|^2) F_N^1 \text{ is relatively compact in } w\text{-}L_t^\infty(L^1_{x_1,v_1}) \\ \text{and } |\xi||U'(|\xi|)|G_N^2 \text{ is relatively compact in } w\text{-}L_t^\infty(L^1_{x_1,v_1})\end{aligned} \tag{2.18}$$

then, up to extraction of a subsequence, $F_N^1 \to F^1$ and $G_N^2 \to G^2$ as $N \to +\infty$ and

$$\tfrac{1}{2} \iiint U'(|\xi|) \frac{\xi}{|\xi|} \left[\frac{G_N^2(t,x_1,v_1,\xi,v_2) - G_N^2(t,x_1-\sigma\xi,v_1,\xi,v_2)}{\sigma} \right] d\xi dv_2 dv_1$$

$$\to \tfrac{3}{16\pi} R_* \nabla_x \cdot \iiint U'(|\xi|) \frac{\xi \otimes \xi}{|\xi|} G^2(t,x_1,v_1,\xi,v_2) d\xi dv_2 dv_1 \,.$$

Eventually,

$$\partial_t \int v_1 F_N^1 dv + \nabla_{x_1} \cdot \int v_1 \otimes v_1 F_N^1 dv_1 =$$

$$\tfrac{3}{16\pi} R_* \nabla_x \cdot \iiint U'(|\xi|) \frac{\xi \otimes \xi}{|\xi|} G^2(t,x_1,v_1,\xi,v_2) d\xi dv_2 dv_1 \,. \tag{2.19}$$

The right hand side of (2.15) is handled by a similar procedure, as follows. First integrate the Liouville equation (2.6) in all variables but t, x_1 and x_2:

$$\partial_t \iint F_N^2 dv_1 dv_2 + \nabla_{x_1} \cdot \iint v_1 F_N^2 dv_1 dv_2 + \nabla_{x_2} \cdot \iint v_2 F_N^2 dv_1 dv_2 = 0 \,. \tag{2.20}$$

Multiply then (2.20) by $U(\frac{|x_1-x_2|}{\sigma})$ and integrate in x_2:

$$\partial_t \iiint U\left(\frac{|x_1-x_2|}{\sigma}\right) F_N^2 dx_2 dv_1 dv_2 + \nabla_{x_1} \cdot \iiint v_1 U\left(\frac{|x_1-x_2|}{\sigma}\right) F_N^2 dx_2 dv_1 dv_2 =$$

$$\frac{1}{\sigma} \iiint U'\left(\frac{|x_1-x_2|}{\sigma}\right) (v_1-v_2) \cdot \frac{x_1-x_2}{|x_1-x_2|} F_N^2(t,x_1,v_1,x_2,v_2) dx_2 dv_1 dv_2$$

which can be recast in terms of G_N^2 as

$$\partial_t \iiint U(|\xi|) G_N^2 d\xi dv_1 dv_2 + \nabla_{x_1} \cdot \iiint v_1 U(|\xi|) G_N^2 d\xi dv_1 dv_2 =$$

$$\frac{1}{\sigma} \iiint U'(|\xi|)(v_1-v_2) \cdot \frac{\xi}{|\xi|} G_N^2(t,x_1,v_1,\xi,v_2) d\xi dv_1 dv_2 \tag{2.21}$$

Substituting (2.21) in (2.15) gives

$$\partial_t \left[\int \tfrac{1}{2}|v_1|^2 F_N^1 dv + \tfrac{1}{4}(N-1)\sigma^3 \iiint U(|\xi|) G_N^2 d\xi dv_1 dv_2 \right]$$

$$+\nabla_{x_1} \cdot \left[\int v_1 \tfrac{1}{2}|v_1|^2 F_N^1 dv_1 + \tfrac{1}{4}(N-1)\sigma^3 \iiint v_1 U(|\xi|) G_N^2 d\xi dv_1 dv_2 \right] =$$

$$-\tfrac{1}{4}(N-1)\sigma^3 \iiint \frac{1}{\sigma}U'\left(\frac{|\xi|}{\sigma}\right)\frac{\xi}{|\xi|}\cdot(v_1+v_2)G_N^2(t,x_1,v_1,\xi,v_2)d\xi dv_2 dv_1\,. \tag{2.22}$$

If the condition (2.18) is strengthened into

$$\begin{gathered}(1+|v_1|^3)F_N^1 \text{ is relatively compact in } L_t^\infty(L^1_{x_1,v_1})\\ (|\xi||U'(|\xi|)|+U(|\xi|))(1+|v_1|+|v_2|)]G_N^2 \text{ is relatively compact in } w\text{-}L_t^\infty(L^1_{x_1,v_1,\xi,v_2})\end{gathered} \tag{2.23}$$

then, again up to extraction of a subsequence, $G_N^2 \to G^2$ as $N \to +\infty$ and, by the same symmetry trick as in (2.17)

$$\begin{aligned}&\partial_t\left[\int \tfrac{1}{2}|v_1|^2F^1dv + \tfrac{3}{16\pi}R_*\iiint U(|\xi|)G^2d\xi dv_1dv_2\right]\\ &+\nabla_{x_1}\cdot\left[\int v_1\tfrac{1}{2}|v_1|^2F^1dv_1 + \tfrac{3}{16\pi}R_*\iiint v_1U(|\xi|)G^2d\xi dv_1dv_2\right]\\ &= -\tfrac{3}{32\pi}R_*\nabla_{x_1}\cdot\iiint U'(|\xi|)\frac{\xi\otimes\xi}{|\xi|}\cdot(v_1+v_2)G^2(t,x_1,v_1,\xi,v_2)d\xi dv_2dv_1\,.\end{aligned} \tag{2.24}$$

At this point, the Euler system for compressible fluids can be derived from the system (2.13)-(2.19)-(2.24) under a closing assumption on F_1 and G^2 which we discuss below.

The classical continuity equation

$$\partial_t\rho + \nabla_{x_1}(\rho u) = 0 \tag{2.25}$$

follows directly from (2.13) without any further assumption, by defining the macroscopic density ρ and bulk velocity u by

$$\int F^1(t,x_1,v_1)dv_1 = \rho(t,x_1)\,,\qquad \int v_1F^1(t,x_1,v_1)dv_1 = \rho u(t,x_1)\,. \tag{2.26}$$

The closure proposed here in order to write the momentum and energy equations consists in assuming that

$$F^1(t,x_1,v_1) = \frac{\rho(t,x_1)}{(2\pi\theta(t,x_1))^{3/2}}\exp\left(-\frac{|v_1-u(t,x_1)|^2}{2\theta(t,x_1)}\right) \tag{2.27}$$

i.e. that F^1 is a local Maxwellian, while G^2 is of the form

$$G^2(t,x_1,v_1,\xi,v_2) =$$

$$\frac{\rho(t,x_1)}{(2\pi\theta(t,x_1))^3}C(|\xi|,\theta(t,x_1))\exp\left(-\frac{|v_1-u(t,x_1)|^2+|v_2-u(t,x_1)|^2+2U(|\xi|)}{2\theta(t,x_1)}\right)\,. \tag{2.28}$$

Then one finds that

$$\partial_t(\rho u)+\nabla_{x_1}(\rho u\otimes u)+\nabla_x p=0 \tag{2.29}$$

with a pressure law given by

$$p=\rho\left[\theta-\tfrac{1}{16\pi}R_*\iiint U'(|\xi|)|\xi|C(|\xi|,\theta)e^{-\frac{U(|\xi|)}{\theta}}\right]\,. \tag{2.30}$$

Now the energy equation reads

$$\partial_t E+\nabla_x\cdot[u(E+p)]=0 \tag{2.31}$$

with energy density

$$E=\rho\left[\tfrac{1}{2}|u|^2+\tfrac{3}{2}\theta+\tfrac{3}{16\pi}R_*\iiint U(|\xi|)C(|\xi|,\theta)e^{-\frac{U(|\xi|)}{\theta}}d\xi\right] \tag{2.32}$$

Thus, we have derived the compressible Euler system (2.25)-(2.29)-(2.31) with the equation of state (2.30)-(2.32), under assumption (2.23). Notice that, if $R_*=0$, the equation of state (2.30)-(2.32) reduces to the usual perfect gas law

$$p=\rho\theta\,,\quad E=\rho\left[\tfrac{1}{2}|u|^2+\tfrac{3}{2}\theta\right]\,. \tag{2.33}$$

It is particularly remarkable that this compressible Euler system for perfect gases can (under certain regularity assumptions, see [Ni], [Ca]) be derived from the Boltzmann equation, for example in the case of a hard sphere gas. The compressible Euler limit of the Boltzmann equation does not depend on the kind of particle interaction considered (cutoff hard potentials — see [Ce] p. 67–71 for this terminology — or hard sphere gases formally converge to the same Euler limit). At this point, it may be worthwhile to recall that the Boltzmann equation has been rigorously derived from the classical dynamics of a gas of N hard spheres of radius σ in the so-called Boltzmann-Grad limit, which means that

$$N\to+\infty \text{ and } \sigma\to 0\,,\qquad \text{with } \frac{N\pi\sigma^2}{\mathcal{V}}\to\frac{1}{l}\in\mathbf{R}_+^*\,. \tag{2.33}$$

In the terminology of (2.3)-(2.5), this corresponds to the scaling where

$$R=\tfrac{4}{3}\frac{\sigma}{l}\,. \tag{2.34}$$

The compressible Euler limit of the Boltzmann equation is obtained under the scaling assumption that the Knudsen number, defined as the ratio of the mean free path to a macroscopic length scale of the flow (which can for example be taken as $\mathcal{V}^{1/3}$)

$$Kn = \frac{l}{\mathcal{V}^{1/3}} \to 0 \,. \tag{2.35}$$

However, there is a double asymptotics in this type of derivation (from particles to Boltzmann and then to the compressible Euler system) which prevents from considering the case where $\sigma \sim l$ as $N \to +\infty$ and $\sigma \to 0$.

Next we discuss our closure assumption (2.33). The limiting form G^2 is suggested by looking at Gibbs distributions for the N particle system. Observe indeed that, since the Hamiltonian (2.1) is invariant under the translations

$$x_1 \mapsto X + x_1 \,, \dots \,, \; x_N \mapsto X + x_N \,,$$

it commutes with the total momentum density

$$m \sum_{i=1}^{N} v_i \,.$$

In particular, a class of special equilibrium solutions of the Liouville equation (2.6) is given by the formula below (which can be referred to as an absolute Gibbs ansatz with parameters $\rho > 0$, $\theta > 0$ and $u \in \mathbf{R}^3$)

$$F_N(x_1, v_1, \dots, x_N, v_N) = \frac{\rho}{(2\pi\theta)^{3N/2}} \exp\left[\frac{1}{2\theta}\left(\sum_{i=1}^{N} |v_i - u|^2 + 2 \sum_{1 \le i < j \le N} U\left(\frac{|x_i - x_j}{\sigma}\right)\right)\right] \tag{2.36}$$

and a straightforward computation shows that

$$G_N^2(x_1, v_1, \xi, v_2) = \frac{\rho}{(2\pi\theta)^3} C_N(\theta, |\xi|) \exp\left[\frac{1}{2\theta}\left(|v_1 - u|^2 + |v_2 - u|^2 + 2U(|\xi|)\right)\right] \tag{2.37}$$

with

$$C_N(\theta, |\xi_2|) = \int \sigma^{3(N-2)} \exp\left[\frac{1}{\theta}\left(\sum_{j=3}^{N} U(|\xi_j|) + \sum_{2 \le i < j \le N} U(|\xi_i - \xi_j)\right)\right] d\xi_3 \dots d\xi_N \,. \tag{2.38}$$

In particular,

$$F_N^1(x_1,v_1)=\frac{\rho}{(2\pi\theta)^{3/2}}e^{-\frac{|v_1-u|^2}{2\theta}}\int\sigma^3C_N(\theta,|\xi|)e^{-\frac{U(|\xi|)}{\theta}}d\xi\,. \tag{2.39}$$

Therefore, in order to be consistant with (2.23), an absolute Gibbs distribution parametrized by $\rho>0$, $\theta>0$ and $u\in\mathbf{R}^3$ should satisfy the conditions

$$\int\sigma^3C_N(\theta,|\xi|)e^{-\frac{U(|\xi|)}{\theta}}d\xi\to 1 \tag{2.40}$$

as well as

$$\int[U(|\xi|)+|\xi||U'(|\xi|)|]C_N(\theta,|\xi|)e^{-\frac{U(|\xi|)}{\theta}}d\xi\to\int[U(|\xi|)+|\xi||U'(|\xi|)|]C(\theta,|\xi|)e^{-\frac{U(|\xi|)}{\theta}}d\xi \tag{2.41}$$

as $N\to+\infty$ (and $\sigma\to 0$ with $N\sigma^3\to R_*$). One can check that there is no contradiction between (2.40) and (2.41). For example, if

$$C_N(\theta,|\xi|)e^{-\frac{U(|\xi|)}{\theta}}=\chi(\sigma|\xi|)$$

and

$$U(|\xi|)=|\xi|^{-3}\text{ or if }U\in C_c^0(\mathbf{R}_+)$$

with

$$\chi\geq 0\,,\quad\int\chi(|\xi|)d\xi=1\,,\qquad\text{and}\int|\xi|^{-3}\chi(|\xi|)d\xi,+\infty\,.$$

one finds that (2.40) holds, while (2.41) becomes

$$\int[U(|\xi|)+|\xi||U'(|\xi|)|]\chi(\sigma|\xi|)d\xi\to -2\int|\xi|^{-3}\chi(\xi)d\xi$$

in the first case or

$$\int[U(|\xi|)+|\xi||U'(|\xi|)|]\chi(\sigma|\xi|)d\xi\to\int[U(|\xi|)+|\xi||U'(|\xi|)|]\chi(0)d\xi$$

in the second.

The closure assumption proposed in (2.23) consists in restricting our attention to Gibbs distributions with parameters that are slowly varying in one coordinate, say x_1. We hope to discuss the possibility of actually constructing such slowly varying Gibbs profiles in a forthcoming publication. Of course, one might think that such a procedure breaks the symmetry (2.9), which, as we have seen in (2.17) and (2.24), is an essential feature of our derivation. However, assumption (2.23) bears only on the limiting form of G_N^2 as $\sigma \to 0$, in which all particles are collapsed on the same position x_1.

As a final remark, we just point out the noticeable difference between the form of G^2 postulated in (2.23) and the fact that, in the Boltzmann-Grad limit, particles are supposed to be uncorrelated before collisions. Indeed, the form (2.23) seems to postulate that two neighboring particles (that is, particles 1 and 2 with $|x_1 - x_2|$ of order σ, which corresponds to the prescription that $|\xi$ is of order 1) are correlated independently of whether they are about to collide or have just collided.

3. The Periodic Lorentz Gas

In this section and the next one, we leave aside the smooth dynamics of N particles interacting via a repulsive potential, and consider instead the large scale discontinuous dynamics corresponding to a dispersive billiards system. This goes under the name of Lorentz gas and is an extremely popular class of models in nonequilibrium statistical mechanics: see [Sp] for a general description.

We are concerned here with a particular example of Lorentz gas. Consider in the euclidian plane $\mathbf{R}^2$ the lattice

$$\Lambda = \mathbf{Z}(1,0) \oplus \mathbf{Z}(\frac{1}{2}, \frac{\sqrt{3}}{2})\,. \tag{3.1}$$

For each positive ϵ and $r \in]0, \frac{1}{2}[$, define $Z(\epsilon, r)$ to be

$$Z(\epsilon, r) = \{x \in \mathbf{R}^2 \mid \text{ dist } (x, \epsilon k) > \epsilon r\}\,; \tag{3.2}$$

see figure 1 below.

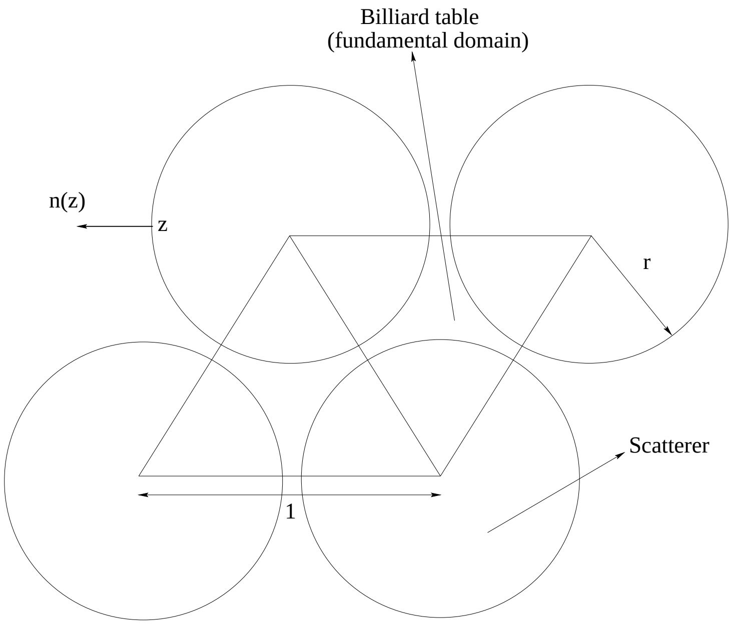

Figure 1: The periodic Lorentz gas: one period

Consider next a gas of like point particles moving freely at unit speed in the domain $Z(\epsilon, r)$. Assume further that, upon impinging on the boundary of $Z(\epsilon, r)$, these particles are specularly reflected and neglect collisions between particles. (That such collisions can be neglected at all results from the assumption that the radius of these particles, and therefore their cross section, is zero). This dynamical system is sometimes referred to as a "billiard system", in which case the domain $Z(\epsilon, r)$ is called the "billiard table". Below, we denote by $x \in Z(\epsilon, r)$ the positions of the particles, and by $v \in S^1$ their velocities. The billiard system generates, for each positive ϵ, a flow on the one-particle phase space $Z(\epsilon, r) \times S^1$, denoted by

$$(X_\epsilon(t; x_0, v_0), V_\epsilon(t; x_0, v_0)) ; \tag{3.3}$$

$X_\epsilon(t; x_0, v_0)$ is the position at time t of a particle which, at time 0 occupied the position x and had instantaneous velocity v_0, while $V_\epsilon(t; x_0, v_0)$ denotes the velocity of this particle. Clearly, this flow is invariant under translations by lattice vectors, i.e.

$$(X_\epsilon(t; x_0 + \epsilon k, v_0), V_\epsilon(t; x_0 + \epsilon k, v_0)) = (X_\epsilon(t; x_0, v_0), V_\epsilon(t; x_0, v_0)) , \qquad k \in \Lambda , \tag{3.4}$$

and scales as follows:

$$(X_\epsilon(t; x_0, v_0), V_\epsilon(t; x_0, v_0)) = (\epsilon X_1(t/\epsilon; x_0/\epsilon, v_0), V_1(t/\epsilon; x_0/\epsilon, v_0)) . \tag{3.5}$$

In 1981, Bunimovich and Sinai announced the following striking result on this billiard system.

Theorem 3.1. *(see [BS], [BSC]) Assume that r satisfies the condition*

$$\frac{\sqrt{3}}{4} < r < \frac{1}{2}, \tag{3.6}$$

and, for all $(x, v) \in Z(1, r) \times S^1$ and all $\epsilon > 0$, set

$$q_\epsilon(t; x, v) = \epsilon X_1(t/\epsilon^2; x, v). \tag{3.7}$$

Call μ_ϵ the probability measure on $C^0(\mathbf{R}_+; \mathbf{R}^2)$ defined as the image of the uniform probability measure on $(Z(1, r)/\Lambda) \times S^1$ under the map

$$(x, v) \mapsto q_\epsilon(\cdot; x_0, v_0). \tag{3.8}$$

Then μ_ϵ converges weakly as $\epsilon \to 0$ to the Wiener measure associated to a Brownian motion with diffusion matrix

$$\sigma^2 = 2E(\tau_1(x_0, v_0)^2 v_0 \otimes v_0) + \sum_{k\geq 1} E(\tau_1(x_0, v_0)\tau_1(x_k, v_k) v_0 \otimes v_k) \tag{3.9}$$

where

- *the expectation is taken with respect to the probability measure proportional to $v \cdot n_1(x) dv dx$ on*
$$\Gamma_+ = \{(x_0, v_0) \in (\partial Z(1, r)/\Lambda) \times S^1 \,|\, v_0 \cdot n(x_0) > 0\} \tag{3.10}$$
with $n_1(x_0)$ denoting the unit inward normal at point $x_0 \in \partial Z(1, r)$;
- *τ_1 is the forward exit time, i.e.*
$$\tau_1(x, v) = \sup\{t \geq 0 \,|\, [x, x + tv] \subset Z(1, r)\}; \tag{3.11}$$
- *the point (x_k, v_k) is the image of (x_0, v_0) under the k-th iterate of the map*
$$\Phi : \Gamma_+ \ni (x, v) \mapsto (x + \tau_1(x, v)v, v - 2v \cdot n_1(x) n - 1(x)) \in \Gamma_+. \tag{3.12}$$

Bunimovich and Sinai based their discussion on a very intricate construction of Markov partitions with countable alphabet for the map Φ above. In particular, this construction helps in proving the subexponential decay of velocity correlations

$$|E(v_0 \otimes v_k)| \leq Ce^{-c\sqrt{k}}, \quad k \geq 0, \tag{3.13}$$

where C and c are two positive constants.

The assumption that $r > \sqrt{3}/4$ implies that the billiard table under consideration has finite horizon, which means that no particle can cross a fundamental domain for the action of Λ on $\mathbf{R}^2$ without colliding with an obstacle. Thus,

$$|\tau_1(x,v)| < 1\,, \qquad \text{for all } (x,v) \in \Gamma_+\,. \tag{3.14}$$

With the above decay (3.13) for the velocity correlations, the bound (3.14) implies that the series defining the diffusion matrix above converges.

These considerations apply to all hyperbolic billiards (see [BSC] for a description of the geometric conditions allowing the application of the theory described above). However, the series (3.9) defining the diffusion coefficient above is neither explicit in the elementary geometric parameters of the billiard table, nor is it very easily computed. Even by taking account of the fast decay of velocity correlations (3.13), one should bear in mind that the constants C and c are not explicit, which makes it hard to predict where the series can safely be truncated; also the billiard map Φ in (3.12), which contains tremendous instabilities, should be computed for sufficiently many points of Γ_+ to allow the use of quadrature formulas in order to compute the expections involved in the truncated series (3.9).

To avoid this difficulty, it was imagined in [Go] to write a kinetic equation for the above billiard system by some analogy with the Boltzmann-Grad limit, and to subsequently approximate the resulting kinetic equation by a diffusion equation, as is customary in neutron transport theory, for example. Here is a quick account of this result.

First, write the Liouville equation satisfied by the 1-particle distribution $f_\epsilon(t,x,v)$ of particles in the scaled billiard table:

$$\epsilon\partial_t f_\epsilon + v\cdot\nabla_x f_\epsilon = 0\,, \quad x \in Z(\epsilon,r)\,,\ v \in S^1\,, \tag{3.15}$$

with the boundary condition expressing that this 1-particle density is invariant under specular reflection at each point of the boundary of $Z(\epsilon,r)$:

$$f_\epsilon(t,x,v) = f_\epsilon(t,x,v-2v\cdot n_\epsilon(x)n_\epsilon(x))\,, \quad x\in\partial Z(\epsilon,r)\,,\ v\in S^1\,. \tag{3.16}$$

Consistently with the notation introduced in Theorem 3.1 above, we denote by $n_\epsilon(x_0)$ the unit inward normal at the point x_0 to $\partial Z(\epsilon,r)$. This Liouville equation (3.15) and the associated boundary condition (3.16) are supplemented by an initial condition of the form

$$f_\epsilon(0,x,v) = f^{in}(x)\,, \quad x\in Z(\epsilon,r)\,,\ v\in S^1\,. \tag{3.17}$$

This Liouville equation (3.15-16) is related to the billiard flow (3.3) defined above by the relation

$$f_\epsilon(t,x,v)=f_\epsilon(t+s,X_\epsilon(s/\epsilon;x,v),V_\epsilon(s/\epsilon;x,v))\,,\quad x\in Z(\epsilon,r)\,,\ v\in S^1\,. \tag{3.18}$$

which, once applied to $s=-t$, gives

$$f_\epsilon(t,x,v)=f^{in}(X_\epsilon(t/\epsilon;x,-v))\,,\quad x\in Z(\epsilon,r)\,,\ v\in S^1\,. \tag{3.19}$$

With the scaling law (3.5) above and the definition (3.7) of q_ϵ, this last formula translates into

$$f_\epsilon(t,x,v)=f^{in}(q_\epsilon(t;x/\epsilon,-v))\,,\quad x\in Z(\epsilon,r)\,,\ v\in S^1\,. \tag{3.20}$$

This last formula should convince the reader discouraged by our shameless introduction of the scaling parameter above that studying the limits of solutions of the Liouville equation (3.15-17), and proving that these limits satisfy a diffusion equation, is just a PDE formulation of the Bunimovich-Sinai result in Theorem 3.1 above. Suffice it to say that the small parameter ϵ can be defined intrinsically as the ratio of the lattice period to the typical wavelengths present in the Fourier transform of the initial data f^{in}.

As it is, the Liouville equation above (3.15-17) is not any simpler than the billiard problem, being essentially equivalent to it. An additional difficulty in analyzing the limit of (3.15-3.17) is that the domain on where this PDE is posed, namely the billiard table, varies with ϵ. One can remedy to that by extending the 1-particle density f_ϵ by 0 inside the obstacles, i.e. by posing

$$F_\epsilon(t,x,v)=f_\epsilon(t,x,v)\ \text{ if }\ x\in Z(\epsilon,r)\,, \tag{3.21a}$$

and

$$F_\epsilon(t,x,v)=0\ \text{ if }\ x\in \overline{Z}(\epsilon,r)^c\,. \tag{3.21b}$$

This defines a bona fide distribution (for example, if f^{in} is a bounded function, F_ϵ is a.e. defined and has the same bound as f^{in}) which satisfies

$$\epsilon\partial_t F_\epsilon+v\cdot\nabla_x F_\epsilon-(v\cdot n_\epsilon(x))\delta_{\partial Z(\epsilon,r)}F_{\epsilon|\partial Z(\epsilon,r)^i}=0\,,\quad x\in\mathbf{R}^2\,,\ v\in S^1\,, \tag{3.22}$$

$$F_{\epsilon|\partial Z(\epsilon,r)^i}=F_{\epsilon|\partial Z(\epsilon,r)^i}\circ\mathcal{R}\quad x\in\partial Z(\epsilon,r)\,,\ v\in S^1\,. \tag{3.23}$$

$$F_\epsilon(0,x,v)=f^{in}(x)\mathbf{1}_{Z(\epsilon,r)}(x)\,. \tag{3.24}$$

In (3.23), the notation $F_{\epsilon|\partial Z(\epsilon,r)^i}$ stands for the trace F_ϵ on $\partial Z(\epsilon,r)$ on the side of $Z(\epsilon,r)$, while $\mathcal{R}$ designates the transformation

$$\mathcal{R}:\ (t,x,v)\mapsto(t,x,v-2n_\epsilon(x)n_\epsilon(x))\,. \tag{3.25}$$

This relation (3.23) can now be used to put (3.22) in the form

$$\epsilon\partial_t F_\epsilon+v\cdot\nabla_x F_\epsilon$$

$$+(v\cdot n_\epsilon(x))_-\delta_{\partial Z(\epsilon,r)}F_{\epsilon|\partial Z(\epsilon,r)^i}-(v\cdot n_\epsilon(x))_+\delta_{\partial Z(\epsilon,r)}F_{\epsilon|\partial Z(\epsilon,r)^i}\circ\mathcal{R}=0\,,\quad x\in\mathbf{R}^2\,,\ v\in S^1\,. \tag{3.26}$$

This last form should be suggestive to anyone familiar with kinetic equations: indeed the term

$$(v\cdot n_\epsilon(x))_-\delta_{\partial Z(\epsilon,r)}F_{\epsilon|\partial Z(\epsilon,r)^i} \tag{3.27}$$

is analogous to the loss term in the Boltzmann collision integral, while the term

$$(v\cdot n_\epsilon(x))_+\delta_{\partial Z(\epsilon,r)}F_{\epsilon|\partial Z(\epsilon,r)^i}\circ\mathcal{R} \tag{3.28}$$

is analogous to the gain term in the same integral. The only difference of course is that these terms are purely local instead of being integral operators as in the case of the Boltzmann collision operator.

This is remedied in the second step of our approach, explained in the following Theorem.

Theorem 3.2. *([Go]) Consider, the family of operators indexed by $\epsilon>0$*

$$L:\ C^0(\mathbf{R}^2\times S^1)\to\mathcal{M}(\mathbf{R}^2\times S^1)$$

defined by

$$L_\epsilon\phi=(v\cdot n_\epsilon(x))_-\delta_{\partial Z(\epsilon,r)}\phi_{|\partial Z(\epsilon,r)^i}-(v\cdot n_\epsilon(x))_+\delta_{\partial Z(\epsilon,r)}\phi_{|\partial Z(\epsilon,r)^i}\circ\mathcal{R} \tag{3.29}$$

and the operator L defined by

$$(L\phi)(x,v)=\sqrt{3}r\left(\phi(x,v)-\frac{1}{2}\int_{S^1}\phi(x,v')|v'-v|dv'\right)\,. \tag{3.30}$$

Then, for any ϕ and $\psi\in C_c^\infty(\mathbf{R}^2\times S^1)$, one has

$$<L_\epsilon\phi,\psi>-\frac{1}{\epsilon}<L\phi,\psi>=O(\epsilon^n)\,,\quad \textit{for all } n\geq 0\,. \tag{3.31}$$

Thus, instead of considering the transport equation with measure coefficients (3.26), one could consider instead

$$\left(1-\frac{2\pi r^2}{\sqrt{3}}\right)(\epsilon\partial_t G_\epsilon + v\cdot\nabla_x G_\epsilon) + \frac{1}{\epsilon}LG_\epsilon = 0\,, \tag{3.32}$$

which is a much more usual object. However, Theorem 3.2 says that, for smooth functions ϕ independent of ϵ, $L_\epsilon\phi$ and $\frac{1}{\epsilon}L\phi$ are close to whithin any power of ϵ, but we cannot claim that the same holds true if ϕ is replaced by F_ϵ.

Nevertheless, this approach shows that one can find a diffusion equation that is close to the original transport equation with measure coefficients (3.26), in the following sense. Consider G the solution to the diffusion problem

$$\partial_t G = \frac{1}{2}D(r)\Delta_x G\,, \quad x\in\mathbf{R}^2\,,\ t>0\,, \tag{3.33}$$

$$G(0,x) = f^{in}(x)\,, \quad x\in\mathbf{R}^2\,, \tag{3.34}$$

where

$$D(r) = \frac{3-2\sqrt{3}\pi r^2}{8r}\,. \tag{3.35}$$

As is well known, the solution G is smooth for all positive times, and, if f^{in} is assumed to be smooth, G is smooth all the way down to $t=0$. By the usual theory of the diffusion approximation of transport equation (see for example [BSS]), one can construct smooth functions G_1 and G_2 of t, x and v such that

$$\left(1-\frac{2\pi r^2}{\sqrt{3}}\right)\left(\partial_t + \frac{1}{\epsilon}v\cdot\nabla_x\right)(G+\epsilon G_1+\epsilon^2 G_2) + \frac{1}{\epsilon^2}L(G+\epsilon G_1+\epsilon^2 G_2) = O(\epsilon)_{L^\infty} \tag{3.36}$$

while

$$(G+\epsilon G_1+\epsilon^2 G_2)_{|t=0} - f^{in} = O(\epsilon)_{L^\infty}\,. \tag{3.37}$$

Next compute

$$\begin{aligned}
&\left(\partial_t + \frac{1}{\epsilon}v\cdot\nabla_x + \frac{1}{\epsilon}L_\epsilon\right)\left[\mathbf{1}_{Z(\epsilon,r)}(G+\epsilon G_1+\epsilon^2 G_2)\right]\\
&= \left(\partial_t + \frac{1}{\epsilon}v\cdot\nabla_x\right)\left[\mathbf{1}_{Z(\epsilon,r)}(G+\epsilon G_1+\epsilon^2 G_2)\right] + \frac{1}{\epsilon}L_\epsilon(G+\epsilon G_1+\epsilon^2 G_2)\\
&= \left(1-\frac{2\pi r^2}{\sqrt{3}}\right)\left(\partial_t + \frac{1}{\epsilon}v\cdot\nabla_x\right)(G+\epsilon G_1+\epsilon^2 G_2) + \frac{1}{\epsilon^2}L(G+\epsilon G_1+\epsilon^2 G_2)
\end{aligned}$$

$$+\left(\partial_t+\frac{1}{\epsilon}v\cdot\nabla_x\right)\left[\left(\mathbf{1}_{Z(\epsilon,r)}-\left(1-\frac{2\pi r^2}{\sqrt{3}}\right)\right)(G+\epsilon G_1+\epsilon^2 G_2)\right]$$
$$+\left(\frac{1}{\epsilon}L-\frac{1}{\epsilon^2}L_\epsilon\right)(G+\epsilon G_1+\epsilon^2 G_2)=0\,. \tag{3.38}$$

Since all the functions G, G_1 and G_2 are smooth,

$$\left(\frac{1}{\epsilon}L-\frac{1}{\epsilon^2}L_\epsilon\right)(G+\epsilon G_1+\epsilon^2 G_2)=O(\epsilon^\infty)_{\mathcal{D}'} \tag{3.39}$$

according to Theorem 3.2, while, by the nonstationary phase lemma one has

$$\left(\mathbf{1}_{Z(\epsilon,r)}-\left(1-\frac{2\pi r^2}{\sqrt{3}}\right)\right)(G+\epsilon G_1+\epsilon^2 G_2)=O(\epsilon^\infty)_{\mathcal{D}'}\,. \tag{3.40}$$

Thus we have proved

Theorem 3.3. *([Go]) Let G be the solution of the diffusion equation (3.33-34) with diffusion coefficient (3.35). Let G_1 and G_2 be defined as*

$$G_1=-L^{-1}v\partial_x G\,,\quad G_2=L^{-1}(vL^{-1}v-\tfrac{1}{2}D(r))\partial_{xx}G\,,$$

where L^{-1} denotes the pseudo-inverse of the Fredholm operator L. Then

$$\left(\partial_t+\frac{1}{\epsilon}v\cdot\nabla_x+\frac{1}{\epsilon}L_\epsilon\right)[\mathbf{1}_{Z(\epsilon,r)}(G+\epsilon G_1+\epsilon^2 G_2)]=O(\epsilon^\infty_{\mathcal{D}'}+O(\epsilon)_{L^\infty} \tag{3.41}$$

Theorem 3.3 shows that replacing the true solution F_ϵ by the truncated asymptotic expansion

$$\mathbf{1}_{Z(\epsilon,r)}(G+\epsilon G_1+\epsilon^2 G_2) \tag{3.42}$$

leads to an approximation of the *equation* (3.26) in the topology of distributions: this corresponds to the notion of consistency.

Comparing the results in Theorem 3.1 and in Theorem 3.3, it seems natural to ask whether the diffusion coefficient given by (3.9) coincides with the one computed by the consistent asymptotic expansion (3.42). In other words, does one have

$$\sigma^2=D(r)\,?$$

In the affirmative, the method based on the search of a consistent asymptotic expansion would lead to a very explicit way of computing the complicated series (3.9).

However, we cannot infer from (3.41) that

$$F_\epsilon - \mathbf{1}_{Z(\epsilon,r)}(G + \epsilon G_1 + \epsilon^2 G_2) \to 0$$

in any reasonable function space. In the language of numerical analysis (referring to the Lax equivalence theorem), this is due to a lack of stability for the transport equation with measure coefficients (3.26).

It is interesting to compare this situation with that considered in section 2. As we said, the Boltzmann equation has been rigorously derived from the Liouville equation for a gas of N colliding hard spheres of radius σ in the Boltzmann-Grad limit: $N \to +\infty$, $\sigma \to 0$, $N\sigma^2 \to 1$. The ideas leading to such a derivation are due of Lanford; see [CIP] for a detailed account of the existing proofs. In the case of the Lorentz gas, the kinetic model (3.32) is not proved to be a mesoscopic limit of the Liouville equation (3.15)-(3.16) — only the consistency to within any order of accuracy in the sense of distributions is established. There are even indications that nothing more than consistency is true: see [BGW], [GW].

4. A Model Knudsen Gas

Thus, the example of the periodic Lorentz gas treated in the previous section leads us to suspect that diffusion coefficients computed by using first a kinetic approximation of the Liouville equation might differ from those computed directly from the definition as the long time limit of the mean square displacement per unit of time. We say "suspect" because, as far as the periodic Lorentz gas is concerned, we know for sure that both diffusion coefficients differ only in the boring case where no diffusion occurs really.

In the present section, we analyze a much simpler example, where it is possible to compute explicitly the difference between the diffusion coefficients computed by each method. This example is an amplification of our previous paper [BGC] (see also [Go2]), which we briefly recall below.

Consider a gas of point particles confined between two infinite plates; as in the case of the Lorentz gas, collisions between particles are neglected, for the same reason (i.e. because these particles have radius — and therefore cross-section — equal to zero). However, as in the case of the Lorentz gas, one takes into account collisions with the plates. These plates are supposed to be rough surfaces, and we shamelessly model the reflection of particles on the plates by a "chaotic" map, as follows.

Each particle has vertical velocity ± 1 and horizontal velocity $a(\omega)$, where $\omega \in \mathbf{T}^2$. This variable ω might look a little obscure, but one could think of ω as a wave vector in a Brillouin zone and of $a(\omega)$ as the gradient of the energy with respect to this wave vector (such models are customary in semiconductors: see for example [Po] for a very nice introduction to these models). Anyway, each time a particle travels freely between the plates, which means that it keeps not only the same horizontal velocity $a(\omega)$, but also the same ω. Each time a particle hits one of the plates, its vertical velocity is changed into its opposite, and its ω changed into $T\omega$, where T is a hyperbolic automorphism of $\mathbf{T}^2$, for example

$$T = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} \quad \text{mod. } 2\pi\,. \tag{4.1}$$

In what follows, we reduce somewhat the model by assuming that the plates are in fact lines. In other words, we suppose that all the values taken by a are colinear and that the initial data depends only on the coordinate in the direction of a: this symmetry is preserved by the evolution of the dynamical system considered. The phase space for this system is therefore the cartesian product of the strip $\mathbf{R} \times [0, h]$ by the set parametrizing velocities i.e. $\mathbf{T}^2 \times \{\pm 1\}$, where $h > 0$ denotes the distance between the plates. (The set $\{\pm 1\}$ is just the set of vertical velocities).

Now, as the particles in this model move without seeing each others, we might have considered instead a phase space consisting of two copies of the strip $\mathbf{R} \times [0, h]$ times $\mathbf{T}^2$, where particles going up move on one of the copy while particles going down move on the other copy. If we sow these two strips together along their boundaries, we obtain a cylinder with two marked generatrices or seams (see figure 2). Particles move on that cylinder as follows:

• their angular velocity around the axis of the cylinder is constant (say 1);

• each time a particle crosses one of the two seams, its ω is changed into $T\omega$ with T defined as in (4.1).

In this model, there is an impingement on the "plates" every h unit of time. In order to observe a hydrodynamic limit, we must first let $h \to 0$. Since we are interested in observing a diffusion in the direction of the seams (or the axis of the cylinder), it is natural to assume that a has mean zero on $\mathbf{T}^2$, and to look at times of the order of $1/h$. However, by doing so, we end up with a phase space that shrinks as $h \to 0$ to become $\mathbf{R} \times \mathbf{T}^2$, and we loose the angle variable.

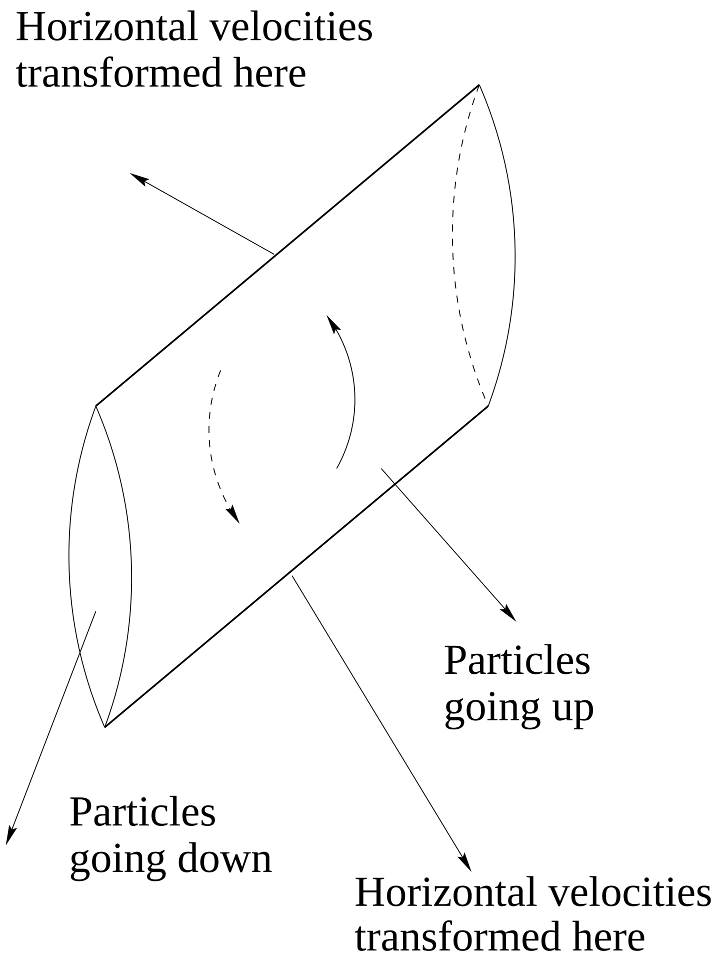

Figure 2: The Knudsen gas model: cylindrical domain.

It is more convenient to look instead at the dynamics on a N-sheet covering of this phase space with $N \to \infty$ as $h \to 0$. This is done as follows:

• the phase space is $\mathbf{R} \times S^1 \times \mathbf{T}^2$;

• each particle has coordinates (x, θ, ω) and moves as follows: call $\epsilon = \frac{2\pi}{N}$, then

$$x'(t) = a(\omega)\,, \quad \theta'(t) = 1\,, \quad \omega'(t) = 0\,, \qquad \text{unless } \theta(t) = k\epsilon \text{ mod. } 2\pi\,, \;\; k \in \mathbf{Z}; \tag{4.2a}$$

in which case, if $\theta(t_0) = k\epsilon$ mod. 2π with $k \in \mathbf{Z}$, then

$$x(t_0 - 0) = x(t_0 + 0)\,, \quad \theta(t_0 - 0) = \theta(t_0 + 0)\,, \quad \omega(t_0 + 0) = T\omega(t_0 - 0)\,. \tag{4.2b}$$

The Liouville equation corresponding to this dynamical system is

$$\epsilon\partial_t f_\epsilon - a(\omega)\partial_x f_\epsilon - \partial_\theta f_\epsilon = 0\,, \quad x \in \mathbf{R}\,,\ \theta \in S^1 \setminus \frac{2\pi}{N}\mathbf{Z}\,,\ t > 0\,, \tag{4.3}$$

with the jump condition

$$f_\epsilon(t, x, k\frac{2\pi}{N} + 0, \omega) = f_\epsilon(t, x, k\frac{2\pi}{N} - 0, T\omega) \tag{4.4}$$

and we assume that the initial data is a smooth function of x only, i.e.

$$f_\epsilon(0, x, \theta, \omega) = \phi(x)\,, \quad x \in \mathbf{R}\,,\ \theta \in S^1 \setminus \frac{2\pi}{N}\mathbf{Z}\,,\ t > 0\,. \tag{4.5}$$

In the sequel, we denote by brackets as in $\langle\,\cdot\,\rangle$ the average in ω. The main result in [BGC] is as follows

Theorem 4.1. *Let $a \in C^3(\mathbf{T}^2)$ be such that $\langle a\rangle = 0$. Assume that $\phi \in C_c^\infty(\mathbf{R})$. Then*

- *the self-correlation $\langle a \circ T^n\, a\rangle \to 0$ exponentially fast as $n \to +\infty$;*
- *the absolutely converging series*

$$D(a) = \sum_{n\in\mathbf{Z}} \langle a \circ T^n a\rangle \geq 0 \tag{4.6}$$

with equality if and only if a is a L^2 coboundary, i.e. of the form

$$a = b - b \circ T \tag{4.7}$$

for some $b \in L^2(\mathbf{T}^2)$;

- *as $\epsilon \to 0$, the number density f_ϵ converges in $C^0([0,\tau], w^* - L^\infty(\mathbf{R} \times S^1 \times \mathbf{T}^2))$ for all $\tau > 0$ to the solution f of the diffusion equation*

$$\partial_t f = \frac{1}{2}D(a)\partial_{xx} f\,, \quad x \in \mathbf{R}\,,\ t > 0\,, \tag{4.8}$$

$$f(0, x) = \phi(x)\,, \quad x \in \mathbf{R}\,. \tag{4.9}$$

Of course, in this case, the diffusion coefficient is not nearly as hard to compute as in the case of the Lorentz gas, in particular because the map T is itself an extremely simple object. For example, if a is a trigonometric polynomial, the series above for $D(a)$ reduces to a few terms and thus can be computed exactly.

Nevertheless, it is instructive to try the detour of a kinetic approximation, as outlined in section 3. Going back to the Liouville equation (4.3-5), we patch together all the restrictions of f_ϵ to each connected component of $\mathbf{R}_t \times \mathbf{R}_x \times (S^1 \setminus \frac{2\pi}{N}\mathbf{Z})_\theta \times \mathbf{T}^2$ and call F_ϵ the function so obtained. This function satisfies the following transport equation on $\mathbf{R}_t \times \mathbf{R}_x \times S^1_\theta \times \mathbf{T}^2$

$$\epsilon\partial_t F_\epsilon + a(\omega)\partial_x F_\epsilon + \partial_z F_\epsilon - \sum_{k=1}^{N} \delta(\theta - k\epsilon)[F_{\epsilon|\theta=k\epsilon+0} - F_{\epsilon|\theta=k\epsilon-0}] = 0\,. \tag{4.10}$$

Averaging this equation in θ and defining

$$G_\epsilon(t,x,\omega) = \frac{1}{2\pi}\int_{S^1} F_\epsilon(t,x,z,\omega)dz \tag{4.11}$$

leads to

$$\epsilon\partial_t G_\epsilon + a(\omega)\partial_x G_\epsilon - \sum_{k=1}^{N}[F_{\epsilon|\theta=k\epsilon+0} - F_{\epsilon|\theta=k\epsilon-0}] = 0\,. \tag{4.12}$$

Next, we use the boundary condition (4.4) to replace the sum above by

$$\sum_{k=1}^{N}[F_\epsilon(t,x,k\epsilon+0,\omega) - F_\epsilon(t,x,k\epsilon-0,\omega)] = \sum_{k=1}^{N}[F_\epsilon(t,x,k\epsilon-0,T\omega) - F_\epsilon(t,x,k\epsilon-0,\omega)]\,. \tag{4.13}$$

Now, if F is a smooth function of θ (which F_ϵ is of course not!)

$$\sum_{k=1}^{N}[F(t,x,k\epsilon,T\omega) - F(t,x,k\epsilon,\omega)]$$

$$= \frac{1}{\epsilon}\left[\int_{S^1} F(t,x,z,T\omega)dz - \int_{S^1} F(t,x,z,\omega)dz\right] + O(\epsilon^\infty)_{\mathcal{D}'_\theta} \tag{4.14}$$

(see [Go] for what exactly is meant by $O(\epsilon^\infty)_{\mathcal{D}'_\theta}$).

In any case, once averaged in θ, the Liouville equation (4.3-5) is weakly consistent to whithin any order of accuracy to the kinetic equation

$$\epsilon\partial_t g_\epsilon + a(\omega)\partial_x g_\epsilon + \frac{1}{\epsilon}(g_\epsilon - g_\epsilon \circ T) = 0\,, \quad x \in \mathbf{R}\,,\ \omega \in \mathbf{T}^2\,, \tag{4.15}$$

$$g_\epsilon(0,x,\omega)=\phi(x)\,,\quad x\in\mathbf{R}\,,\ \omega\in\mathbf{T}^2\,, \tag{4.16}$$

where $g_\epsilon\circ T$ is a shorthand notation for

$$(t,x,\omega)\mapsto g_\epsilon(t,x,T\omega)\,. \tag{4.17}$$

The proof of consistency to within any order of accuracy in the sense of distributions rests on the Euler-Mc Laurin formula and is as in [Go].

Now we can discuss the limit of (4.15-16) as $\epsilon\to 0$. One finds that the bulk density $\langle g_\epsilon\rangle$ is, in the limit as $\epsilon\to 0$ governed by a diffusion equation. The proof is not nearly as simple as the classical proof of diffusion approximation in the case of the neutron transport equation because the jump in ω is purely deterministic. However, the same kind of techniques as in [BGC] gives the following

Theorem 4.2. *Let $a\in C^3(\mathbf{T}^2)$ be such that $\langle a\rangle=0$. Assume that $\phi\in C_c^\infty(\mathbf{R})$. Then as $\epsilon\to 0$, the family g_ϵ converges in $L^\infty(\mathbf{R}_+\times\mathbf{R}\times\mathbf{T}^2))$ weak-* to the solution g of the diffusion equation*

$$\partial_t g=\frac{1}{2}D'(a)\partial_{xx}g\,,\quad x\in\mathbf{R}\,,\ t>0\,, \tag{4.18}$$

$$g(0,x)=\phi(x)\,,\quad x\in\mathbf{R}\,. \tag{4.19}$$

where the diffusion coefficient is given by

$$D'(a)=2\sum_{n\geq 0}\langle a\circ T^n\,a\rangle\,. \tag{4.20}$$

Sketch of the proof. First one has the following a priori estimates: by the maximum principle

$$\|g_\epsilon\|_{L^\infty(\mathbf{R}_+\times\mathbf{R}\times\mathbf{T}^2)}\leq\|\phi\|_{L^\infty(\mathbf{R})}\,; \tag{4.21}$$

then, multiplying (4.15) by g_ϵ and integrating in x and ω (taking account of the fact that, by the finite speed of propagation for the transport (4.15) — which is precisely $\|a\|_{L^\infty}/\epsilon$ — each function g_ϵ vanishes at infinity in x as ϕ does) one finds

$$\frac{1}{2}\|g_\epsilon(t)\|_{L^2(\mathbf{R}\times\mathbf{T}^2)}+\frac{1}{2\epsilon^2}\int_0^t\int_{\mathbf{R}}\langle g_\epsilon-g_\epsilon\circ T\rangle dxds=\frac{1}{2}\|\phi\|_{L^2(\mathbf{R})}\,. \tag{4.22}$$

Then, one can average the transport equation 4.15 with respect to ω, to find

$$\partial_t\langle g_\epsilon\rangle+\partial_x\frac{1}{\epsilon}\langle ag_\epsilon\rangle=0\,. \tag{4.23}$$

Next, consider the approximate homological equation for the unknown $b_\epsilon \equiv b_\epsilon(\omega)$

$$\epsilon^2 b_\epsilon + b_\epsilon - b\epsilon \circ T^{-1} = a\,. \tag{4.24}$$

Since T preserves the Lebesgue measure on $\mathbf{T}^2$, the operator $a \mapsto a \circ T$ is a unitary transformation of L^2 and the b_ϵ can be defined by the normally converging series

$$b_\epsilon = \sum_{n\geq 0} \frac{1}{(1+\epsilon^2)^{n+1}}\, a \circ T^{-n}\,. \tag{4.25}$$

Then

$$\begin{aligned}\frac{1}{\epsilon}\langle a g_\epsilon\rangle &= \langle \epsilon b_\epsilon g_\epsilon\rangle + \langle b_\epsilon \frac{1}{\epsilon}(g_\epsilon - g_\epsilon \circ T)\rangle \\ &= \langle \epsilon b_\epsilon g_\epsilon\rangle - \partial_t \langle \epsilon b_\epsilon g_\epsilon\rangle - \partial_x \langle b_\epsilon a g_\epsilon\rangle\,.\end{aligned} \tag{4.26}$$

The first equality uses again that the operator $\psi \mapsto \psi \circ T$ is unitary on $L^2(\mathbf{T}^2)$ with adjoint $\psi \mapsto \psi \circ T^{-1}$; the second equality uses the transport equation(4.15) to replace the $O(1/\epsilon)$ term $\frac{1}{\epsilon}(g_\epsilon - g_\epsilon \circ T)$ by a term involving first order derivatives.

Now, we claim that b_ϵ satisfies

$$\langle b_\epsilon\rangle = 0\,, \qquad \epsilon\langle b_\epsilon^2\rangle = O(1)\,, \tag{4.27}$$

$$\langle b_\epsilon a\rangle \to \frac{1}{2} D'(a) \qquad \text{as } \epsilon \to 0\,. \tag{4.28}$$

The first relation in (4.27) is a trivial consequence of (4.24); (4.28) follows from the exponential decay of the self-correlation coefficients of a stated in Theorem 4.1 and the dominated convergence theorem. As for the second relation in (4.27), one writes

$$\epsilon^2 \langle b_\epsilon^2\rangle + \langle b_\epsilon(b_\epsilon - b_\epsilon \circ T)\rangle = \langle b_\epsilon a\rangle \tag{4.29}$$

and use that the second term in the left hand side of (4.29) is nonnegative since

$$\langle b_\epsilon(b_\epsilon - b_\epsilon \circ T)\rangle = \frac{1}{2}\langle (b_\epsilon - b_\epsilon \circ T)^2\rangle\,.$$

The last and main step in the proof is provided by the following decorrelation properties:

$$\langle b_\epsilon a g_\epsilon\rangle - \langle b_\epsilon a\rangle\langle g_\epsilon\rangle \to 0\,, \tag{4.30}$$

and

$$\langle \epsilon b_\epsilon g_\epsilon\rangle - \langle \epsilon b_\epsilon\rangle\langle g_\epsilon\rangle \to 0\,, \tag{4.31}$$

These are obtained from two ingredients. One is the representation of the solution g_ϵ as

$$g_\epsilon(t,x,\omega) = \mathbf{E}\phi\left(x + \epsilon \sum_{n=0}^{N(t/\epsilon^2)} \tau_n a(T^n\omega)\right) \tag{4.32}$$

where τ_n, $n = 0, \ldots$ is a sequence of independent, exponentially distributed random jump times (i.e. Prob $\{\tau_n > t\} = e^{-t}$ for all positive t). The other one is the mixing property enjoyed by T and analogous to the so-called "weak Bernoulli mixing" stated as Proposition 6 of [BGC] (see especially formula (37), p. 43 of [BGC]).

With (4.30) and (4.31), properties (4.27) and (4.28) of b_ϵ, plus the weak compactness of the family $\langle g_\epsilon \rangle$ guaranteed by the maximum principle (4.21) show that the family of averages $\langle g_\epsilon \rangle$ converges to the solution g of (4.18-19). Finally, by convexity and weak limit, (4.22) shows that any weak-* limit point of g_ϵ as $\epsilon \to 0$ is invariant under the transformation T acting on the ω variable. Since T is ergodic, this shows that such weak-* limit points as $\epsilon \to 0$ must be independent of ω and therefore equal to the solution g of (4.18-19). //

The main interest (if any) of this little computation is essentially the following consequence of Theorems 4.1 and 4.2.

Corollary 4.3. *For all $a \in C^3(\mathbf{T}^2)$ such that $\langle a \rangle = 0$, the "true" diffusion coefficient $D(a)$ and the diffusion coefficient $D'(a)$ computed by the kinetic theory differ by*

$$D'(a) - D(a) = \langle a^2 \rangle\,. \tag{4.33}$$

In particular, the kinetic theory approach gives a positive diffusion coefficient even if a is a coboundary. This is completely analogous to the case of the Lorentz gas with touching obstacles: in this case, each particle stays confined in the same period and the "true" diffusion coefficient is zero. In any case, (4.22) shows that the kinetic model (4.15-16) is dissipative while the Liouville equation is not; thus there should be little surprise in the fact that the diffusion coefficient computed by the kinetic approach is higher than the "true" diffusion coefficient.

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