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On the mean free path for a periodic array of spherical obstacles

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Abstract. *We prove theorems pertaining to periodic arrays of spherical obstacles which show how the macroscopic limit of the mean free path depends on the scaling of the size of the obstacles. We treat separately the cases where the obstacles are totally and partially absorbing, and we also distinguish between two-dimensional arrays, where our results are optimal, and higher dimensional arrays where they are not. The cubically symmetric arrays to which these results apply do not have finite horizon.*

1. Introduction.

The idea of the "mean free path" for large ensembles of particles interacting among themselves (or moving among obstacles or within an enclosure) is quite intuitive, and

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lies at the foundations of kinetic theory as conceived by Maxwell and Boltzmann in the late nineteenth century. For a given physical system, estimates of the mean free path are important in determining the sort of dynamics that predominates. However, actually calculating the mean free path—even in many simplified models—is problematic, and it is often necessary to resort to dimensional arguments that are not wholly rigorous. One family of simplified models that has played an important role in statistical mechanics and kinetic theory is the so-called Lorentz gas in a plane dispersive billiard consisting of a periodic array of circular obstacles, together with its higher dimensional analogues. In kinetic theory, it is particularly interesting to study the behavior of particles in such billiards in the macroscopic limit (i.e., as the size of the array is reduced to zero). In this article, we prove theorems pertaining to periodic arrays of spherical obstacles which show how the macroscopic limit of the mean free path depends on the scaling of the size of the obstacles. We treat separately the cases where the obstacles are totally and partially absorbing, and we also distinguish between two-dimensional arrays, where our results are optimal, and higher dimensional arrays where they are not. The interesting aspect of these results is that the (hyper-) cubically symmetric arrays to which they apply do not have *finite horizon* (i.e., the arrays have unbounded trajectories).

The Lorentz gas has been widely studied: in Refs. [4] and [5], Bunimovich and Sinai, then Bunimovich, Sinai, and Chernov construct (analogues of) Markov partitions to analyze the "hydrodynamic limit" (in this case a Brownian motion) of a Lorentz gas with finite horizon. But the hydrodynamic limit corresponds to cases where the mean free path tends to zero, something that is assured in [4] and [5] by the scaling and the geometric hypothesis of finite horizon. The "kinetic" regime (also known as the Boltzmann-Grad limit) corresponds to cases where the limiting value of the mean free path is of the order of the unit length: hence this limit appears for periodic Lorentz gases only in cases where the finite horizon hypothesis does not hold. The Boltzmann-Grad limit of the Lorentz gas has been studied by many authors, but essentially only for random distributions of obstacles; see Gallavotti [9], Spohn [16], and Boldigrini, Bunimovich, and Sinai [3]. The Boltzmann-Grad limit for clouds of interacting particles (leading to the nonlinear Boltzmann equation) was investigated on a rigorous basis by Lanford [12], and subsequently by Illner and Pulvirenti [11] (in the two dimensional case), and by Pulvirenti [13].

However, as can be seen from the discussion below, the case of a square (or cubic, or hypercubic) array of spherical obstacles involves number theoretic questions (essentially rational approximation) in a *structural* way. Because of this, the results we find in (space) dimensions higher than two are not as good as those we find in two dimensions. The higher dimensional case involves "simultaneous rational approximation" (of several real numbers by fractions with the same denominator), while the two-dimensional case entails approximation of one real number by a sequence of rationals, where the algorithm of continued fractions is known to be in some sense optimal. For discussions of these questions, we refer the interested reader to Cassels [6] and Schmidt [14].

2. The n-Dimensional Dispersive Billiard and its Mean Free Path

The n-dimensional analogue of a periodic, planar array of circular scatterers with square symmetry is simply the periodic array of spherical obstacles defined as follows. First, denote by $\mathcal{L}_\varepsilon \equiv a\varepsilon\mathbf{Z}^n$ the (hyper-) cubic lattice in $\mathbf{R}^n$ with interstitial spacing $a\varepsilon$. The billiard domain is then

$$Z_\varepsilon \;=\; \{x \in \mathbf{R}^n \;\big|\; \mathrm{dist}\{x, \mathcal{L}_\varepsilon\} > r\varepsilon^\gamma\}. \tag{1}$$

Here $\varepsilon > 0$ is a small parameter which controls the spacing between obstacles in the array, while the exponent γ controls the way the size of the obstacles scales with ε (we assume that $\gamma \geq 1$ and $0 < 2r < a$ so that obstacles do not overlap in the macroscopic limit $\varepsilon \to 0$).

Using dimensional arguments, it is possible to estimate the order of magnitude of the mean free path for a population of point particles moving between the obstacles with constant speed c (neglecting collisions between particles)*. To see this, note that for a given geometry, the mean free path diminishes as the volume-density of obstacles—or as the size of the obstacles—increases. It therefore seems plausible to suppose that the order of magnitude of the mean free path is given by

$$\frac{1}{N_\varepsilon S_\varepsilon} \tag{2}$$

where N_ε is the density of obstacles per unit n-dimensional volume and S_ε is an $n-1$-dimensional volume element (so that the above expression has the dimension of length) measuring the size of the obstacles. For example, for S_ε, one could take the $n-1$-dimensional volume (physically, the "cross-section") of the transverse section of an individual obstacle, so that $S_\varepsilon = |\mathbf{B}^{n-1}|r^{n-1}\varepsilon^{\gamma(n-1)}$ (here $|\mathbf{B}^{n-1}|$ denotes the $n-1$-dimensional volume of the unit ball $\mathbf{B}^{n-1}$ in $\mathbf{R}^{n-1}$; for example $|\mathbf{B}^1| = 2$, $|\mathbf{B}^2| = \pi$, $|\mathbf{B}^3| = \frac{4}{3}\pi$, etc.). Using this ansatz together with (2), we arrive to the following estimate of the order of magnitude of the mean free path in Z_ε:

$$\frac{a^n}{|\mathbf{B}^{n-1}|r^{n-1}}\varepsilon^{n-\gamma(n-1)}. \tag{3}$$

The same expression is found after a more detailed analysis using diffusive billiard dynamics for Z_ε in the sense of "weak consistency" (see Golse [10]). Regardless of the process used to obtain the estimate of the mean free path (3), it suggests that the value $\gamma_c = \frac{n}{n-1}$ of the parameter γ is critical in the following sense:

• For $1 \leq \gamma < \gamma_c$, the mean free path tends to zero with ε. Assuming specular reflection of particles from the obstacles, one expects the movement of the particles in Z_ε to be given by an equation of hydrodynamic type (see Bunimovich-Sinai [4]).

• For $\gamma > \gamma_c$, the mean free path tends to infinity as $\varepsilon \to 0$. It is then trivial to show that the motion of the particles in Z_ε is governed by a free-transport equation.

* *One could reduce the number of parameters in the problem by adapting the length and time scales so that $a = 1$ and $c = 1$. However, we kept these extra parameters so that expressions like (3)—see below—clearly define a length.*

Perhaps the most crucial question along these lines is the following:

- For $\gamma = \gamma_c$, is the mean free path of order 1 as $\varepsilon \to 0$, and can one describe the corresponding motion of the particles in Z_ε by a kinetic equation?

The methods described below do not answer this question; we refer instead to the forthcoming article [18] for partial results in that direction. In this paper, we show rigorously that in dimension 2, γ_c has the value suggested by formula (3); and in higher dimensions, we obtain estimates of γ_c which are consistent with (3).

In any case, no rigorous calculation of the mean free path in Z_ε exists, in part because of the presence of unbounded trajectories (e.g. some trajectories parallel to the axes of the lattice $\mathcal{L}_\varepsilon$ are unbounded), and the presence of arbitrarily long trajectories.

3. Transport Equation Formalism.

We shall consider two types of problems: Case A, where particles are totally absorbed at the boundary of Z_ε; and Case B, where, upon reaching the boundary of Z_ε, particles are partially absorbed, then reflected with coefficient of reflection α ($0 < \alpha < 1$; our methods unfortunately do not apply to the case of total reflection $\alpha = 1$).

Let $f_\varepsilon(t, x, \omega)$ be the density of particles at the point x, at time t, moving in the direction $\omega \in \mathbf{S}^{n-1}$. We write

$$\Gamma_\varepsilon^+ = \{(x,\omega) \in \partial Z_\varepsilon \times \mathbf{S}^{n-1} \mid \omega \cdot n_x > 0\}, \tag{4}$$

where n_x is the inward normal at the point $x \in \partial Z_\varepsilon$. (Here "inward" means toward the interior of Z_ε; away from the centers of the balls Z_ε^c.) The equation satisfied by f_ε is

$$\partial_t f_\varepsilon + c\omega \cdot \nabla_x f_\varepsilon = 0, \qquad x \in Z_\varepsilon \tag{5}$$

with initial data

$$f_\varepsilon(0, x, \omega) = \phi(x, \omega), \qquad x \in Z_\varepsilon \tag{6}$$

and with either the condition of totally absorbing boundaries (Case A):

$$f_\varepsilon(t,x,\omega) = 0\,, \qquad (x,\omega) \in \Gamma_\varepsilon^+\,, \tag{7A}$$

or the condition of partially absorbing/partially reflecting boundaries (Case B):

$$f_\varepsilon(t,x,\omega) = \alpha f_\varepsilon(t,x,\mathcal{R}(n_x)\omega)\,, \qquad (x,\omega) \in \Gamma_\varepsilon^+\,. \tag{7B}$$

Here $\mathcal{R}(n_x)\omega$ represents specular reflection: $\mathcal{R}(n_x)\omega = \omega - 2(\omega \cdot n_x)n_x$; and ϕ is a nonnegative function defined on the whole of $\mathbf{R}^n \times \mathbf{S}^{n-1}$.

We may write the solution of (5)-(6)-(7A) using the method of characteristics. Let $\tau_\varepsilon(x,\omega)$ be the time of exit from Z_ε, in other words

$$\tau_\varepsilon(x,\omega) = \inf\{t > 0 \mid x - tc\omega \in \partial Z_\varepsilon\}\,. \tag{8}$$

For fixed $x \in Z_\varepsilon$, $\tau_\varepsilon(x,\omega)$ is finite for almost every $\omega \in \mathbf{S}^{n-1}$. (In fact, for "irrational" ω; that is, ω such that $\forall k \in \mathbf{Z}^n \setminus \{0\}$, $k \cdot \omega \neq 0$ it is well known that the trajectory of every point of the torus $\mathbf{T}^n \equiv \mathbf{R}^n/\mathbf{Z}^n$ is dense in $\mathbf{T}^n$; in other words, the linear flow in the direction ω on $\mathbf{T}^n$ is topologically transitive.) The solution of (4)-(5)-(6A) is given by

$$f_\varepsilon(t,x,\omega) \;=\; \mathbf{1}_{0 \le t < \tau_\varepsilon(x,\omega)}\phi(x - tc\omega, \omega) \tag{9}$$

and this formula shows that if $\tau_\varepsilon(x,\omega) \to 0$ as $\varepsilon \to 0$, then $f_\varepsilon(t,x,\omega) \to 0$. On the other hand, if, for any initial data ϕ bounded on $\mathbf{R}^n$ we had $f_\varepsilon \to 0$ as $\varepsilon \to 0$, this would mean that the equivalent effective cross section of absorption (as $\varepsilon \to 0$) of the array of obstacles Z_ε is infinite, or, what amounts to the same thing, that the mean free path tends to 0 with ε. Formula (8) therefore shows that in order to establish that $\gamma < \gamma_c$, it suffices to show that $f_\varepsilon \to 0$ for the initial data $\phi = 1$.

Remark 1. Usually, the types of questions addressed in the present article are solved by considering the "free path distribution," i.e.

$$\mu_\varepsilon(t) = \text{meas}\left(\{(x,\omega) \in Z_\varepsilon \times \mathbf{S}^{n-1} \,|\, \tau_\varepsilon(x,\omega) > t\}\right).$$

Relation (9) links the free path distribution μ_ε to the number density of particles f_ε in the following way: for any nonnegative initial number density ϕ

$$\text{meas}\left(\{(x,\omega)\in Z_\varepsilon\times \mathbf{S}^{n-1}\,\big|\, f_\varepsilon(t,x,\omega)\neq 0\}\right)\leq \mu_\varepsilon(t)\,.$$

On the other hand, if one chooses $\phi\equiv 1$, the inequality above becomes an equality. So, for fixed $t>0$, showing that $\mu_\varepsilon(t)\to 0$ is equivalent to showing that $f_\varepsilon(t,\cdot,\cdot)$ converges to 0 in the measure sense. Thus, by using this remark, all the results contained in the present paper could easily be rephrased in terms of the limiting behavior of the free path distribution.

Here we have chosen to use the formalism of transport equations rather than free path distributions for the following reasons:

— transport equations are the unifying concept common to both the approach involving weak consistency (developed in [10]) and to the present paper;

— the treatment of the subcritical case ($\gamma>\gamma_c$) is particularly simple if one uses PDE techniques: see Remark 5 following Theorem 2B, and the proof thereafter.

4. Principal Results.

We give several results affirming formula (3). For two-dimensional arrays, we state theorems implying $\gamma_c=2$. For higher dimensional arrays, we state similar but slightly weaker theorems which show that $\frac{n}{n-2/3}\leq\gamma_c\leq\frac{n}{n-1}$. As before, we divide these statements into those for totally absorbing obstacles, and those for partially absorbing obstacles.

A. *The Case of Total Absorption*

As mentioned above, the best result concerns the case where the dimension of the space is two.

Theorem 1A. *Let $n=2$, and choose $1\leq\gamma<2$, $T>0$, and a compact "observation set" $K\subset\mathbf{R}^2$. Then given any number s with $1<s<(\gamma-1)^{-1}$, there exists a constant A*

such that for any initial data $\phi \in L^\infty(\mathbf{R}^2 \times \mathbf{S}^1)$, the family f_ε of solutions of the problem (5)-(6)-(7A) satisfies

$$\left| \int_0^T \int_{K \cap Z_\varepsilon} \int_{\mathbf{S}^1} |f_\varepsilon(t,x,\omega)| d\omega dx dt \right| \leq A\varepsilon^{(1+s-\gamma s)/2} \|\phi\|_{L^\infty}.$$

The proof of this theorem (as well as the proofs of those below) relies on certain estimates of the "ergodization time for linear flows on tori" which we discuss (and prove in the two-dimensional case) in Section 5. These two-dimensional estimates are optimal in a sense which is clarified in Section 5. However, for tori of dimension greater than two, the estimates available on ergodization times are less precise. This is because in two dimensions, they are obtained using a continued fraction expansion of the slope of the direction vector, which is known to be an optimal approximation. In higher dimensions, this method no longer works, as it leads to a problem of *simultaneous* approximation of several irrationals by rational numbers.

Despite the lack of sharpness of the higher-dimensional estimates due to H.S. Dumas [8], our result based on them is as follows:

Theorem 2A. *Let $n > 2$, and choose $1 \leq \gamma < \frac{n}{n-2/3}$, $T > 0$, and a compact set $K \subset \mathbf{R}^n$. Then given any number s with $1 < s < (\gamma - 1)^{-1}$, there exists a constant A such that for any initial data $\phi \in L^\infty(\mathbf{R}^n \times \mathbf{S}^{n-1})$, the family f_ε of solutions of the problem (5)-(6)-(7A) satisfies*

$$\left| \int_0^T \int_{K \cap Z_\varepsilon} \int_{\mathbf{S}^{n-1}} |f_\varepsilon(t,x,\omega)| d\omega dx dt \right| \leq A\varepsilon^{(1+s-\gamma s)/2} \|\phi\|_{L^\infty}.$$

Remark 2. The estimates provided in Theorems 1A and 2A are not optimal. This is one of the shortcomings of our method, which uses L^∞ bounds for τ_ε rather than L^1 bounds or bounds on the free path distribution $\mu_\varepsilon(t)$. In the case of a Poisson random distribution of scatterers, as discussed in [3], the right hand side of the estimate in Theorem 1A decays exactly like $\varepsilon^{n-\gamma(n-1)}$. We doubt however that such an estimate can be obtained in the periodic case. A slightly weaker estimate may be obtained using methods very different from those presented here: see [18].

B. *The Case of Partial Absorption/Reflection*

We next state theorems for partially absorbing obstacles which closely parallel those for totally absorbing obstacles. However, the proofs of the theorems below are considerably more complicated, and lead to less precise estimates of the rate of decay of the mean free path.

Theorem 1B. *Let $n = 2$, and choose $1 \leq \gamma < 2$, $0 \leq \alpha < 1$, $T > 0$, and a compact set $K \subset \mathbf{R}^2$. Then there exist constants $b > 0$, $B > 0$, and $\varepsilon_0 > 0$ such that for any initial data $\phi \in L^\infty(\mathbf{R}^2 \times \mathbf{S}^1)$, and for $0 < \varepsilon \leq \varepsilon_0$, the family f_ε of solutions of the problem (5)-(6)-(7B) satisfies*

$$\left| \int_0^T \int_{K \cap Z_\varepsilon} \int_{\mathbf{S}^1} |f_\varepsilon(t,x,\omega)| d\omega dx dt \right| \leq B\varepsilon^b \|\phi\|_{L^\infty} .$$

Theorem 2B. *Let $n > 2$, and choose $1 \leq \gamma < \frac{n}{n-2/3}$, $0 \leq \alpha < 1$, $T > 0$, and a compact set $K \subset \mathbf{R}^n$. Then there exist constants $b > 0$, $B > 0$, and $\varepsilon_0 > 0$ such that for any initial data $\phi \in L^\infty(\mathbf{R}^n \times \mathbf{S}^{n-1})$, and for $0 < \varepsilon \leq \varepsilon_0$, the family f_ε of solutions of the problem (5)-(6)-(7B) satisfies*

$$\left| \int_0^T \int_{K \cap Z_\varepsilon} \int_{\mathbf{S}^{n-1}} |f_\varepsilon(t,x,\omega)| d\omega dx dt \right| \leq B\varepsilon^b \|\phi\|_{L^\infty} .$$

Remark 3. These results partly correct the errors that appear in the Note [1].

Remark 4. Theorems 1A and 2A (total absorption) apply to a more general class of scatterers than the spheres described in Eq. (1). In fact, Theorems 1A and 2A clearly apply to any class of scatterers which *contains* the scatterers defined as the complement of Z_ε in Eq. (1). More specifically: let Z'_ε be a family of open sets such that $Z'_\varepsilon \subset Z_\varepsilon$ for all $\varepsilon > 0$; then if τ'_ε denotes the exit time relative to Z'_ε, one has $\tau'_\varepsilon(x,\omega) \leq \tau_\varepsilon(x,\omega)$ for all $x \in Z'_\varepsilon$. In particular, if $\tau_\varepsilon(x,\omega) \to 0$ a.e., then $\tau'_\varepsilon(x,\omega) \to 0$ a.e..

Remark 5. Using elementary distributional calculus, it is not difficult to show that for any dimension n, $\gamma_c \leq \frac{n}{n-1}$. It therefore follows from Theorems 1A and 1B that, in two dimensions, $\gamma_c = 2$, as predicted by dimensional analysis (2), (3). On the other hand, Theorems 2A and 2B show that $\frac{n}{n-2/3} \leq \gamma_c \leq \frac{n}{n-1}$ in higher dimensions.

To see that $\gamma_c \leq \frac{n}{n-1}$, first note that if $\alpha = 1$ (total reflection) is allowed in Eq. (7B), then by the Maximum Principle, nonnegative initial data $\phi \geq 0$ give rise to nonnegative solutions $f_\varepsilon \geq 0$ with $\|f_\varepsilon\|_{L^\infty} \leq \|\phi\|_{L^\infty}$ for all $t \geq 0$. In fact, the same inequality holds for any α ($0 \leq \alpha \leq 1$), since, for fixed ϕ and fixed t, $\|f_\varepsilon\|_{L^\infty}$ is monotone decreasing with α.

Let $\{\ \}$ denote the operator which nullifies functions over obstacles; in other words, $\{f_\varepsilon\}(t,x,\omega) = 0$ for $x \notin Z_\varepsilon$, and $\{f_\varepsilon\}$ agrees with f_ε otherwise. It not difficult to see that

$$\partial_t\{f_\varepsilon\} = \{\partial_t f_\varepsilon\} \quad \text{and} \quad \partial_x\{f_\varepsilon\} = \{\partial_x f_\varepsilon\} + n_x\big(f_\varepsilon\big|_{\partial Z_\varepsilon^+}\big)\delta_{\partial Z_\varepsilon}, \tag{10}$$

where n_x is the inward unit normal to ∂Z_ε at x, $\delta_{\partial Z_\varepsilon}$ is the Dirac delta density concentrated on ∂Z_ε, and $f_\varepsilon\big|_{\partial Z_\varepsilon^+}$ is the "jump," or exterior limit, of f_ε at ∂Z_ε (see, e.g., Schwartz [15], Ch. 2, §3, Ex. 1). Therefore $\{\partial_t f_\varepsilon\} + c\omega \cdot \{\partial_x f_\varepsilon\} = 0$ leads to

$$\partial_t\{f_\varepsilon\} + c\omega \cdot \partial_x\{f_\varepsilon\} = c\omega \cdot n_x\big(f_\varepsilon\big|_{\partial Z_\varepsilon^+}\big)\delta_{\partial Z_\varepsilon}. \tag{11}$$

Now integrating the right hand side over $[0,T] \times K \times \mathbf{S}^{n-1}$, we find

$$\begin{aligned}\int_0^T \int_K \int_{\mathbf{S}^{n-1}} c\omega \cdot n_x\big(f_\varepsilon\big|_{\partial Z_\varepsilon^+}\big) d\omega\, \delta_{\partial Z_\varepsilon} dt &\leq 2\pi c\|\phi\|_{L^\infty} T \int_K \delta_{\partial Z_\varepsilon} \leq \\ 2\pi c\|\phi\|_{L^\infty} T\Big(\frac{\mathrm{diam} K}{a\varepsilon}\Big)^n |\mathbf{S}^{n-1}|(r\varepsilon^\gamma)^{n-1} &= O(\varepsilon^{\gamma(n-1)-n})\end{aligned} \tag{12}$$

from which it follows that, for every $\gamma > \frac{n}{n-1}$, we have $\partial_t\{f_\varepsilon\} + c\omega \cdot \partial_x\{f_\varepsilon\} \to 0$ in the sense of distributions as $\varepsilon \to 0$. In other words, $\gamma > \frac{n}{n-1}$ leads to a free transport equation in the macroscopic limit, so that $\gamma_c \leq \frac{n}{n-1}$.

Remark 6. As long as one is interested in estimating the mean free path, one can argue that it suffices to treat the fully absorbing case. However, as we shall see below, bounds on the exit time in a given direction ω depend crucially on how "rationally independent" the components of ω are. Specular reflection can change a direction with rationally independent components into a direction with rationally dependent components. In other words, the bound on the exit time which we have can be destroyed by the interaction with the scatterers. For this reason, we treat the case of partial absorption as well below.

5. Ergodization Rates for Linear Flow on the Torus.

This section is a self-contained discussion of the ergodization rates for linear flow on the torus developed in Dumas [8] and used in the proofs of the principal results announced above. We also derive an ergodization rate in the two-dimensional case which is mentioned in Remark 3.2 of [8], but is not explicitly calculated there.

5.1 *Linear Flow on* $\mathbf{T}^n$ *: Definitions and Notation.*

Given a direction vector $\omega \in \mathbf{S}^{n-1}$, we define the *linear flow on* $\mathbf{T}^n \equiv \mathbf{R}^n/\mathbf{Z}^n$ *associated to* ω as the family of maps

$$\omega_t : \mathbf{T}^n \to \mathbf{T}^n \quad \text{given by} \quad \theta \mapsto \theta + t\omega\,, \quad t \in \mathbf{R}\,. \tag{13}$$

The maps ω_t are well defined: if $y - y' \in \mathbf{Z}^n$, then clearly $(y+t\omega)-(y'+t\omega) \in \mathbf{Z}^n$; moreover, since the translations by the vector $t\omega$ form a one-parameter group of C^∞ transformations of $\mathbf{R}^n$, by passing to the quotient, we deduce that ω_t defines a one-parameter group of C^∞ transformations of $\mathbf{T}^n$.

A *rectilinear orbit segment of* $\mathbf{T}^n$ *starting at* θ is a parametrized curve of the form

$$\bigcup_{a<t<b} \omega_t(\theta) \tag{14}$$

where a and b are real numbers. Of course, the complete orbit of θ is obtained when $a = -\infty$ and $b = +\infty$.

Given $\theta \in \mathbf{T}^n$, there is an open neighborhood U of θ in $\mathbf{T}^n$ diffeomorphic to an open set V in $\mathbf{R}^n$; we equip U with the pull-back metric of the Euclidean metric on V. In fact, it is the unique metric on $\mathbf{T}^n$ which is invariant under all transformations ω_t for all $t \geq 0$ and every $\omega \in \mathbf{S}^{n-1}$. $\mathbf{T}^n$ equipped with this metric is a complete Riemannian manifold called the flat torus of dimension n. Its geodesic curves are the rectilinear orbit segments defined above. The associated geodesic distance is

$$\mathrm{dist}\{\theta, \theta'\} = \inf\{|x - x'| \mid \theta = x \bmod 1\,,\ \theta' = x' \bmod 1\}\,. \tag{15}$$

Fix $1 \geq R > 0$ and let $\mathcal{B}_{R/2}(\theta)$ be the ball of diameter R centered on $\theta \in \mathbf{T}^n$. We say that the flow ω_t with direction vector $\omega \in \mathbf{S}^{n-1}$ ergodizes $\mathbf{T}^n$ to within R after time T if and only if

$$\bigcup_{0 \leq t \leq T} \omega_t\big(\mathcal{B}_{R/2}(\theta)\big) \ = \ \mathbf{T}^n \tag{16}$$

for every $\theta \in T^n$. This condition is clearly independent of θ: for all θ, $\phi \in \mathbf{T}^n$,

$$\bigcup_{0 \leq t \leq T} \omega_t\big(\mathcal{B}_R(\theta)\big) \ = \ \bigcup_{0 \leq t \leq T} \omega_t\big(\mathcal{B}_R(\phi)\big) \ + \ \{\theta - \phi\} \tag{17}$$

so that

$$\text{if} \quad \bigcup_{0 \leq t \leq T} \omega_t\big(\mathcal{B}_R(\phi)\big) = \mathbf{T}^n, \quad \text{then} \quad \bigcup_{0 \leq t \leq T} \omega_t\big(\mathcal{B}_R(\theta)\big) = \mathbf{T}^n. \tag{18}$$

5.2 *The Special Case of Linear Flow on* $\mathbf{T}^2$.

On $\mathbf{T}^2$, we restrict ourselves to the class of flows with directions $\omega = (\omega_1, \omega_2)$ "between $0°$ and $45°$"; i.e., directions belonging to the eighth-circle $\mathcal{F}$ defined as

$$\mathcal{F} \ = \ \{(\omega_1, \omega_2) \in \mathbf{S}^1 \mid \sqrt{2}/2 < \omega_1 < 1 \text{ and } 0 < \omega_2/\omega_1 < 1\}. \tag{19}$$

(Note: We use ω_1, ω_2 to denote the components of the direction ω, even though the subscript t appears in our use of ω_t to designate the flow with direction ω. Since we never consider the time-1 or time-2 maps of ω_t, this should not cause confusion.)

Since we are only interested in directions with irrational slope (directions with rational slope do not generate ergodic flows), we have eliminated the directions $\omega = (1, 0)$ and $\omega = (\sqrt{2}/2, \sqrt{2}/2)$. The entirety of linear flows on $\mathbf{T}^2$ is then obtained by considering the seven remaining open sectors of directions in $\mathbf{S}^1$ which we reduce to $\mathcal{F}$ by symmetry.

5.3 *The Correspondence Between Rotations of* $\mathbf{T}^1 = \mathbf{R}/\mathbf{Z}$ *and Linear Flows on* $\mathbf{T}^2$.

For $0 < \beta < 1$, we define the rotation $\mathcal{R}_\beta : \mathbf{T}^1 \to \mathbf{T}^1$ by $\mathcal{R}_\beta(x) = x + \beta \bmod 1$. We say that $\mathcal{R}_\beta$ fills $\mathbf{T}^1$ to within R $(0 < R < 1)$ after N iterations if and only if for every $x \in \mathbf{T}^1$

$$\bigcup_{k=1}^{N} \mathcal{R}_\beta^k(I_R(x)) \;=\; \mathbf{T}^1, \tag{20}$$

where $I_R(x)$ designates the closed interval of length R centered at $x \in \mathbf{T}^1$.

There is a one-to-one correspondence between rotations on $\mathbf{T}^1$ and linear flows on $\mathbf{T}^2$:

• For $\omega = (\omega_1, \omega_2) \in \mathcal{F}$, the Poincaré map of ω_t induced on a vertical section of $\mathbf{T}^2$ is the rotation $\mathcal{R}_{\omega_2/\omega_1}$.

• Conversely, given a rotation $\mathcal{R}_\beta : \mathbf{T}^1 \to \mathbf{T}^1$ with $0 < \beta < 1$, the linear suspension of $\mathcal{R}_\beta$ on $\mathbf{T}^2$ is the linear flow $\omega_t : \mathbf{T}^2 \to \mathbf{T}^2$ with direction $\omega = (\frac{1}{\sqrt{1+\beta^2}}, \frac{\beta}{\sqrt{1+\beta^2}})$.

This correspondence also establishes a link between the ergodization time for linear flows of $\mathbf{T}^2$ and the number of iterations of the corresponding rotation necessary to fill $\mathbf{T}^1$:

Lemma 1. *Let* $\omega = (\omega_1, \omega_2) \in \mathcal{F}$ *(cf. (11)) and set* $\beta = \omega_1/\omega_2$. *If* $\mathcal{R}_\beta$ *fills* $\mathbf{T}^1$ *to within* R *after* N *iterations, then* ω_t *ergodizes* $\mathbf{T}^2$ *to within* $\omega_1 R$ *after time* $T = N/\omega_1$.

Proof. (Elementary geometry)

Remark 7. In particular, Lemma 1 shows that ω_t ergodizes $\mathbf{T}^2$ to within R after time $T = \sqrt{2}N$, since $\sqrt{2}/2 < \omega_1 < 1$.

5.4 *The Ergodization Time for Flows in Two Dimensions*

We now introduce the set $\mathcal{D}_n(s, C)$ of “highly irrational” direction vectors satisfying Diophantine conditions:

$$\mathcal{D}_n(s, C) = \{\omega \in \mathbf{S}^{n-1} \;\big|\; |\omega \cdot k| \geq C|k|^{-s} \;\forall k \in \mathbf{Z}^n \setminus \{0\}\}\,. \tag{21}$$

We recall that, for $s > n-1$, $\mathcal{D}_n(s, C)$ is nonempty for small enough $C > 0$, and in fact $\operatorname{meas}\{\mathcal{D}_n(s, C)^c\} \to 0$ as $C \to 0$ (here the superscript c denotes the complement in $\mathbf{S}^{n-1}$).

The main results here are the following theorem and its corollary.

Theorem 3. *Let $0 < R < 1$, $\omega \in \mathcal{F}$ (cf. (9)) and set $\beta = \omega_2/\omega_1$. If $\omega \in \mathcal{D}_2(s,C)$, then $\mathcal{R}_\beta$ fills $\mathbf{T}^1$ to within R after $[(3\sqrt{2})^s/(CR^s)]$ iterations. (Here $[x]$ is the integer part of x.)*

The result we use to prove Theorems 1A and 1B is the following

Corollary 1. $\omega \in \mathcal{D}_2(s,C) \implies \omega_t$ *ergodizes $\mathbf{T}^2$ to within R after time* $T = \dfrac{3^s(\sqrt{2})^{s+1}}{CR^s}$.

Proof. Apply Lemma 1 to Theorem 3.

5.5 *The Ergodization Time for Flows in Higher Dimensions*

Before proceeding to the proof of Theorem 3, for comparison we next state the best ergodization time known to us in higher dimensions $n > 2$, then follow with a simple conjecture and a remark on how the class $\mathcal{D}_n(s,C)$ may be enlarged while maintaining the ergodization time.

Theorem 4. $\omega \in \mathcal{D}_n(s,C) \implies \omega_t$ *ergodizes $\mathbf{T}^n$ to within R after time* $T = \dfrac{\kappa}{CR^{s+n/2}}$.

The constant κ appearing in Theorem 4 depends only on n and s, and involves the Sobolev norm of a certain "smoothest test function." It is given explicitly in [8], where complete proofs of Theorem 4 (called Theorem 1 in [8]) and related results appear.

Remark 8. Based on the way this estimate enters into the proofs of Theorems 2A and 2B, we note that it would be consistent with $\gamma_c = \frac{n}{n-1}$ if the optimal ergodization time appearing above in Theorem 4 were of the form $T = \kappa/(CR^s)$. In fact Remark 5, above, together with the proof of Theorem 2A show that this is the best possible ergodization time, at least in terms of its dependence on an inverse power of R.

Remark 9. Although we do not make use of it in this article, it is worth noting that the class of direction vectors $\omega \in \mathbf{S}^{n-1}$ whose ergodization times are comparable to those of Theorems 3 and 4 is in fact larger than $\mathcal{D}_n(s,C)$. This is because given a fixed $R > 0$, even $\omega \in \mathbf{S}^{n-1}$ with rationally related components will fill $\mathbf{T}^n$ to within R, provided the rational relations occur at sufficiently high order. This can be quantified by defining the set of "nearly highly irrational" direction vectors satisfying Diophantine conditions *truncated at order* N:

$$\mathcal{D}_n(s,C,N) = \{\omega \in \mathbf{S}^{n-1} \mid |\omega \cdot k| \geq C|k|^{-s} \ \forall k \in \mathbf{Z}^n \text{ with } 0 < |k| \leq N\}. \tag{22}$$

It is easy to see that $\mathcal{D}_n(s,C)$ is a Cantor set in $\mathbf{S}^{n-1}$, and that for each $N < \infty$, $\mathcal{D}_n(s,C,N)$ is an approximating superset of $\mathcal{D}_n(s,C)$ consisting of finitely many connected components with nonempty interior. In higher dimensions $n > 2$, it is possible to show that there exists a "critical cutoff" N_{crit} such that $N \geq N_{\text{crit}}$ ensures that flows with direction vectors $\omega \in \mathcal{D}_n(s,C,N)$ retain the ergodization time of Theorem 4 up to a factor depending on N. Details and an estimate of N_{crit} may be found in [8]. In two dimensions, the situation is considerably simpler: the proof of Theorem 3 which we give below shows that $N_{\text{crit}} \leq 3/R$.

5.6 *Proof of Theorem 3.*

Proof.

Part 1. *A bound on the growth of the denominators in the continued fraction expansion of* $\beta = \omega_2/\omega_1$.

Let the rational number p_n/q_n be the n^{th} convergent in the continued fraction expansion of $\beta = \omega_2/\omega_1$. We use the following properties of the sequence of convergents $\{p_n/q_n\}_{n=1}^{\infty}$ of $\beta \notin \mathbf{Q}$, $0 < \beta < 1$ (cf. for example Arnold [2] or Schmidt [14]).

(i) (rational approximation) $\forall k, \quad \left|\beta - \dfrac{p_k}{q_k}\right| < \dfrac{1}{q_k q_{k+1}} < \dfrac{1}{q_k^2}$

(ii) (growth of denominators for $\beta \notin \mathbf{Q}$) $q_1 = 1, \;\; q_k < q_{k+1}, \;$ and $\; q_k \to \infty$

(iii) (convergents not greater than 1) $\forall k, \;\; 1 \leq p_k \leq q_k$

According to (ii), we may choose an index k so that $q_k \leq 3/R < q_{k+1}$. Fixing this value of k, and multiplying the first inequality of (i) by $\omega_1 q_k$, we obtain

$$\frac{1}{q_{k+1}} > \frac{\omega_1}{q_{k+1}} > |\omega_2 q_k - \omega_1 p_k| = |\omega \cdot (-p_k, q_k)| \geq C\|(-p_k,q_k)\|^{-s}$$

$$= C(p_k^2+q_k^2)^{-s/2} \ \geq \ C(2q_k^2)^{-s/2} \ \geq \ \frac{CR^s}{(3\sqrt{2})^s}. \tag{23}$$

From this we deduce that $q_{k+1} \ < \ \left[\frac{(3\sqrt{2})^s}{CR^s}\right]$.

Part 2. *Shadowing of the (periodic) orbits of* $\mathcal{R}_{p_{k+1}/q_{k+1}}$ *by orbits of* $\mathcal{R}_\beta$.

Set $r = p_{k+1}/q_{k+1}$, which is rational in lowest terms. The sequence $\{\mathcal{R}_r^j(x)\} \subset \mathbf{T}^1$ is clearly periodic with period q_{k+1} for all $x \in \mathbf{T}^1$. In fact, $\mathcal{R}_r$ fills $\mathbf{T}^1$ to within exactly $1/q_{k+1} < R/3$ after q_{k+1} iterations. It is easy to see that the first q_{k+1} iterations of $\mathcal{R}_r$ are shadowed by those of $\mathcal{R}_\beta$.

More precisely: for every $1 \leq j \leq q_{k+1}$ and all $x \in \mathbf{T}^1$, we have:

$$\mathrm{dist}\{\mathcal{R}_r^j(x), \mathcal{R}_\beta^j(x)\} \ \leq \ |j(\frac{p_{k+1}}{q_{k+1}} - \frac{\omega_2}{\omega_1})| \ < \ q_{k+1}\frac{1}{q_{k+1}^2} \ = \ \frac{1}{q_{k+1}} \ < \ R/3 \tag{24}$$

Now, since $\mathcal{R}_r$ fills $\mathbf{T}^1$ to within $R/3$ after q_{k+1} iterations, and since each iterate $\mathcal{R}_r^j(x)$ is shadowed to within $R/3$ by $\mathcal{R}_\beta^j(x)$ $(1 \leq j \leq q_{k+1})$, it follows that $\mathcal{R}_\beta$ fills $\mathbf{T}^1$ to within R after $q_{k+1} \ < \ \left[\frac{(3\sqrt{2})^s}{CR^s}\right]$ iterations. //

Remark 10. In Part 1 above, whether $\beta = \omega_2/\omega_1$ is rational (so that its continued fraction expansion terminates) or irrational, it is still possible to choose k so that $q_k \leq 3/R < q_{k+1}$ provided $\omega \in \mathcal{D}_n(s, C, N)$ with $N \geq 3/R$, as the reader may easily check. This establishes the last part of Remark 9, above (since the rest of the proof goes through unchanged).

6. Proofs of Principal Results.

The proofs of Theorems 1A,B and 2A,B above differ only in the estimate of the ergodization time, which in turn depends on the dimension of the ambient space. We therefore give complete details of the proofs in the two-dimensional cases only (Theorems 1A and 1B).

6.1 *Proof of Theorem 1A.*

Proof. We begin by estimating the measure of the complement of $\mathcal{D}_2(s,C)$ in $\mathbf{S}^1$ (with respect to the uniform measure μ on $\mathbf{S}^1$). From elementary geometry, we have

$$\mu\{\mathcal{D}_2(s,C)^c\} \;=\; \mu\{\mathbf{S}^1 \setminus \mathcal{D}_2(s,C)\} \;\leq\; K_1 \sum_{0\neq k\in \mathbf{Z}^2} \frac{C}{|k|^{s+1}} \;=\; CK_1\rho(s+1) \tag{25}$$

for some constant $K_1 > 0$, and where $\rho(s+1) = \sum_{0\neq k\in\mathbf{Z}^2} |k|^{-(s+1)}$ converges for $s > 1$.

It is clear (see the definition) that if the flow ω_t with direction vector ω ergodizes $\mathbf{T}^2_{a\varepsilon} \equiv \mathbf{R}^2/(a\varepsilon\mathbf{Z})^2$ to within $2r\varepsilon^\gamma$ after time T_ε, then $\forall x \in Z_\varepsilon$ the collision time $\tau_\varepsilon(x,\omega) \leq T_\varepsilon$. We showed in the previous section (see Corollary 1) that every flow with direction $\omega \in \mathcal{D}_2(s,C)$ ergodizes $\mathbf{T}^2 = \mathbf{R}^2/\mathbf{Z}^2$ to within $\frac{2r}{a}\varepsilon^{\gamma-1}$ after time $3^s(\sqrt{2})^{s+1}C^{-1}(\frac{2r}{a}\varepsilon^{\gamma-1})^{-s}$. Consequently, every vector $\omega \in \mathcal{D}_2(s,C)$ ergodizes $\mathbf{T}^2_{a\varepsilon} = \mathbf{R}^2/(a\varepsilon\mathbf{Z})^2$ to within $2r\varepsilon^\gamma$ after time

$$T_\varepsilon \;=\; a\varepsilon\frac{3^s(\sqrt{2})^{s+1}}{C(\frac{2r}{a}\varepsilon^{\gamma-1})^s} \;=\; a^{1+(\gamma-1)s}\frac{3^s(\sqrt{2})^{s+1}}{C(2r)^s}\varepsilon^{1-(\gamma-1)s}\,. \tag{26}$$

Now let s be such that $1 < s < (\gamma-1)^{-1}$. According to the formula above, at any $x \in Z_\varepsilon$, directions ω belonging to $\mathcal{D}_2(s,C)$ have collision times $\tau_\varepsilon(x,\omega)$ which we estimate as

$$(x,\omega) \in Z_\varepsilon \times \mathcal{D}_2(s,C) \implies \tau_\varepsilon(x,\omega) \;\leq\; \frac{K_2}{C}\varepsilon^{1-(\gamma-1)s}, \tag{27}$$

where

$$K_2 \;=\; a^{1+(\gamma-1)s}\frac{3^s(\sqrt{2})^{s+1}}{c(2r)^s} \tag{28}$$

and we see that τ_ε vanishes together with ε on $Z_\varepsilon \times \mathcal{D}_2(s,C)$. We therefore decompose the initial data ϕ into the disjoint sum

$$\phi \;=\; \phi\mathbf{1}_{\mathcal{D}_2(s,C)} \;+\; \phi\mathbf{1}_{\mathcal{D}_2(s,C)^c} \tag{29}$$

and we consider the corresponding decomposition of the solution of (5)-(6)-(7A)

$$f_\varepsilon \;=\; g_\varepsilon\mathbf{1}_{\mathcal{D}_2(s,C)} \;+\; h_\varepsilon\mathbf{1}_{\mathcal{D}_2(s,C)^c}\,. \tag{30}$$

It follows that

$$\int_0^T \int_{K\cap Z_\varepsilon} \int_{\mathbf{S}^1} |f_\varepsilon(t,x,\omega)| d\omega dx dt \quad =$$

$$\int_0^T \int_{K\cap Z_\varepsilon} \int_{\mathcal{D}_2(s,C)} |g_\varepsilon(t,x,\omega)| d\omega dx dt \quad + \quad \int_0^T \int_{K\cap Z_\varepsilon} \int_{\mathcal{D}_2(s,C)^c} |h_\varepsilon(t,x,\omega)| d\omega dx dt \quad \leq$$

$$\frac{K_2}{C}\varepsilon^{1-(\gamma-1)s}\text{meas}\{K\}2\pi\|\phi\|_{L^\infty} \quad + \quad T\text{meas}\{K\}CK_1\rho(1+s)\|\phi\|_{L^\infty} \quad \leq$$

$$\frac{A}{2}\Big(C + \frac{\varepsilon^{1-(\gamma-1)s}}{C}\Big)\|\phi\|_{L^\infty} \tag{31}$$

where

$$A \;=\; 2\,\text{meas}\{K\}\cdot\max\big\{TK_1\rho(1+s)\,,\; 2\pi K_2\big\}. \tag{32}$$

The bound on the right-hand side of (31) is minimized by choosing $C = \varepsilon^{(1+s-\gamma s)/2}$ (the so-called "distinguished limit"), in which case the integral on the left-hand side of (31) is bounded by $A\varepsilon^{(1+s-\gamma s)/2}\|\phi\|_{L^\infty}$, as desired. //

Remark 11. If, instead of Theorems 1A and 2A as stated (with their order estimates of the rate of decay of the integral with ε), one wishes to prove only that

$$\lim_{\varepsilon\to 0}\int_0^T \int_{K\cap Z_\varepsilon} \int_{\mathbf{S}^{n-1}} |f_\varepsilon(t,x,\omega)| d\omega dx dt \;=\; 0, \tag{33}$$

it suffices to note (see the first part of the proof above for $n = 2$) that

$$\text{meas} \bigcap_{\substack{s>n-1\\ C>0}} (\mathcal{D}_n(s,C))^c \;=\; 0 \tag{34}$$

from which it follows that for almost every $(x,\omega) \in Z_\varepsilon \times \mathbf{S}^{n-1}$, the time to collision $\tau_\varepsilon(x,\omega)$ vanishes with ε.

6.2 *Proof of Theorem 1B.*

Because it is somewhat longer than the proof just given, we break the proof of Theorem 1B into Parts a) through f).

Proof.

a) Solution of the Transport Equation

We denote by $(X_\varepsilon(t,x,\omega), \Omega_\varepsilon(t,x,\omega))$ the "reverse broken flow" of the system (5)-(6)-(7B) on $\overline{Z_\varepsilon} \times \mathbf{S}^1$. More explicitly, using the method of characteristics we may write this flow as the solution of the system

$$\frac{dX_\varepsilon}{dt} = -\Omega_\varepsilon, \quad \frac{d\Omega_\varepsilon}{dt} = 0, \qquad X_\varepsilon \in Z_\varepsilon \tag{35}$$

$$X_\varepsilon(0,x,\omega) = x, \quad \Omega_\varepsilon(0,x,\omega) = \omega \tag{36}$$

$$X_\varepsilon(t+0) = X_\varepsilon(t-0), \quad \Omega_\varepsilon(t+0) = \mathcal{R}(n_{X_\varepsilon})\Omega_\varepsilon(t-0), \qquad X_\varepsilon \in \partial Z_\varepsilon . \tag{37}$$

We denote by $\mathcal{N}_\varepsilon(t,x,\omega) = \mathrm{card}\{0 \le \tau < t \mid X_\varepsilon(\tau,x,\omega) \in \partial Z_\varepsilon\}$ the number of collisions experienced by a particle with initial condition (x,ω), moving backward in $\overline{Z}_\varepsilon$ for a time $t > 0$. The value of f_ε after time t is then

$$f_\varepsilon(t,x,\omega) = \alpha^{\mathcal{N}_\varepsilon(t,x,\omega)} \phi(X_\varepsilon(t,x,\omega), \Omega_\varepsilon(t,x,\omega)) . \tag{38}$$

b) Decomposition of the Solution

As in the proof of Theorem 1A, we decompose the solution f_ε into a disjoint sum of Diophantine and non-Diophantine directions:

$$f_\varepsilon \ = \ g_\varepsilon \ + \ h_\varepsilon \, , \qquad \text{where} \qquad g_\varepsilon \ = \ f_\varepsilon \mathbf{1}_{\mathcal{D}_2(s,C_0)}, \quad h_\varepsilon \ = \ f_\varepsilon \mathbf{1}_{\mathcal{D}_2(s,C_0)^c} \, , \tag{39}$$

and where $C_0 > 0$ will be determined later.

c) Decomposition of the Integral

As in the proof of Theorem 1A, we write

$$\Big| \int_0^T \int_{K \cap Z_\varepsilon} \int_{\mathbf{S}^1} |f_\varepsilon(t,x,\omega)| d\omega dx dt \Big| \quad \le$$

$$T \|\phi\|_{L^\infty} \mathrm{meas}\{K\} C_0 K_1 \rho(1+s) \ + \ \int_0^T \int_{K \cap Z_\varepsilon} \int_{\mathcal{D}_2(s,C_0)} |g_\varepsilon(t,x,\omega)| d\omega dx dt \ \le$$

$$T\|\phi\|_{L^\infty}\mathrm{meas}\{K\}C_0K_1\rho(1+s) \ + \ \|\phi\|_{L^\infty}\int_0^T\int_{K\cap Z_\varepsilon}\int_{\mathcal{D}_2(s,C_0)}\alpha^{\mathcal{N}_\varepsilon(t,x,\omega)}d\omega dx dt. \quad (40)$$

Now we know that $(x,\omega)\in Z_\varepsilon\times\mathcal{D}_2(s,C_0) \implies \tau_\varepsilon(x,\omega) \le K_2C_0^{-1}\varepsilon^{1-(\gamma-1)s}\equiv T_\varepsilon^0$ (cf. Eqns. (26)–(28)). We shall later choose C_0 so that $T_\varepsilon^0\to 0$ as $\varepsilon\to 0$, so we may assume that ε_0 is small enough to ensure that $2T_\varepsilon^0\le T$ for $0<\varepsilon\le\varepsilon_0$. We then split the last integral into an integration over the time intervals $[0,2T_\varepsilon^0]$ and $[2T_\varepsilon^0,T]$ as follows:

$$\int_0^T\int_{K\cap Z_\varepsilon}\int_{\mathcal{D}_2(s,C_0)}\alpha^{\mathcal{N}_\varepsilon(t,x,\omega)}d\omega dx dt \quad =$$

$$\int_0^{2T_\varepsilon^0}\int_{K\cap Z_\varepsilon}\int_{\mathcal{D}_2(s,C_0)}\alpha^{\mathcal{N}_\varepsilon(t,x,\omega)}d\omega dx dt \ + \ \int_{2T_\varepsilon^0}^T\int_{K\cap Z_\varepsilon}\int_{\mathcal{D}_2(s,C_0)}\alpha^{\mathcal{N}_\varepsilon(t,x,\omega)}d\omega dx dt. \quad (41)$$

The first integral on the right hand side of (41) is easily bounded by $2T_\varepsilon^0\mathrm{meas}\{K\}2\pi = 2K_2C_0^{-1}\varepsilon^{1-(\gamma-1)s}\mathrm{meas}\{K\}2\pi$. As for the second integral on the right hand side of (41), we modify the argument of $\mathcal{N}_\varepsilon$ in two ways which do not increase $\mathcal{N}_\varepsilon$.

First, for all $(x,\omega)\in(K\cap Z_\varepsilon)\times\mathcal{D}_2(s,C_0)$, we have $\tau_\varepsilon(x,\omega)\le T_\varepsilon^0$; in particular, for such (x,ω) and for all $t\in[2T_\varepsilon^0,T]$, we have $t>\tau_\varepsilon(x,\omega)$, so that on the interval of integration $[2T_\varepsilon^0,T]$, we may shift the time by $\tau_\varepsilon(x,\omega)$ and particles along their trajectories a distance $c\tau_\varepsilon(x,\omega)$ to obtain

$$\mathcal{N}_\varepsilon(t,x,\omega) \ \ge \ \mathcal{N}_\varepsilon(t-\tau_\varepsilon(x,\omega),x-c\tau_\varepsilon(x,\omega)\omega,\omega). \quad (42)$$

Second, for all $t\in[2T_\varepsilon^0,T]$ and all $(x,\omega)\in(K\cap Z_\varepsilon)\times\mathcal{D}_2(s,C_0)$, we have $t/2\ge\tau_\varepsilon(x,\omega)$. Since $\mathcal{N}_\varepsilon$ is monotone increasing in its first argument, it follows that for such (t,x,ω),

$$\mathcal{N}_\varepsilon(t-\tau_\varepsilon(x,\omega),x-c\tau_\varepsilon(x,\omega)\omega,\omega) \ \ge \ \mathcal{N}_\varepsilon(t/2,x-c\tau_\varepsilon(x,\omega)\omega,\omega). \quad (43)$$

The right hand side of Eq. (41) is therefore bounded by

$$2T_\varepsilon^0\mathrm{meas}\{K\}2\pi \ + \ I_\varepsilon \quad = \quad 2\frac{K_2}{C_0}\varepsilon^{1-(\gamma-1)s}\mathrm{meas}\{K\}2\pi \ + \ I_\varepsilon\,, \quad (44)$$

where

$$I_\varepsilon \ = \ \int_{2T_\varepsilon^0}^T\int_{K\cap Z_\varepsilon}\int_{\mathcal{D}_2(s,C_0)}\alpha^{\mathcal{N}_\varepsilon(t/2,x-c\tau_\varepsilon(x,\omega)\omega,\omega)}d\omega dx dt. \quad (45)$$

d) Passage Through Reflection

We introduce the periodicized (or punctured toroidal) domain Y_ε associated to Z_ε by writing $Y_\varepsilon = Z_\varepsilon/(a\varepsilon\mathbf{Z})^2$. We note that Y_ε has compact closure, and that its boundary is a single circular obstacle of radius $r\varepsilon^\gamma$. We also define the boundary domains Δ_ε^+ and $\Delta_\varepsilon^+(s,C)$ by

$$\Delta_\varepsilon^+ \;=\; \{(y,\omega)\in\partial Y_\varepsilon\times\mathbf{S}^1 \;\big|\; \omega\cdot n_y>0\}\,, \tag{46}$$

$$\Delta_\varepsilon^+(s,C) \;=\; \Delta_\varepsilon^+\cap\big(\partial Y_\varepsilon\times\mathcal{D}_2(s,C_0)\big)\,, \tag{47}$$

where n_y is the inward normal at the point $y\in\partial Y_\varepsilon$.

Now let

$$\mathcal{Q}_\varepsilon \;=\; \{(y,\omega)\in\partial Y_\varepsilon\times\mathbf{S}^1 \;\big|\; \exists k\in\mathbf{Z}^2\setminus\{0\}\text{ s.t. }\mathcal{R}(n_y)\omega\cdot k=0\}\,. \tag{48}$$

The set $\mathcal{Q}_\varepsilon$ is clearly of $dyd\omega$-measure 0. On the other hand, linear flows on the torus with irrational slope are topologically transitive (i.e. the orbit of each point is dense). It follows in particular that for all $(y,\omega)\notin\mathcal{Q}_\varepsilon$, one has $\tau_\varepsilon(y,\mathcal{R}(n_y)\omega)<+\infty$. We may then define the boundary (or reflection) map

$$\mathcal{T}:\Delta_\varepsilon^+\setminus\mathcal{Q}_\varepsilon\to\Delta_\varepsilon^+ \qquad\text{by}\qquad \mathcal{T}(y,\omega) \;=\; \big(y-\tau_\varepsilon(y,\mathcal{R}(n_y)\omega)\mathcal{R}(n_y)\omega,\mathcal{R}(n_y)\omega\big) \tag{49}$$

and the "nice" set

$$\mathcal{E}_\varepsilon^N(s,C) \;=\; \bigcap_{k=0}^N \mathcal{T}^{-k}(\Delta_\varepsilon^+(s,C)) \tag{50}$$

consisting of elements $(y,\omega)\in\Delta_\varepsilon^+(s,C)\setminus\mathcal{Q}_\varepsilon$ whose first N iterates under $\mathcal{T}$ belong to $\Delta_\varepsilon^+(s,C)$.

Now consider the measure $d\nu_\varepsilon=|\omega\cdot n_y|dyd\omega$ on Δ_ε^+. We have

$$\nu_\varepsilon(\mathcal{E}_\varepsilon^N(s,C)^c) \;=\; \nu_\varepsilon(\Delta_\varepsilon^+\setminus\mathcal{E}_\varepsilon^N(s,C)) \;=\; \nu_\varepsilon\Big(\bigcup_{k=0}^N\mathcal{T}^{-k}(\Delta_\varepsilon^+(s,C)^c)\Big) \;\le$$

$$\sum_{k=0}^N\nu_\varepsilon\big(\mathcal{T}^{-k}(\Delta_\varepsilon^+(s,C)^c)\big) \;=\; (N+1)\nu_\varepsilon(\Delta_\varepsilon^+(s,C)^c) \;\le\; (N+1)2\pi r\varepsilon^\gamma CK_1\rho(s+1)\,, \tag{51}$$

where we have used the fact that $\mathcal{T}$ preserves the measure ν_ε (see, e.g., Bunimovich-Sinai [4]).

e) Further Estimates

We return to the problem of estimating the integral I_ε in Eq. (45). First, we define the "lift" $\mathcal{A}_\varepsilon^N(s,C) \subset Z_\varepsilon \times \mathbf{S}^1$ of the nice set $\mathcal{E}_\varepsilon^N(s,C)$ by

$$\mathcal{A}_\varepsilon^N(s,C) \;=\; \{(x,\omega) \in Z_\varepsilon \times \mathbf{S}^1 \,\big|\, [(x,\omega)] \in \mathcal{E}_\varepsilon^N(s,C)\}\,, \tag{52}$$

where $[(x,\omega)]$ is the equivalence class of (x,ω) for the relation $(x,\omega) \sim (x',\omega) \Longleftrightarrow x - x' \in (a\varepsilon\mathbf{Z})^2$.

We introduce an ε-dependent order parameter $C_1 > 0$ (to be chosen later so that $C_1 \to 0$ as $\varepsilon \to 0$), and we separate I_ε into an integral over initial conditions giving rise to trajectories whose directions after one collision belong to the nice set $\mathcal{A}_\varepsilon^N(s,C_1)$, and an integral over the complement of those initial conditions. In other words,

$$I_\varepsilon \quad \leq \quad J^\varepsilon \quad + \quad L^\varepsilon\,, \tag{53}$$

where

$$J^\varepsilon = \int_0^T \int_{K\cap Z_\varepsilon} \int_{\mathcal{D}_2(s,C_0)} \alpha^{\mathcal{N}_\varepsilon(t/2,x-c\tau_\varepsilon(x,\omega)\omega,\omega)} \mathbf{1}_{\{(x-c\tau_\varepsilon(x,\omega)\omega,\omega)\in\mathcal{A}_\varepsilon^N(s,C_1)\}}\, d\omega\, dx\, dt\,, \tag{54}$$

$$L^\varepsilon = \int_0^T \int_{K\cap Z_\varepsilon} \int_{\mathcal{D}_2(s,C_0)} \alpha^{\mathcal{N}_\varepsilon(t/2,x-c\tau_\varepsilon(x,\omega)\omega,\omega)} \mathbf{1}_{\{(x-c\tau_\varepsilon(x,\omega)\omega,\omega)\in(\mathcal{A}_\varepsilon^N(s,C_1))^c\}}\, d\omega\, dx\, dt. \tag{55}$$

In order to estimate J^ε, we introduce yet another ε-dependent order parameter θ_ε, to be chosen shortly, and we write

$$J^\varepsilon \quad = \quad J_1^\varepsilon \quad + \quad J_2^\varepsilon\,, \tag{56}$$

where

$$J_1^\varepsilon \;=\; \int_0^{\theta_\varepsilon} \int_{K\cap Z_\varepsilon} \int_{\mathcal{D}_2(s,C_0)} \alpha^{\mathcal{N}_\varepsilon(t/2,x-c\tau_\varepsilon(x,\omega)\omega,\omega)} \mathbf{1}_{\{(x-c\tau_\varepsilon(x,\omega)\omega,\omega)\in\mathcal{A}_\varepsilon^N(s,C_1)\}}\, d\omega\, dx\, dt \tag{57}$$

and

$$J_2^\varepsilon \;=\; \int_{\theta_\varepsilon}^T \int_{K\cap Z_\varepsilon} \int_{\mathcal{D}_2(s,C_0)} \alpha^{\mathcal{N}_\varepsilon(t/2,x-c\tau_\varepsilon(x,\omega)\omega,\omega)} \mathbf{1}_{\{(x-c\tau_\varepsilon(x,\omega)\omega,\omega)\in\mathcal{A}_\varepsilon^N(s,C_1)\}} d\omega dx dt. \quad (58)$$

We set $\theta_\varepsilon = 2K_2NC_1^{-1}\varepsilon^{1-(\gamma-1)s}$, where N and C_1 will be chosen later so that $N \to \infty$, $C_1 \to 0$, and $\theta_\varepsilon \to 0$ as $\varepsilon \to 0$. We restrict $\varepsilon_0 > 0$ so that $0 < \varepsilon \le \varepsilon_0 \Longrightarrow \theta_\varepsilon \le T$. We have

$$J_1^\varepsilon \quad\le\quad \theta_\varepsilon \mathrm{meas}\{K\}2\pi \quad=\quad 2K_2NC_1^{-1}\varepsilon^{1-(\gamma-1)s}\mathrm{meas}\{K\}2\pi. \qquad (59)$$

On the other hand, if $t \ge \theta_\varepsilon$ and if $(x,\omega) \in \mathcal{A}_\varepsilon^N(s,C_1)$, then because of the way θ_ε is defined, at least N collisions occur on the interval $[0,t/2]$; i.e., $(t,x,\omega) \in [\theta_\varepsilon,T]\times\mathcal{A}_\varepsilon^N(s,C_1) \Longrightarrow \mathcal{N}_\varepsilon(t/2,x,\omega) \ge N$. Therefore

$$J_2^\varepsilon \quad\le\quad T\alpha^N \mathrm{meas}\{K\}2\pi. \qquad (60)$$

In order to estimate the integral L^ε in Eq. (54), we are going to define a new compact set K' which is slightly bigger than K, and which encompasses the first collisions of all particles emanating from K in the directions $\mathcal{D}_2(s,C_0)$. By restricting ε_0 such that $0 < \varepsilon \le \varepsilon_0 \Longrightarrow cT_\varepsilon^0 \le 1$, we ensure that no particle travels more than unit distance on the time interval $[0,T_\varepsilon^0]$. We may then take

$$K' \quad=\quad \{x\in\mathbf{R}^2 \,\big|\, \mathrm{dist}\{x,K\}\le 1\}. \qquad (61)$$

Let $d\lambda_\varepsilon$ be the image measure of $dxd\omega$ under the map $(x,\omega)\mapsto(x-c\tau_\varepsilon(x,\omega)\omega,\omega)$. In other words, $d\lambda_\varepsilon$ is the measure on Γ_ε^+ given by $d\lambda_\varepsilon = \tau_\varepsilon^+(x,\omega)(n_x\cdot\omega)dxd\omega$, where $\tau_\varepsilon^+(x,\omega) = \tau_\varepsilon(x,-\omega)$ is the "forward" time to collision, and n_x is the inward unit normal to ∂Z_ε at x. Below we shall also denote $\Gamma_\varepsilon^+(s,C_0) = \Gamma_\varepsilon^+ \cap \big[(\partial Z_\varepsilon\cap K')\times\mathcal{D}_2(s,C_0)\big]$. With these conventions, we see that the image of $(K\cap Z_\varepsilon)\times\mathcal{D}_2(s,C_0)$ under the map $(x,\omega)\mapsto(x-c\tau_\varepsilon(x,\omega)\omega,\omega)$ is contained in $\Gamma_\varepsilon^+(s,C_0)$, and we may therefore write

$$L^\varepsilon \;\le\; \int_0^T \int_{\Gamma_\varepsilon^+(s,C_0)\cap(\mathcal{A}_\varepsilon^N(s,C_1))^c} \alpha^{\mathcal{N}_\varepsilon(t/2,x,\omega)} d\lambda_\varepsilon dt. \qquad (62)$$

Rewriting L^ε in this way amounts to a change of variables that is well known in the theory of neutron transport; see Cessenat [7]. Since the compact set K' contains no more than $(\mathrm{diam}K'/a\varepsilon)^2$ obstacles, it follows that

$$L^\varepsilon \;\le\; T\frac{K_2}{C_0}\varepsilon^{1-(\gamma-1)s}\Big(\frac{\mathrm{diam}K'}{a\varepsilon}\Big)^2(N+1)2\pi r\varepsilon^\gamma C_1K_1\rho(s+1). \tag{63}$$

f) Order Parameters and Final Estimate

In view of the inequalities and Eqs. (40) – (63), we have shown that the following bound holds:

$$\Big|\int_0^T\int_{K\cap Z_\varepsilon}\int_{\mathbf{S}^1}|f_\varepsilon(t,x,\omega)|d\omega dx dt\Big| \quad\le$$
$$\|\phi\|_{L^\infty}\big(K_3C_0 \;+\; K_4C_0^{-1}\varepsilon^{1-(\gamma-1)s} \;+\; J_1^\varepsilon \;+\; J_2^\varepsilon \;+\; L^\varepsilon\big) \quad\le$$
$$\|\phi\|_{L^\infty}\Big(K_3C_0+K_4\frac{\varepsilon^{1-(\gamma-1)s}}{C_0}+K_4\frac{N\varepsilon^{1-(\gamma-1)s}}{C_1}+K_5\alpha^N+K_6\frac{NC_1}{C_0}\varepsilon^{(\gamma-1)(1-s)}\Big), \tag{64}$$

where

$$K_3 \;=\; TK_1\rho(s+1)\mathrm{meas}\{K\}, \qquad K_4 \;=\; 4\pi K_2\mathrm{meas}\{K\}$$

$$K_5 \;=\; 2\pi T\mathrm{meas}\{K\}, \qquad K_6 \;=\; 4\pi rTK_1K_2\rho(s+1)(\mathrm{diam}K'/a)^2. \tag{65}$$

We now choose the order parameters and constants C_0, C_1, N, b, B, s and ε_0 so that the integral in (64) vanishes with ε, and the conclusion of Theorem 1B holds. By hypothesis, $1\le\gamma<2$. First, choose $b>0$ such that $0<b<(2-\gamma)/9<(2-\gamma)/8$. For $\gamma=1$, the desired inequalities below hold for any $s>1$; for $1<\gamma<2$, set $s=(2b+\gamma-1)/(\gamma-1)>1$. Finally, take

$$C_0 \;=\; \varepsilon^{2-\gamma-8b}, \quad C_1 \;=\; \varepsilon^{2-\gamma-4b}, \quad N \;=\; \varepsilon^{-b}, \tag{66}$$

and restrict $0<\varepsilon_0<1$ so that $0<\varepsilon\le\varepsilon_0\Longrightarrow\alpha^N=\alpha^{\varepsilon^{-b}}\le\varepsilon^b$. Then, taking all restrictions on ε_0 into account, for $0<\varepsilon\le\varepsilon_0$ it is not difficult to verify that $C_0\to0$, $C_1\to0$, $N\to\infty$, $T_\varepsilon^0\to0$, $\theta_\varepsilon\to0$, as $\varepsilon\to0$, and that

$$\Big|\int_0^T\int_{K\cap Z_\varepsilon}\int_{\mathbf{S}^1}|f_\varepsilon(t,x,\omega)|d\omega dx dt\Big| \quad\le\quad B\varepsilon^b\|\phi\|_{L^\infty} \tag{67}$$

where

$$B \quad = \quad K_3 \; + \; 2K_4 \; + \; K_5 \; + \; K_6. \tag{68}$$

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Remark 12. In order to carry out the proofs of Theorems 2A and 2B, it suffices to repeat the proofs just given, replacing as appropriate the estimate of the ergodization time in two dimensions (Section 5, Corollary 1) with the estimate in higher dimensions (Section 5, Theorem 4).

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