Limit theorems for deterministic Knudsen flows between two plates

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Abstract

We investigate the model dynamics of a test particle which moves between two parallel plates and is reflected at the walls according to some deterministic periodic reflection law. For a particular continuous velocity model, a diffusion limit is derived using the Markov partition approach. It is shown that at least for a large class of discrete velocity models such a limit is not possible. Numerical aspects are discussed.

1 Introduction

Dynamics of test particles moving within small gaps between two parallel plates or within thin tubes are relevant for a number of applications, for example for the investigation of gas surface interactions (see the paper [8] from 1930 and the literature cited in [2] documenting ongoing interest in this problem in recent years) or for the modelling of the dynamic behaviour of slider heads of magnetic disk storage devices [6].

Diffusion limits for a test particle moving between two parallel plates have been studied recently in a couple of papers [2, 3, 4, 6]. In most of these papers, the particle was assumed to move uniformly between the plates and to be reflected according to some stochastic reflection law at the walls. The results obtained there where either based on some stochastic limit theorems or on some functional analytic properties of the reflection operator associated to the reflection law. In [3], a diffusion limit could be proven for a Lorentz gas test particle - again under a stochastic reflection law.

Recently the diffusive behaviour of a deterministic test particle dynamics was studied in [7] using Markov partitions. This result encourages to investigate the existence of diffusion limits for *deterministic* Knudsen flows between parallel walls. One aim of the paper is to make the Markov partition approach more transparent and accessible to further applications.

The basic idea of the paper is roughly as follows. We investigate the dynamics of a particle between two walls located at $x_1 = 0$ and $x_1 = h$. For simplicity, consider the reflection law at $x_1 = h$ to be specular reflection at a flat wall. The law at $x_1 = 0$ is chosen as to mimic specular reflection at a periodic surface. (Some aspects of the limiting behaviour of such boundaries have been studied in [?].) Let's construct the phase space of the particle. Suppose the finite interval $[0, a_0] \subset \mathbb{R}^k$ represents one period of the wall at $x_1 = 0$, and the set of admissible velocities pointing off from the wall is indexed by another interval $[0, b_0] \subset \mathbb{R}^l$. Denote $I := [0, a_0] \times [0, b_0]$. A particle leaving the wall at a point $z = (a, b)^T \in I$ hits the flat plane at some later plane, is specularly reflected and gets into contact with the wall again. After reflection it ends up in another position $z' = (a', b')^T$, from which it leaves the wall again. For Knudsen flows and deterministic reflection laws, z' is given by some mapping $S : I \to \mathbb{R}^k \times [0, b]$. We distinguish between microscopic and macroscopic dynamics of the particle. The phase space of the microscopic dynamics is the interval $I = [0, a_0] \times [0, b_0]$. The microscopic dynamics T is defined as a mapping on I by truncating the position vector: $Tz = (a' \bmod a_0, b')$. The mapping D takes values in $\mathbb{R}^m$ and is defined by $Dz = a' - (a' \bmod a_0)$. Finally, the macroscopic dynamics is defined by

$$X_n(z) := \sum_0^{n-1} D(T^i z) \tag{1.1}$$

which gives approximately (i.e. up to the part contained in $T^{n-1}z$) the position after the n^{th} contact with the wall. The macroscopic dynamics is completely ruled by T which describes a deterministic - by choice even reversible - dynamics. The basic aim of the paper is to study the limiting behaviour of X_n and to derive - if possible - a diffusion limit.

The plan of the paper is as follows. In section two, we collect some more or less classical results necessary to formulate limit theorems for Knudsen flows between two parallel plates. In section 3 we investigate a discrete velocity model under a periodic deterministic reflection law and show that a diffusion limit cannot be expected in general. In section 4 a diffusion limit is derived for a continuous velocity model under a periodic model reflection law which mimics specular reflection on a rough surface. Section 5 finishes with some numerical aspects: about the role of truncation errors which transform continuous velocity models into discrete models, and about the dimension reduction in the diffusion limit.

2 The mathematical framework

2.1 Automorphisms and stationary measures

This section shortly introduces into the mathematical framework enabling to formulate diffusion limits for deterministic flows. It follows widely the exposition in [9, Chapter 8 §1]. We start recalling some standard definitions. Suppose given a measure space $(\Omega, \mathcal{O}, \mu)$. (Without stating it explicitely all the time, μ is assumed to be normalized, i.e. $\mu(\Omega) = 1$.) An *automorphism* T is a one-to-one map of Ω onto itself such that for all $A \in \mathcal{O}$ holds TA, $T^{-1}A \in \mathcal{O}$, and μ is $T-$invariant, i.e. $\mu(A) = \mu(TA) = \mu(T^{-1}A)$. A *partition* ξ of Ω is an at most countable collection of measurable sets in Ω, $\xi = (C_1, \ldots, C_m)$ with $1 \leq m \leq \infty$, which covers Ω, and for which $\mu(C_i \cap C_j) = 0$ if $i \neq j$. Denote for $M = \{1, \ldots, m\}$ the product space

$$Y := \prod_{i=-\infty}^{\infty} M^{(i)} \tag{2.2}$$

with $M^{(i)} := M$ as the set of infinite sequences in M, and the $\sigma-$algebra $\mathcal{Q}$ as the set of all subsets of Y.

Given T and ξ as above, a map $\phi = (\phi_i)_{i=-\infty}^{\infty} : \Omega \to Y$ may be defined by

$$\phi_i(x) = k \Longleftrightarrow T^i x \in C_k \tag{2.3}$$

Through ϕ, a measure ν is induced on $\mathcal{Q}$ by

$$\nu(A) := \mu(\phi^{-1}(A)) \tag{2.4}$$

Since T is an automorphism, it follows easily that ν is *stationary* - i.e. is invariant with respect to the shift operator S on Y which is defined by $(Sy)_i := y_{i+1}$.

Similarly, for given $f : M \to \mathbb{R}^p$ define the sequence $f \circ \phi$ in $\mathbb{R}^p$ by

$$(f \circ \phi)_i(x) := f(\phi_i(x)) = f(k) \text{ if } T^i x \in C_k \tag{2.5}$$

and the corresponding measure $\nu_f := \nu \circ f^{-1}$. Let's agree to call $f \circ \phi$ *equivalent* to a stationary stochastic process $R_n$on $\mathbb{R}^p$ if the stationary measure of R_n is equal to ν_f.

The results to be derived in this section are related to certain properties of ν_f for a given automorphism T. A special role is played by socalled Bernoulli automorphisms. The shift operator S defined above is (as an automorphism on $(Y, \mathcal{Q}, \nu)$) called *Bernoulli automorphism*, if the S-invariant measure ν is a product measure

$$\nu = \bigotimes_{i=-\infty}^{\infty} \eta^{(i)} \tag{2.6}$$

with an appropriate measure $\eta = \eta^{(i)}$ on M. In this case $f \circ \phi$ is equivalent to a sequence of independent identically distributed random variables ζ_i. In the case of finite expectation $\mathcal{E}(\zeta_i)$ and finite covariance matrix, this gives rise to a central limit theorem for sums

$$\frac{1}{\sqrt{n}} \sum_{i=0}^{n-1} ((f \circ \phi)_i - \mathcal{E}(\zeta_i)) \tag{2.7}$$

and thus to a diffusion limit. This procedure is described in the next section.

Another relevant class are Markov automorphisms. The shift operator S is called *Markov automorphism* if ν is defined via a measure η on M and a stochastic matrix $P = (p_{ij})_{1 \le i,j \le m}$ as follows. For finite-dimensional cylinders

$$A = \{y \in Y : y_i \in A_1, \cdots, y_{i+r} \in A_r\} \tag{2.8}$$

with $A_i \subset M$, $\nu(A)$ is given by

$$\nu(A) = \sum_{i(1) \in A_1} \eta_{i(1)} \sum_{i(2) \in A_2} p_{i(1),i(2)} \cdots \sum_{i(r) \in A_r} p_{i(r-1),i(r)} \tag{2.9}$$

This means that ν (and with this also ν_f) is equivalent to a Markov process. Certain Markov automorphisms are related to Bernoulli automorphisms as follows. Pick up a fixed element $e \in M$ such that $p_{i,e} > 0$ for all $i \in M$, and consider $Y_e := \{y \in Y : y_0 = e\}$. Obviously $\nu(Y_e) > 0$ and ν-almost sure, for $y \in Y_e$ there exists a strictly increasing infinite sequence $(n_i)_{i \in \mathbb{N}}$ with $y_{n_i} = e$. We can choose this sequence such that it meets all indices j such that $y_j = e$. This means that almost all $y \in Y_e$ can be seen as a infinite sequence of finite sequences $z_i := (y_{n_i+1}, \ldots, y_{n_{i+1}-1}, y_{n_{i+1}})$ of which only the last element is equal to e. Denote by Z the set of all such finite sequences. Then it is seen easily that the (normalized) measure ν on Y_e is equivalent to a product measure on the sequence space $\prod_{i=-\infty}^{\infty} Z^{(i)}$, with $Z^{(i)} = Z$.

A third class are the Markov automorphisms reflecting deterministic behaviour, i.e. those for which the elements of the stochastic matrix are of the form $p_{ij} = \delta_{\chi(i),j}$. Here, δ_{ij} denotes the Kronecker symbol and $\chi : M \to M$ is fixed. Clearly, in this situation for almost all $x \in \Omega$, $f \circ \phi(x)$ leads (possibly after a few steps) to periodic behaviour, and no regular diffusion limit may be obtained.

2.2 Diffusion limits for Bernoulli automorphisms $[ch_6]$

Let the measure space $(\Omega, \mathcal{O}, \mu)$ and an automorphism T on Ω be given as in the previous section. Suppose further given a measurable function $D = (d_i)_{i \le p} : \Omega \to \mathbb{R}^p$ with finite expectation $\bar{d} = (\bar{d}_i)$:

$$\bar{d}_i = \int_\Omega d_i(x) d\mu(x) < \infty \tag{2.10}$$

and finite, positive definite covariance matrix $\Sigma_D = (d_{ij})$ defined by

$$d_{ij} := \int_\Omega (d_i - \bar{d}_i)(d_j - \bar{d}_j)(x) d\mu(x) \tag{2.11}$$

Our aim is to develop diffusion limits for

$$X_n := \sum_{i=0}^{n-1} D(T^i x) \tag{2.12}$$

respectively its continuous-time extension $X(t)$ defined by

$$t \longrightarrow X_{[nt]} + (nt - [nt]) D(T^{[nt]+1} x) \tag{2.13}$$

It is evident that if X_n is equivalent to some stochastic process R_n the measures on $C([0, t_0]$, $t_0 > 0$ defined by the continuous-time extensions are equal. On $\mathbb{R}^p$ consider random walks R_n defined by

$$R_n = \sum_{i=1}^{n} \zeta_i \tag{2.14}$$

where ζ_i are independent and identically distributed random variables with finite expectation $\bar{\zeta} = \mathcal{E}(\zeta_i)$ and finite, positive definite covariance matrix Σ. The continuous version $R(t)$ is defined as above. The diffusion limit for $R(t)$ is a classical result.

Proposition 2.1: *For* $\epsilon \to 0$,

$$\sqrt{\epsilon}\left(R(\frac{t}{\epsilon}) - \frac{t}{\epsilon}\bar{\zeta}\right) \tag{2.15}$$

converges in distribution to the Wiener process W_Σ *with covariance matrix* Σ.

A proof for the one-dimensional version may be found in [5, Theorem 10.1]. The generalization to arbitrary dimensions is immediate.

Now suppose that there is a partition $\xi = (C_1, \dots, C_m)$ of Ω satisfying

Assumptions 2.2:

1. *D restricted to C_i is constant: $D|_{C_i} \equiv D_i$.*
2. *The corresponding shift operator S on $Y = \prod M$ is a Bernoulli automorphism.*

Then for arbitrary pairwise different indices $j_1, \dots, j_k \in \mathbb{N}$ and for arbitrary indices $n_1, \dots, n_k \in M$,

$$\mu\{x \in \Omega : D(T^{j_i}) = D_{n_i}, i = 1, \dots, k\} = \nu\{y \in Y : y_{j_i} = j_i, i = 1, \dots, k\} = \prod_{i=1}^{k} p_{n_i} \tag{2.16}$$

where $p_i = \nu(y_1 = i)$. This means that X_n is distributed like a sum of independent random variables on $\{D_1, \dots, D_m\}$ with probabilities p_i. It follows

Proposition 2.3: *Under the assumptions 3.2, X_n is equivalent to some random walk $R_n = \sum_{i=0}^{n-1} \zeta_i$. Denote $\bar{\zeta} = \mathcal{E}(\zeta)$. Then in particular $\sqrt{\epsilon}(X(t/\epsilon) - (t/\epsilon) \cdot \bar{\zeta})$ converges in distribution to a Wiener process W_Σ.*

Finally, we introduce a time change. Suppose given a measurable function $\tau : \Omega \to \mathbb{R}_+$ with finite expectation $0 < \bar{t} = \int \tau(x) d\mu(x)$, satisfying

Assumption 2.4: *For μ-almost all x*

$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=0}^{n-1} \tau(T^i x) = \bar{t} \tag{2.17}$$

This assumption is in particular satisfied if T is ergodic on $(\Omega, \mathcal{O}, \mu)$. Define $t_n := \sum_{i=0}^{n-1} \tau(T^i x)$ and $\bar{X}(t_n) := X_n$ with affine linear continuous-time extension as above. The diffusion limit carries over to this case. Since this has been demonstrated for similar situations e.g. in [2, 3] we restrict here to a heuristic argument. From (2.17) follows that $t_n \approx n \cdot \bar{t}$. Therefore,

$$\bar{X}(\frac{t}{\epsilon}) = \sum_{i=0}^{[\frac{1}{\epsilon} \cdot \frac{t}{\bar{t}}]-1} D(T^i x) + O(1) \tag{2.18}$$

The latter sum is distributed like

$$\sum_{i=0}^{[\frac{1}{\epsilon} \cdot \frac{t}{\bar{t}}]-1} \zeta_i = R(\frac{1}{\epsilon} \cdot \frac{t}{\bar{t}}) + O(1) \tag{2.19}$$

In fact, one can prove

Corollary 2.5: *Under the assumptions 2.2 and 2.4,* $\sqrt{\epsilon}(\bar{X}(t/\epsilon)-(1/\epsilon)\cdot(t/\bar{t})\cdot\bar{\zeta})$ *converges in distribution to the Wiener process* $W_{\Sigma'}$ *with*

$$\Sigma' = \frac{1}{\bar{t}^2}\Sigma \tag{2.20}$$

Following the remarks above, the generalization to a Markov automorphism is immediate, e.g. by conditioning on the first visit at a fixed set C_i.

3 Discrete velocity models

3.1 The setting

We consider a particle flow in the physical domain $\Xi = [0,h] \times \mathrm{I\!R}$. The particles assume velocities out of a finite set $\Gamma = \Gamma_+ \cup \Gamma_-$ of admissible velocities, $\Gamma_+ = \{\underline{u}_1, \ldots, \underline{u}_N\}$, $\Gamma_- = \{\underline{v}_1, \ldots, \underline{v}_N\}$. $\underline{u}_i = (u_{i1}, u_{i2})$ and $\underline{v}_i = (v_{i1}, v_{i2})$ are elements of $\mathrm{I\!R}^2$ with $\underline{u}_i$ pointing to the upper boundary $\partial_+\Xi = \{h\} \times \mathrm{I\!R}$ (i.e. $u_{i1} > 0$), and $\underline{v}_i$ to the lower boundary $\partial_-\Xi = \{0\} \times \mathrm{I\!R}$ (i.e. $v_{i1} < 0$). In the interiour $\mathring{\Xi}$ of Ξ, particles move with constant velocities. Density functions $f_i = f_i(t, \underline{x})$ for $\underline{u}_i$ and $g_i = g_i(t, \underline{x})$ for $\underline{v}_i$ describing the time evolution according to this law are governed by the partial differential equations

$$\left(\frac{\partial}{\partial t} + \underline{u}_i \cdot \nabla_{\underline{x}}\right) f_i = 0 \tag{3.1}$$

and

$$\left(\frac{\partial}{\partial t} + \underline{v}_i \cdot \nabla_{\underline{x}}\right) g_i = 0 \tag{3.2}$$

where $\underline{x} = (x_1, x_2)$ denotes the position vector in physical space. At the boundaries $\partial_\pm\Xi$, the particles are reflected back into $\mathring{\Xi}$ by changing the velocities according to some deterministic reflection laws. For simplicity, we assume at the upper boundary the uniform law $\underline{u}_i \to \underline{v}_i$ with the corresponding boundary condition for the densities f_i, g_i

$$|v_{i1}| g_i(t, (h, x_2)) = u_{i1} f_i(t, (h, x_2)) \tag{3.3}$$

(See, e.g. [1] for the derivation of boundary conditions from reflection laws.) At the lower boundary, we consider periodic boundary conditions as follows. Suppose given two functions $A_k : \{1, \ldots, N\} \longrightarrow \{1, \ldots, N\}$, $k = 1, 2$. If a particle hits at a position $\underline{x} = (0, x_2)$ with $x_2 \bmod 2 \in [0, 1)$ then v_i is changed into $u_{A_1(i)}$, otherwise into $u_{A_2(i)}$. The corresponding boundary conditions are

$$u_{j1} f_j(t, (0, x_2)) = \sum_{i:A_k(i)=j} |v_{i1}| g_i(t, (0, x_2)) \tag{3.4}$$

where $k \in \{1,2\}$ has to be chosen according to the value of x_2. Let us point out that if the A_i define one-to-one mappings, then the situation describes a completely reversible dynamics ("S-reversible" in the sense of Illner and Neunzert [10]).

In [1] it was shown how the boundary value problem (4.1) to (4.4) (completed with some initial condition) on $\Xi \times \Gamma$ may be transformed to an integral equation on $(\partial_- \Xi \times \Gamma_+) \cup (\partial_+ \Xi \times \Gamma_-)$. In a similar manner we investigate now the particle flow by registrating only scattering events at the boundaries. Since the reflection law at $x_1 = h$ is very simple, it is sufficient to project the dynamics to scattering events at $x_1 = 0$.

Suppose that a particle is reflected back from some point $\underline{x} = (0, x)$ at the lower boundary, $x \in [0,2)$, with some velocity $\underline{u}_i$. Then it hits at some later time the plane $x_1 = h$, is reflected back with velocity $\underline{v}_i$ and hits again $x_1 = 0$ at some point $(0, \tilde{x})$, where it is scattered back into some velocity $\underline{\tilde{u}} = \underline{u}_j$. Write $\tilde{x}$ as the unique decomposition $\tilde{x} = \delta + z$ where $T_1(x,i) := \delta \in [0,2)$, and $D(x,i) := z$ is an even integer. Denote further $T_2(x,i) := j = A_{k(\delta)}(i)$ indicating the new velocity $\underline{\tilde{u}}$, and $T := (T_1, T_2)$. T is defined on the state space $\Omega = [0,2) \times \{1, \dots, N\}$. We provide Ω with the σ-algebra $\mathcal{O}$ which is the product of the Borel σ-algebra on $[0,2)$ with the natural algebra for the finite set $\{1, \dots, N\}$. Whenever it is convenient, we identify $[0,2)$ with the torus $\mathbb{R}$ mod 2 and interpret elements $x \in \mathbb{R}$ as elements in $\mathbb{R}$ mod 2. As measure μ on Ω we define the measure obtained (after normalization) from the Borel measure on $[0,2)$ and the measure counting elements in subsets of $\{1, \dots, N\}$.

We consider T as the microscopic dynamics which may or may not exhibit some ergodic property, while it is the evolution of $n \longrightarrow D \circ T^n$which is responsible for macroscopic effects like the existence or non-existence of a diffusion limit. The shift in state space after the n-th iteration is given by

$$H_n(x,i) := \sum_{l=0}^{n-1} D \circ T^l(x,i) + r_n(x,i) \tag{3.5}$$

with a bounded error term r_n. If the orbit $n \to T^n(x,i)$ is asymptotically periodic (i.e. periodic after a finite number of steps), then

$$H(x,i) := \lim_{n \to \infty} \frac{1}{n} H_n(x,i) \tag{3.6}$$

exists, and

$$\frac{1}{\sqrt{n}}(H_n - n \cdot H) \to 0 \tag{3.7}$$

3.2 Periodic and nonperiodic orbits

We will derive criteria under which with a strictly positive probability (with respect to the measure ν), the dynamics is asymptotically periodic. One criterion is the existence of an appropriate partition of Ω. We denote by $\Im$ the set of semi-open intervals $[a,b)$

which are either contained in $[0,1)$ or in $[1,2)$. Given $i \in \{1,\ldots,N\}$, an interval $I \in \Im$ is shifted under the dynamics $T_1(.,i)$ by the value $h_i = T_1(0,i)$, i.e. $T_1(I,i) = h_i + I$. Considered as a subset of the torus, this set splits up into two sets $P_i^{(1)}I := T_1(I,i) \cap [0,1)$ and $P_i^{(2)}I := T_1(I,i) \cap [1,2)$ which are both elements of $\Im$. As the crucial property of D, observe that $D(.,i)$ is constant on an interval $I \in \Im$ if $T_1(I,i) \in \Im$, i.e. if $T_1(I,i)$ does not contain elements both in $[0,1)$ and in $[1,2)$ (which means that one of the two sets $P_i^{(k)}I$ is empty). This follows immediately from the dynamics defined in the previous section.

We reach our goal quickly, if we use the following

Assumption 3.1: *There exists a finite partition $\xi = (C_1,\ldots,C_m)$ of $[0,2)$ such that*

1. *for all $j \in \{1,\ldots,m\}$, $C_j \in \Im$;*
2. *for all $i \in \{1,\ldots,N\}$ and $j \in \{1,\ldots,m\}$, either $P_i^{(1)}C_j$ or $P_i^{(2)}C_j$ is empty;*
3. *for all $i \in \{1,\ldots,N\}$, $j \in \{1,\ldots,m\}$ and $k \in \{1,2\}$ there exists a $j' \in \{1,\ldots,m\}$ such that $P_i^{(k)}C_j \subseteq C_{j'}$.*

In fact, from the above statement we conclude that

$$x \longrightarrow D((x,i)) \tag{3.8}$$

is constant on the sets C_j, and we may interpret this as a function of the pair (j,i): $D(j,i) := D((x,i))$ for $x \in C_j$. By induction it follows that there exists a mapping

$$F : \{1,\ldots,m\} \times \{1,\ldots,N\} \longrightarrow \{1,\ldots,m\} \times \{1,\ldots,N\} \tag{3.9}$$

such that $D(T^n(x,i)) = D(F^n(j,i))$. However, $n \to F^n(j,i)$ is a deterministic dynamics on the finite set $\{1,\ldots,m\}\times\{1,\ldots,N\}$ and thus becomes periodic after at most $m\cdot N-1$ steps. This proves

Proposition 3.2: *Under the assumption 3.1, for all $x \in [0,2)$ the mapping $n \to D(T^n(x,i))$ is asymptotically periodic.*

Corollary 3.3: *Suppose that all numbers $h_i := T_1(0,i)$ are rationals. Then all mappings $n \to D(T^n(x,i))$ are asymptotically periodic.*

P r o o f : Write $h_i = p_i/q_i$ with $p_i, q_i \in \mathbb{N}$ and take a number $q \in \mathbb{N}$ which is a multiple of all q_i. Then the collection of sets $[(j-1)/q, j/q)$ for $j = 1,\ldots,2q$ satisfies the assumptions. □

In general, no statement about the existence of periodic orbits can be made. In fact, there are examples (also for non-rational numbers h_i) with asymptotically periodic behaviour a.s., and others with non-periodic behaviour a.s. A useful criterion for finding periodic orbits is derived now.

For $(x,i)\in\Omega$ denote for short $T^n x$ the x-component $T_1^n(x,i)$ of the n-th iterate. Define by $r^n(x,i)$ the distance on the right to the next "critical" point 1 or 2:

$$r_n(x,i) := \begin{cases} 2 - T^n x & : \quad T^n x \in [1,2) \\ 1 - T^n x & : \quad T^n x \in [0,1) \end{cases} \tag{3.10}$$

and

$$r(x,i) := \liminf_{n\to\infty} r_n(x,i) \tag{3.11}$$

This function allows to classify periodic and non-periodic states.

Proposition 3.4: *a) If $r(x,i) > 0$ then there exists an $h > 0$ such that for all $\tilde{x} \in [x, x+h)$, $n \to T_1^n(\tilde{x}, i)$ is asymptotically periodic.*
b) If $r(x,i) = 0$ then $n \to T_1^n(x,i)$ is not asymptotically periodic.

P r o o f : a) Define $\delta := \liminf_n r_n(x,i)$, and $h := \inf_n r_n(x,i)$. Since $r_n(x,i) > 0$ we conclude that h is strictly positive. By definition of T_1 and induction follows for all $n \in \mathbb{N}$, $T_1^n([x,x+h),i) \in \Im$, and for all $\tau \in [0,h)$, $T^n(x+\tau) = T^n + \tau$, and

$$r(x+\tau,i) = \delta - \tau = r(T_1^m(x+\tau,i)) \text{ for arbitrary } m \in \mathbb{N} \tag{3.12}$$

Now choose $m, n \in \mathbb{N}$, $m > n$, such that

$$T_2^m(x,i) = T_2^n(x,i) =: \hat{i} \tag{3.13}$$

and

$$T_1^m([x,x+h),i) \cap T_1^n([x,x+h),i) \neq \emptyset \tag{3.14}$$

If $y \in T_1^m([x,x+h),i) \cap T_1^n([x,x+h),i)$ then

$$(y,\hat{i}) = T_1^m(x+\tau_1,i) = T_1^n(x+\tau_2,i) \tag{3.15}$$

From

$$\delta - \tau_1 = r(T_1^m(x+\tau_1)) = r(y) = r(T_1^n(x+\tau_2)) = \delta - \tau_2 \tag{3.16}$$

follows $\tau_1 = \tau_2$ and with this $T_1^m x = T_1^n x$; from this we conclude that $T_1^m([x,x+h),i) = T_1^n([x,x+h),i)$, and all orbits starting from $[x,x+h) \times \{i\}$ are asymptotically periodic.
b) follows immediately from the strict positivity of $r(.,.)$. $\square$

We obtain as an immediate sufficient criterium

Corollary 3.5: *If the numbers $1, h_1, \ldots, h_N$ are rationally independent, then $r(.,.) \equiv 0$.*

("Rationally independent" means: If

$$s_0 + \sum_{i=1}^{m} s_i h_i = 0 \tag{3.17}$$

for some $m \in \mathbb{N}$ and for integers s_i, $i = 0, \ldots, m$, then $s_0 = \cdots = s_m = 0$.)

P r o o f : Suppose $r(x', i') > 0$. Then from the theorem follows that there exist $n > m \geq 0$ such that $T^n(x', i') = T^m(x', i')$. Denote $(x, i) := T^m(x', i')$. Obviously $r(x, i) > 0$, and $(x, i) = T^{n-m}(x, i)$. From this we conclude

$$x = (x + h_{j_1} + \cdots + h_{j_{n-m}}) \bmod 2 \tag{3.18}$$

with $j_k = T_2^k(x, i)$, and thus

$$h_{j_1} + \cdots + h_{j_{n-m}} = 2l \text{ for some } l \in \mathbb{N} \tag{3.19}$$

which is a contradiction to the independence. □

Let us consider the case when the mappings A_k on $\{1, \ldots, N\}$ are one-to-one. Then T is reversible and an automorphism with respect to the measure μ. It follows that all asymptotically periodic orbits are periodic and that $r(x, i) = \min_{n \in \mathbb{N}} r_n(x, i)$. From the proof follows that $r(., i)$ is strictly monotonically decreasing to 0 in $[x, x + \delta)$ if $r(x, i) = \delta$. Denote

$$J_i := \{x \in [0, 2) : r(x, i) > 0\} \tag{3.20}$$

and assign to each $x \in J_i$ the interval $[x - \tau, x + r(x, i))$ where

$$\tau = \max\{s \geq 0 : r(x', i) \geq r(x, i) \text{ for all } x' \in [x - s, x] \tag{3.21}$$

Collecting all these intervals decomposes J_i into a collection of disjoint intervals in $\Im$. This collection can be at most countable. This proves

Corollary 3.6: *If the A_k are one-to-one, then for each $i \in \{1, \ldots, N\}$ with $J_i \neq \emptyset$ there exists an at most countable collection $\xi_i = (C_k^{(i)})_{1 \leq k \leq r}$ of sets in $\Im$ which cover J_i.*

4 A continuous-velocity model

4.1 Specular reflection at a rough surface

As in section 4, we consider a two-dimensional flow between two walls at $x_1 = 0$ and $x_1 = h$, but now with a continuous set $\Gamma \subset \mathbb{R}^2$ of velocities. As boundary conditions we model specular reflection which does not change modulus of the velocities. Therefore we may choose without restriction a set of velocities with constant modulus. Therefore $\Gamma := \{(\cos\alpha, \sin\alpha)^T, \alpha \in I\}$ where $I \subset [-\pi, \pi]$ is a union of intervals to be specified later.

Between the walls, the particles move with constant velocities. The evolution equation for the density function $f = f(t, \underline{x}, \alpha)$ is

$$\left(\frac{\partial}{\partial t} + (\cos\alpha, \sin\alpha)^T \cdot \nabla_{\underline{x}} \right) f = 0 \tag{4.22}$$

At the upper boundary, particles are reflected specularly at a flat wall in the plane $x_1 = h$. This means that the velocities $\underline{v} = (\cos\alpha, \sin\alpha)^T$, $\alpha \in (-\pi/2, \pi/2)$ change into $(-\cos\alpha, \sin\alpha)^T$. The corresponding boundary condition for f is

$$f(t, (h, x_2), \alpha') = f(t, (h, x_2), \alpha) \text{ for } \alpha \in (-\pi, \pi) \tag{4.23}$$

where α and $\alpha' \in [-\pi, -\pi/2] \cup [\pi/2, \pi]$ are related by

$$\begin{pmatrix} \cos\alpha' \\ \sin\alpha' \end{pmatrix} = \begin{pmatrix} -\cos\alpha \\ \sin\alpha \end{pmatrix} \tag{4.24}$$

At the lower boundary, a model reflection law is chosen which mimics specular reflection at a rough surface with periodic profile. This model is to be derived now.

Consider a wall with a profile which in a neighborhood of $x_2 = 0$ is given by $(H(x_2), x_2)^T$ with an even C^2-function H. Denote by $\eta(x_2)$ the normal vector at $(H(x_2), x_2)^T$ pointing at the upper wall. It is given by $\eta(x_2) = c \cdot (H'(x_2), -1)^T$, where $c = 1/\sqrt{1 + (H'(x_2))^2}$ is the normalizing constant. Suppose a particle hits the wall at $(H(x_2), x_2)^T$ with a velocity $\underline{v}$ satisfying $\underline{v} \cdot \eta < 0$, and is specularly reflected. Then $\underline{v}$ is changed into

$$A_{x_2}(\underline{v}) := \underline{v} - 2(\underline{v} \cdot \eta)\eta \tag{4.25}$$

With such a reflection law, multiple scatterings at the wall between contacts with the plane $x_1 = h$ as well as velocities $(\cos\alpha, \sin\alpha)^T$ close to parallel to the wall (i.e. α close to $\pm\pi/2$) cannot be avoided. This causes difficulties which are hard to handle. Therefore we redefine the reflection law by some kind of linearization argument.

Close to $x_2 = 0$, the wall profile $(H(x_2), x_2)^T$ may well be approximated by some parametrized curve

$$\phi \to r \cdot (\cos\phi - h_0, \sin\phi)^T \tag{4.26}$$

where r is the radius of curvature of H at $x_2 = 0$. The normal vector at $r \cdot (\cos\phi - h_0, \sin\phi)^T$, which for simplicity we again denote by $\eta = \eta(\phi)$, is defined by $\eta(\phi) = (\cos\phi, \sin\phi)^T$. Under specular reflection, a velocity $\underline{v} = (-\cos\alpha, \sin\alpha)^T$ thus changes to a new vector which for small angles α, ϕ is approximated by

$$A_{x_2}(\underline{v}) \approx \begin{pmatrix} -\cos\alpha \\ \sin\alpha \end{pmatrix} + 2\cos(\alpha - \phi) \begin{pmatrix} \cos\alpha \\ \sin\alpha \end{pmatrix} \approx \begin{pmatrix} \cos(\alpha + 2\phi) \\ \sin(\alpha + 2\phi) \end{pmatrix} \tag{4.27}$$

Notice that $x_2 \approx r \cdot \phi$. We interpret the approximation as a model law for the plane $x_1 = 0$. In order to get a periodic law mapping incident velocities (i.e. $v_1 < 0$)

into reflected ones ($v_1 > 0$) we introduce a final modification. Define the canonical projection $\Pi : \mathbb{R} \to \mathbb{R}/Z$, $\Pi(x) := x \bmod 1$ and the invertible function $\Upsilon : \mathbb{R} \to \mathbb{R}$, $\Upsilon(x) := 2\alpha_0 \cdot (x - 0.5)$ for some fixed $\alpha_0 \in (0, \pi/2)$, which maps $[0,1]$ onto $[-\alpha_0, \alpha_0]$. Our final reflection law now changes velocities $\underline{v} = (-\cos\alpha, \sin\alpha)^T$, $\alpha \in [-\alpha_0, \alpha_0]$ into new velocities $\underline{v}' := (\cos\alpha', \sin\alpha')$ with $\alpha' =: R_{x_2}(\alpha) \in [-\alpha_0, \alpha_0]$ defined by

$$R_{x_2}(\alpha) := \Upsilon \circ \Pi \circ \Upsilon^{-1}(\alpha + 2x_2/r). \tag{4.28}$$

Notice that for x_2 and α in a neighborhood of 0, this is precisely the approximation given in the above formula. For all x_2, R_{x_2} is a one-to-one mapping on $[-\alpha_0, \alpha_0]$. The corresponding reflection law for the densities f reads

$$\cos\alpha \cdot f(t, (0, x_2), \alpha) = |\cos\tilde{\alpha}| \cdot f(t, (0, x_2), \tilde{\alpha}) \tag{4.29}$$

where $\tilde{\alpha} \in [-\pi, -\pi + \alpha_0] \cup [\pi - \alpha_0, \pi]$ is related to $R_{x_2}^{-1}(\alpha)$ via

$$\begin{pmatrix} \cos\tilde{\alpha} \\ \sin\tilde{\alpha} \end{pmatrix} = \begin{pmatrix} -\cos R_{x_2}^{-1}(\alpha) \\ \sin R_{x_2}^{-1}(\alpha) \end{pmatrix} \tag{4.30}$$

4.2 Diffusion limit for a model problem

For given $\alpha \in [-\alpha_0, \alpha_0] \cup [-\pi, -\pi + \alpha_0] \cup [\pi - \alpha_0, \pi]$, define $\bar{\alpha} := \arcsin(\sin\alpha)$. For α_0 small, $\overline{\cos}\alpha := \pm(1 - \bar{\alpha}^2/2)$ and $\overline{\sin}\alpha := \bar{\alpha} - \bar{\alpha}^3/2 = \bar{\alpha} \cdot \overline{\cos}\alpha$ are third order approximations of $\cos\alpha$ resp. $\sin\alpha$. (This may serve as a motivation concerning the domain of validity of the model discussed now.)

We are going to study (for arbitrary but fixed $\alpha_0 \in (0, \pi/2)$ the particle dynamics corresponding to the boundary value problem

$$\left(\frac{\partial}{\partial t} + (\overline{\cos}\alpha, \overline{\sin}\alpha)^T \cdot \nabla_x\right) f(t, \underline{x}, \alpha) = 0 \tag{4.31}$$

with the boundary conditions defined in the previous subsection. As in section 4 we do this just by registrating scattering events at the lower boundary. Suppose a particle starts at time $t = 0$ from the lower boundary at $x_2 = x_0$ at state $\alpha \in [-\alpha_0, \alpha_0]$. Then it hits the plane $x_1 = h$ at time $t = h/\overline{\cos}\alpha$ at $x_2 = x_0 + h\alpha$ and is reflected back into the state given by the reflection law, which does not change the moduli of the velocity components. Finally it hits the plane $x_1 = 0$ again at $x_2 = x_0 + 2h\alpha$ at time $t = 2h/\overline{\cos}\alpha$ and is reflected into the state $\alpha' = R_{x_2}(\alpha) = \Upsilon \circ \Pi \circ \Upsilon^{-1}(\alpha + 2(x_0 + 2h\alpha)/r)$. Notice that this describes a completely deterministic and reversible dynamics. The time discretization describing scattering events with the wall is given by the mapping

$$(x_0, \alpha) \longrightarrow (x_0 + 2h\alpha, \Upsilon \circ \Pi \circ \Upsilon^{-1}(\alpha + 2(x_0 + 2h\alpha)/r)) \tag{4.32}$$

For our analysis it is crucial that this mapping can be transformed into a group automorphism on the torus $\mathrm{Tor}^2 := \mathbb{R}^2/\mathbf{Z}^2$. To this aim we assume that

$$\frac{2}{r} =: q \in \mathbb{N} \tag{4.33}$$

and

$$2h =: p \in \mathbb{N} \tag{4.34}$$

From (4.12) follows that

$$\Pi \circ \Upsilon^{-1}(\alpha + \frac{2x}{r}) = \Pi \circ \Upsilon^{-1}(\alpha + \frac{2x'}{r}) \tag{4.35}$$

if $\Upsilon^{-1}(x) - \Upsilon^{-1}(x') \in \mathbf{Z}$. Therefore we define as microscopic dynamics the mapping on $[-\alpha_0, \alpha_0]^2$ given by

$$(x, \alpha) \longrightarrow (\Upsilon \circ \Pi \circ \Upsilon^{-1}(x + p\alpha), \Upsilon \circ \Pi \circ \Upsilon^{-1}(\alpha + q(x + p\alpha))) \tag{4.36}$$

Again, the macroscopic dynamics is defined by

$$D(x, \alpha) := x - \Upsilon \circ \Pi \circ \Upsilon^{-1}(x + p\alpha) \tag{4.37}$$

and

$$X_n := \sum_{i=0}^{n-1} D(T^i(x'\alpha)) \tag{4.38}$$

Under the transformation $(z, \beta) = (\Upsilon^{-1}x, \Upsilon^{-1}\alpha) =: \Upsilon^{-1}(x, \alpha)$ the microscopic dynamics transforms to

$$T(z, \beta) = (\Pi(z + p\beta), \Pi(qz + (1 + pq)\beta)) \tag{4.39}$$

The corresponding linear lifting is the linear mapping on $\mathbb{R}^2$ defined by the matrix

$$A = \begin{pmatrix} 1 & p \\ q & 1 + pq \end{pmatrix} \tag{4.40}$$

The coefficients of A are positive integers, and $\det A = 1$. Thus T is a group automorphism on Tor^2. Such transformations are well-studied in literature, see e.g. [12, Chapters I.12, II.3]. T is ergodic with respect to the Haar measure μ on Tor^2. In particular,

$$\bar{t} := \lim_{n \to \infty} \frac{1}{n} \sum_{i=0}^{n-1} t(T^i(z, \beta)) \tag{4.41}$$

with $t(z, \beta) = 2h/\overline{\cos}(\Upsilon\beta)$ exists a.s. and is independent of (z, β). Furthermore, as was shown in [11], T is equivalent to a Bernoulli shift B.

Here, we provide a partition adapted to the macroscopic dynamics giving rise to an appropriate Markov automorphism and thus to a diffusion limit.

Denote $w := \sqrt{pq \cdot (pq+4)}$. Then the eigenvalues of A are

$$\lambda_1 = \frac{pq+2+w}{2} > 1 \tag{4.42}$$

and

$$\lambda_2 = \frac{pq+2-w}{2} = \frac{1}{\lambda_1} < 1 \tag{4.43}$$

with the corresponding eigenvectors

$$v_1 = (p, \lambda_2 - 1)^T \tag{4.44}$$

and

$$v_2 = (p, \lambda_1 - 1)^T \tag{4.45}$$

It is convenient to call lines parallel to v_1 unstable and those parallel to v_2 stable. We consider partitions $\xi = (C_i)_{1 \le i \le M}$ into parallelograms the edges of which are parallel to the eigenvectors. Such a partition is called Markov partition if the stable parts of the boundaries are transformed under A to (subsets of) the stable part of $\cup \partial C_i$, and the unstable under A^{-1} to the unstable part. A Markov partition into two parallelograms for a given automorphism T is provided by [9, end of section 8, §1]. In our case it is $\xi' = (C_1', C_2')$, C_1' resp. C_2' being the parallelograms spanned by the vectors

$$p_1 = \frac{w - pq}{2pw} \cdot v_1, \text{ and } p_2 = -\frac{1}{w} \cdot v_2 \tag{4.46}$$

resp.

$$q_1 = -\frac{1}{w} \cdot v_1, \text{ and } q_2 = -\frac{w + pq}{2pw} \cdot v_2 \tag{4.47}$$

We demonstrate this for the case $p = 2$, $q = 3$. Fig. 1 shows the torus (thick solid lines), two eigenvectors (thick dashed lines) and the two parallelograms (thin solid lines). (Of course points outside of the unit interval are to be interpreted as elements of the torus under the natural projection.) The thin dashed lines are auxiliary lines for the construction of ξ'. In Fig. 2, the marked region represents the image of the smaller parallelogram under T. (The image of the other parallelogram is then obviously the complementary set.) The condition for a Markov partition concerning the stable part of the boundaries can be readily read off from this picture. For the general case, the conditions for a Markov partition follow from a straightforward[1] calculation yielding

$$A \cdot p1 = \lambda_2 \cdot q_2 + (1, q)^T \tag{4.48}$$

$$A \cdot q_1 = \lambda_2 \cdot p_2 - (p, pq + 1)^T \tag{4.49}$$

$$A^{-1} p_2 = \lambda_2 q_1 + (-p, 1)^T \tag{4.50}$$

and

$$A^{-1} q_2 = \lambda_2 \cdot p_1 - (pq + 1, -q) \tag{4.51}$$

This is not the partition we are looking for, since the macroscopic contributions $D(.)$ are not constant on C_i'. However, this can be achieved by splitting up the parallelograms along all lines parallel to v_1 which are transformed under T to the stable part of the initial partition. More specifically, the new partition ξ is obtained from ξ' as the set of all subsets of Ω of the form

$$C_i' \cap \{x \in \mathrm{Tor}^2 : D(x) = D_k, Tx \in C_j'\} \tag{4.52}$$

for fixed $i, j \in \{1, 2\}$ and D_k in the image of D which consists of a finite number of numbers. The new partition for the special case cited above is shown in Fig. 3. Combining these results with those of section 2.2 we end up with

Corollary to Proposition 2.3: *Under the scaling of Proposition 2.3, $X(.)$ converges in distribution to a Wiener process.*

[1]The precise formulas - as well as the preceding ones - have been found using the mathematics package DERIVE. It is, however, indeed straightforward to verify them by hand.

5 Some numerical aspects

Finally we concentrate on two numerical aspects coming out of the analysis so far. These are:

- We have seen a fundamental difference of the behaviour of discrete velocity models and continuous ones. How does e.g. the truncation error of a computer affect the dynamics?

- While the kinetic dynamics lives on a two-dimensional space-velocity phase space, the diffusion limit reduces to the one-dimensional physical space. Can this reduction of the dimension even be performed on the kinetic level and nevertheless describe the correct macroscopic dynamics?

For a dynamics composed by different periodic cycles with different expectations, we have to expect a variance growing quadratically in time. Such an effect has to appear in discrete velocity models with rational increments (Corollary 3.3). In a first numerical simulation we tested a continuous velocity model as described in section 4.2, but with truncation of the velocities after the n-th decimal at each time step. The corresponding variances of the complete system are shown in Fig. 4 from $n = 2$ (thin solid line) over $n = 4$ and $n = 6$ to the truncation error of the computer (thick solid line). While the latter curve agrees with the expected linear growth in time, deviations from linearity increase with increasing truncation error.

A look at Fig.2 suggests that the macroscopic behaviour should depend only on the component of a phase space vector in direction of the unstable manifold, i.e. in direction of p_1. The increment of the macroscopic variable is essentially determined from the number of crossings of the stable manifold when stretching the unstable part according to the larger eigenvalue λ_1. Thus the same macroscopic behaviour should exhibit for the stationary measure on the two-dimensional phase space and for the measure given by projection onto the unstable manifold (with (p_1, p_2) as an orthogonal system). In a second numerical experiment we compared the distribution of the macroscopic increments when starting from a 10×10-discretization of the smaller parallelogram C_1 with that of a 100-point discretization of p_1. The results after 1000 time steps are shown in Fig.5 and exhibit a quite reasonable agreement. This result may encourage to consider aspects of dimension reduction for kinetic schemes when passing to the macroscopic limit.

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