Entropy, Lyapunov exponents and mean free path for billiards

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April 25, 1997

Abstract

We review known results and derive some new ones about the mean free path, Kolmogorov-Sinai entropy and Lyapunov exponents for billiard type dynamical systems. We focus on exact and asymptotic formulas for these quantities. The dynamical systems covered in the paper include periodic Lorentz gas, stadium and its modifications, and the gas of hard balls, for which we prove rigorously the classical Boltzmann formula for the intercollision time. Some open questions and numerical observations are discussed.

Keywords: Billiards, hard balls, Lorentz gas, entropy, mean free path, Lyapunov exponents.

1 Basic facts about billiards

Hamiltonian systems with elastic collisions or specular reflections are often called billiards. In particular, these include gases of hard balls, Lorentz gases, and stadia. Below we recall basic definitions and facts about billiards.

Let Q be a compact closed connected domain in $\mathbb{R}^d$ or on a d-torus $\mathrm{T}^d = \mathbb{R}^d/\mathbb{Z}^d$. Let the boundary ∂Q be a finite union of smooth (of class C^3) compact manifolds of codimension one, $\partial Q = \Gamma_1 \cup \cdots \cup \Gamma_r$, $r \geq 1$. We call Q a billiard table and ∂Q its wall. Let the set

$$\Gamma^* = \cup_{i \neq j}(\Gamma_i \cap \Gamma_j)$$

be a finite union of smooth compact submanifolds of codimension ≥ 2. This set includes all the corner points of the wall ∂Q. We will call it the singular part of ∂Q. The points $q \in (\partial Q) \setminus \Gamma^*$ are said to be regular.

The billiard dynamical system in Q is generated by the free motion of a pointlike particle at unit speed in the table Q with specular reflections at the wall ∂Q. The reflection rule "the angle of incidence equals the angle of reflection" is specified by the equation[1]

$$v_+ = v_- - 2\,(n(q) \cdot v_-)\,n(q) \tag{1.1}$$

[1] Here and on $(u \cdot v)$ means the scalar product of vectors u and v.

where v_- and v_+ are the incoming and outgoing velocity vectors, and $n(q)$ is the inward unit normal vector to the wall ∂Q at the point of reflection q. The vector $n(q)$ is well defined at all regular points of ∂Q. If the particle hits the singular set Γ^* (a corner point of the wall), its further trajectory is not defined.

The phase space of the billiard system is $M = Q \times S^{d-1}$, where S^{d-1} is the unit sphere of velocity vectors. We denote phase points by $x = (q, v)$, where q is the configuration point (the position of the billiard particle in Q), and v is its velocity vector. We denote by Π_Q and Π_V the natural projections of M onto Q and S^{d-1}, respectively. The billiard dynamics generates a flow, Φ^t, on M. This flow preserves the normalized Liouville measure $d\mu = c_\mu \, dq \, dv$, where dq and dv are the Lebesgue measures on Q and S^{d-1}, respectively, and

$$c_\mu = \left(|Q| \cdot |S^{d-1}|\right)^{-1}$$

is the normalizing factor. Here $|Q|$ is the volume of the domain Q and

$$|S^{d-1}| = \frac{2\pi^{d/2}}{\Gamma(d/2)}$$

is the $(d-1)$-dimensional volume of the unit sphere in $\mathbb{R}^d$. Here $\Gamma(x)$ is the gamma function, $\Gamma(n+1) = n!$, $\Gamma(x+1) = x\Gamma(x)$, and $\Gamma(1/2) = \sqrt{\pi}$.

The billiard flow Φ^t has a natural cross-section associated to the wall of the billiard table. Let

$$\Omega = \{(q, v) \in M : \ q \in \partial Q \ \text{ and } \ (v \cdot n(q)) \geq 0\}$$

The first return map $T : \Omega \to \Omega$ takes a point $x \in \Omega$ to the point on the trajectory of x immediately after its first reflection in ∂Q. This is called the billiard ball map. The map T preserves the probability measure $d\nu = c_\nu\,(v\cdot n(q))\,dq\,dv$, where dq is now the Lebesgue measure on ∂Q, and c_ν is the normalizing factor. It is a simple calculation, cf. [8], that

$$c_\nu = \left(|\partial Q|\cdot|B^{d-1}|\right)^{-1}$$

Here $|\partial Q|$ is the $(d-1)$-dimensional volume of the wall ∂Q, and $|B^{d-1}| = |S^{d-2}|/(d-1)$ is the volume of the unit ball in $\mathbb{R}^{d-1}$.

For every phase point $x = (q,v) \in M$ let $\tau_+(x) = \min\{t > 0 : \Phi^{t+0}x \in \Omega\}$ and $\tau_-(x) = \max\{t < 0 : \Phi^{t+0}x \in \Omega\}$ be the first positive and negative moments of reflection, respectively. We then have two canonical projections of M onto Ω: $\tilde\pi_\pm x = \Phi^{\tau_\pm(x)+0}x$. Note that $T^{\pm 1}x = \tilde\pi_\pm x$ for $x \in \Omega$.

Any point $x = (q,v) \in M$ can be specified by the point $\tilde x = (\tilde q, v) = \tilde\pi_-(x) \in \Omega$ and the positive number $t = |\tau_-(x)| \geq 0$. In this way $(\tilde q, v, t)$ make a coordinate system in M, with $\tilde q \in \partial Q$, $v \in S^{d-1}$, and $t > 0$. In these coordinates

$$d\mu = c_\mu\,(v\cdot n(\tilde q))\,d\tilde q\,dv\,dt \tag{1.2}$$

where $d\tilde q$ is the Lebesgue measure on ∂Q, cf. [8]. Actually, it is Eq. (1.2) on which the invariance of the measure ν under T is based, see also [8].

2 Mean free path

For every phase point $x \in M$ the free path is the distance the billiard particle covers before it collides with ∂Q. Since the speed of the particle is unit, the free path is

$\tau(x) = \tau_+(x) = \min\{t > 0 : \Phi^{t+0} x \in \Omega\}$.

As for the *mean* free path, there is a natural ambiguity in this concept, since one can integrate $\tau(x)$ with respect to either the Liouville measure μ or the "boundary" measure ν arriving at two different values.

It is, however, more sensible and traditional to define the mean free path by

$$\bar{\tau} = \int_\Omega \tau(x)\, d\nu(x) \tag{2.1}$$

which is the definition we adopt here. The main reason for this is the 'dynamical' interpretation of $\bar{\tau}$: it is the time average of the free paths along typical trajectories. Precisely, the Birkhoff ergodic theorem implies that for almost every $x \in \Omega$ we have

$$\frac{\tau(x) + \tau(Tx) + \cdots + \tau(T^{n-1}x)}{n} \to \hat{\tau}(x) \quad \text{as} \quad n \to \infty \tag{2.2}$$

Then the mean value of $\hat{\tau}(x)$ coincides with $\bar{\tau}$:

$$\int_\Omega \hat{\tau}(x)\, d\nu(x) = \bar{\tau} \tag{2.3}$$

If the billiard ball map T is ergodic, then we simply have $\hat{\tau}(x) = \bar{\tau}$ a.e.

There is a remarkably simple formula for the mean free path in *any* billiard table Q in terms of its geometric parameters:

$$\bar{\tau} = \frac{|Q| \cdot |S^{d-1}|}{|\partial Q| \cdot |B^{d-1}|} \quad \left(= \frac{c_\nu}{c_\mu} \right) \tag{2.4}$$

This follows from Eq. (1.2):

$$\int_\Omega \tau(x)\, d\nu(x) = c_\nu \int_\Omega \tau(x)\, (v \cdot n(\tilde{q}))\, d\tilde{q}\, dv = c_\nu \int_M (v \cdot n(\tilde{q}))\, d\tilde{q}\, dv\, dt = c_\nu / c_\mu$$

In particular, for planar billiard tables $d = 2$, and we have

$$\bar{\tau} = \frac{\pi\,|Q|}{|\partial Q|} \tag{2.5}$$

and for 3-D billiard tables we have

$$\bar{\tau} = \frac{4\,|Q|}{|\partial Q|} \tag{2.6}$$

We emphasize that (2.4)-(2.6) are *exact* formulas.

The formulas (2.4)-(2.6) with the definition (2.1) of $\bar{\tau}$ are known in integral geometry and geometric probability, see, e.g., Eq. (4-3-4) in [24]. Eq. (2.5) is often referred to as Santalo's formula, since it is given in Santalo's book [26].

The formulas (2.4)-(2.6) with the dynamical interpretation (2.2)-(2.3) of $\bar{\tau}$ have been also discussed and derived from (1.2) at Moscow seminar on dynamical systems directed by Sinai and Alekseev in the seventies. Regrettably, it has never been considered to be worth publishing, so I could not locate any reference to it until mid-eighties. Wojtkowski proved the 2-D formula (2.5) based on Eq. (1.2) in Ref. [36]. A proof of Eq. (2.4) in any dimension based on (1.2) was given in [8]. Another proof of (2.4), based on Green's theorem in vector analysis, was independently found by Golse (private communication [17]). Unfortunately, the lack of references to the above formulas leads to repeated attempts by various researches to estimate $\bar{\tau}$ numerically or heuristically for particular billiard tables. This section is intended to help fill this gap.

3 Entropy and Lyapunov exponents

Billiards belong to a rather general class of smooth dynamical systems with singularities. An exact definition of this class and its extensive study may be found in the book by Katok and Strelcyn [18]. The main results of that book are the existence of local stable and unstable manifolds and exact formulas for the entropy. It was also shown in that book that the billiard ball map in a planar billiard table under certain very mild conditions belongs in the class of smooth maps with singularities. For multidimensional billiards, the same was shown in [8] under the assumption that the sectional curvature of the smooth components of the boundary ∂Q is C^2 smooth up to the singular set Γ^*. In particular, the sectional curvature must be uniformly bounded. This assumption is pretty mild and possibly can be relaxed.

Thus, all the results of the book [18] carry over to generic billiards. These produce the following three theorems.

Theorem 3.1 (Lyapunov exponents) *For ν-almost every point $x \in \Omega$ there is a DT-invariant decomposition of the tangent space*

$$\mathcal{T}_x\Omega = \oplus_{i=1}^{s(x)} H_i(x)$$

such that, uniformly in the vectors $w \in H_i(x)$, $||w|| = 1$, we have the limit

$$\lim_{n \to \pm\infty} n^{-1} \ln ||DT_x^n(w)|| = \chi_i(x)$$

for $i = 1, \ldots, s(x)$. Here $\chi_1(x) < \chi_2(x) < \cdots < \chi_{s(x)}(x)$ are Lyapunov exponents of the billiard ball map T at the point x.

Remark. This theorem immediately follows from the Oseledec multiplicative theorem, see [18], and the following fact:

$$\int_{\Omega} \log^{+} ||DT_x^{\pm}||\, d\nu(x) < \infty$$

where $\log^{+} a = \max\{\log a, 0\}$.

Remark. The functions $s(x)$, $\chi_i(x)$ and $\dim H_i(x)$ (the multiplicity of the exponent $\chi_i(x)$) are invariant under both T and T^{-1}. In particular, if the billiard ball map T is ergodic, then these functions are a.e. constant on Ω.

As a corollary to the above theorem, there is an a.e. DT-invariant decomposition

$$\mathcal{T}_x\Omega = E_x^u \oplus E_x^s \oplus E_x^0$$

where the subspaces E_x^u, E_x^s and E_x^0 correspond to positive, negative and zero exponents, respectively. Any vector $w \in E_x^u$ under the iterations of DT exponentially grows in the future and exponentially contracts in the past. A time-symmetric statement holds for vectors $w \in E_x^s$. The space E_x^u is said to be unstable, E_x^s stable and E_x^0 neutral. We denote $d^u(x) = \dim E_x^u$ and $d^s(x) = \dim E_x^s$.

If positive and negative Lyapunov exponents exist on a subset of positive measure, but there are zero Lyapunov exponents as well, the map T is said to be *partially hyperbolic.* An example is a 3-D billiard table made by placing a vertical cylinder in a 3-D cube, i.e., $Q = \{-1 \le x, y, z \le 1, \text{ and } x^2 + y^2 \ge r^2\}$ for some $r < 1$. Here $\dim \Omega = 4$, there are one positive and one negative Lyapunov exponents a.e., as well as two zero Lyapunov exponents. There are also billiard trajectories in this domain that never hit the cylinder

$x^2 + y^2 = r^2$, their all Lyapunov exponents are zero, but they make a set of measure zero in the phase space.

If all the Lyapunov exponents are nonzero a.e., the map T is said to be (fully) hyperbolic, in which case T is often said to be *chaotic*, quite informally.

At present, the following classes of billiards are known to be fully hyperbolic: dispersing, some semidispersing, and planar billiards bounded by the so-called absolutely focusing arcs. A billiard Q is said to be dispersing (semidispersing) if its boundary ∂Q is strictly (nonstrictly) concave outward at all its regular points. All dispersing billiards are hyperbolic, ergodic, K-mixing and Bernoulli, see [27, 31, 10]. Semidispersing billiards are generally hyperbolic, but not necessarily, as the above example shows.

Planar billiards whose boundary contains concave inward (focusing) components are sometimes hyperbolic, too. This happens, e.g., if all the focusing components of ∂Q are arcs of some circles, and all those circles lie entirely in Q, as it was shown by Bunimovich [4, 5]. Much more general classes of planar hyperbolic billiards with focusing components of the boundary have been later found by Wojtkowski [35], Markarian [23], Bunimovich [6] and Donnay [12]. We will call such components *absolutely focusing arcs*, following [6].

Normally, hyperbolic billiards are ergodic, but not necessarily. An example of a fully hyperbolic nonergodic billiard table was given by Wojtkowski in [35].

Theorem 3.2 (Stable and unstable manifolds) *For ν-almost every point $x \in \Omega$ there are smooth submanifolds W_x^u and W_x^s in Ω, which contain the point x and satisfy the fol-*

lowing:

$$\max_{n\geq 0}\{\operatorname{diam} T^n W_x^s, \operatorname{diam} T^{-n} W_x^u\} \leq C_x \gamma_x^n$$

for some $C_x > 0$ and $\gamma_x \in (0,1)$. In other words, the images of the manifolds W_x^s and W_x^u under the iterations of T and T^{-1}, respectively, exponentially contract. The tangent spaces to W_x^u and W_x^s at the point x are E_x^u and E_x^s, respectively. In particular, $\dim W_x^{u,s} = d^{u,s}(x)$. *If $d^u(x) = 0$ or $d^s(x) = 0$, then the corresponding manifold is degenerate – it is just one point x.*

Remark. The above two theorems hold for the billiard flow Φ^t with obvious modifications, which we do not elaborate. We will denote by $\tilde{\chi}_i(x)$ the Lyapunov exponents for the flow Φ^t, by $\tilde{H}_i(x)$ the corresponding subspaces of $\mathcal{T}_x M$, by $\mathcal{E}_x^{u,s,0}$ the unstable, stable and neutral subspaces, respectively, and by $\mathcal{W}_x^{u,s}$ the unstable and stable manifolds.

The Lyapunov exponents for T are proportional to those of Φ^t, and their subspaces are related by $(D\tilde{\pi}_-)\tilde{H}_i(x) = H_i(\tilde{\pi}_- x)$. Since $\dim M$ $=\dim \Omega + 1$, the flow Φ^t has an extra Lyapunov exponent. It is a zero exponent for the velocity vector $w = v$ (this vector is the kernel of the projection $D\tilde{\pi}_-$). It then follows that $(D\tilde{\pi}_-)\mathcal{E}_x^{u,s} = E_{\tilde{\pi}_- x}^{u,s}$ and $\tilde{\pi}_- \mathcal{W}_x^{u,s} = W_{\tilde{\pi}_- x}^{u,s}$.

Theorem 3.3 (Formulas for the entropy) *The measure-theoretic (Kolmogorov-Sinai) entropy of the billiard ball map T with respect to the measure ν is given by*

$$h(T) = \int_\Omega \sum{}^{+} \chi_i(x) \dim H_i(x)\, d\nu(x) \tag{3.1}$$

where the sum $\sum^+$ runs over all positive Lyapunov exponents. It is also given by

$$h(T) = \int_\Omega \ln |DT_x^u|\, d\nu(x) \tag{3.2}$$

where $|DT_x^u|$ is the Jacobian of the derivative DT_x restricted to the unstable space E_x^u (i.e., this is the expansion factor of the volume of the unstable space E_x^u).

The formula (3.1) is known as Pesin's identity. It was proved in [25] for general smooth dynamical systems and in [18] for systems with singularities. Note that the Lyapunov exponents, hence the integral in (3.1), do not depend on the choice of Riemannian metric in $\mathcal{T}(\Omega)$. The function $\ln |DT_x^u|$ definitely depends on the choice of metric, but the value of the integral in (3.2) does not, as it follows from the invariance of the measure ν under T.

4 Operator techniques

For any point $x = (q, v) \in M$ we denote by $dx = (dq, dv)$ tangent vectors in $\mathcal{T}_x M$, so that $dq \in \mathcal{T}_q Q$ and $dv \in \mathcal{T}_v S^{d-1}$. Suppose that the segment $\{\Phi^s x,\ 0 \le s \le t\}$ does not contain points of reflection. Then, working with $dx = (dq, dv)$ as with an infinitesimal vector in M, we get

$$\Phi^t(q, v) = (q + tv, v) \quad \text{and} \quad \Phi^t(q + dq, v + dv) = (q + dq + t(v + dv), v + dv)$$

so that

$$D\Phi^t(dq, dv) = (dq + t\,dv, dv) \tag{4.1}$$

At a point $x = (q, v)$ of reflection at ∂Q, we have an instantaneous transformation of the velocity vector (1.1). This results in an instantaneous transformation of tangent vectors, $(dq_-, dv_-) \mapsto (dq_+, dv_+)$. To describe it, denote by $U : \mathcal{T}_q Q \to \mathcal{T}_q Q$ the reflection across the hyperplane $\mathcal{T}_q(\partial Q)$, i.e. $U(w) = w - 2\,(n(q) \cdot w)\,n(q)$ for every $w \in \mathcal{T}_q Q$. In particular, $U(dv_-) = dv_+$. Then we have

$$dq_+ = U(dq_-) \quad \text{and} \quad dv_+ = U(dv_-) + \Theta(dq_-) \tag{4.2}$$

Here Θ is a special operator in $\mathcal{T}_q Q$ associated with the given reflection. It is defined as follows:

(i) it acts like U on vectors parallel to v_-, i.e. it takes v_- to v_+;

(ii) denote by J_- and J_+ hyperplanes in $\mathcal{T}_q Q$ perpendicular to v_- and v_+, respectively; then for any vector $w \in J_-$ we have

$$\Theta(w) = 2\,(v_+ \cdot n(q))\,V_+ K_q V_-(w) \,\in J_+$$

Here V_- is the projection of J_- onto $\mathcal{T}_q(\partial Q)$ parallel to the velocity vector v_-, and V_+ is the projection of $\mathcal{T}_q(\partial Q)$ onto J_+ parallel to the normal vector $n(q)$. Also, K_q is the curvature operator of the wall ∂Q at q defined by $n(q + dq) = n(q) + K_q(dq)$ for $dq \in \mathcal{T}_q(\partial Q)$. Since K_q is a self-adjoint operator, so is ΘU^{-1}.

The formula (4.2) is a multi-dimensional version of the classical mirror equation in geometrical optics, see a remark in [35]. It first appeared, apparently, in [28]. Its proof may be also found in [29], cf. [31].

Equations (4.1) and (4.2) completely determine the action of $D\Phi^t$, for all $-\infty < t < \infty$.

Remark. Since $dv \in \mathcal{T}_v S^{d-1}$, the vector dv is orthogonal to v. Put $(q_t, v_t) = \Phi^t(q, v)$ and $(dq_t, dv_t) = D\Phi^t(dq, dv)$. It follows from (4.1) and (4.2) that the scalar product $(dq_t \cdot v_t)$ is constant in time. Therefore, for any unstable or stable vector $(dq, dv) \in \mathcal{E}_x^{u,s}$ the component dq must be also orthogonal to v, otherwise the vector (dq_t, dv_t) would fail to contract exponentially as $t \to \pm\infty$.

Denote by J_x the hyperspace in $\mathcal{T}_q Q$ orthogonal to the velocity vector v. It can be naturally identified with $\mathcal{T}_v S^{d-1}$.

The billiard dynamics is a Hamiltonian one. Thus, symplectic geometry is applicable. We consider the space $J_x \times J_x \subset \mathcal{T}_q Q \times \mathcal{T}_v S^{d-1}$, so that the second copy of J_x is identified with $\mathcal{T}_v S^{d-1}$. In this space, we take a symplectic form defined by $\omega(dx', dx'') = (dq' \cdot dv'') - (dq'' \cdot dv')$ for any two vectors $dx' = (dq', dv')$ and $dx'' = (dq'', dv'')$ in $J_x \times J_x$. It is known that the operator $D\Phi^t$ is symplectic for every t, see, e.g., [36], i.e. it preserves the form ω. It then follows that ω vanishes on $\mathcal{E}_x^u$, so that for any two vectors $dx', dx'' \in \mathcal{E}_x^u$ we have

$$\omega(dx', dx'') = 0, \quad \text{or} \quad (dq' \cdot dv'') = (dq'' \cdot dv') \tag{4.3}$$

(otherwise the vectors $D\Phi^t(dx')$ and $D\Phi^t(dx'')$ would fail to contract exponentially as $t \to -\infty$). The same holds for $\mathcal{E}_x^s$. Since the form ω is nondegenerate, we get $\dim \mathcal{E}_x^{u,s} \leq d-1$. Therefore, the point x is fully hyperbolic, or, equivalently, the multiplicity of its zero Lyapunov exponent for the billiard flow Φ^t is one, iff $\dim \mathcal{E}_x^{u,s} = d-1$, i.e. iff both

$\mathcal{E}_x^{u,s}$ are Lagrangian subspaces of $J_x \times J_x$.

In any case the unstable space $\mathcal{E}_x^u$ is a subspace in $J_x \times J_x \subset \mathcal{T}_q Q \times \mathcal{T}_v S^{d-1}$. Its projections under $D\Pi_Q$ and $D\Pi_V$ down to $J_x \subset \mathcal{T}_q Q$ and $J_x = \mathcal{T}_v S^{d-1}$ are two subspaces of J_x denoted by J_x^u and V_x^u, respectively.

We would like to have a one-to-one projection of $\mathcal{E}_x^u$ onto J_x^u. If this is not the case, then there is a nonzero vector $(0, dv) \in \mathcal{E}_x^u$. This situation does not survive under small variation of t in (4.1). In fact, for any nonzero vector $(dq, dv) \in \mathcal{E}_x^u$ the equation $dq + t\,dv = 0$ has a solution iff the vectors dq and dv are parallel, and then $t = \pm||dq||/||dv||$. Thus, on any segment $\{\Phi^s x,\, 0 \le s \le t\}$ there might be at most a finite number of points $y = \Phi^s x$ where the projection of $\mathcal{E}_y^u$ onto J_y^u fails to be one-to-one. We say that such points are *focusing* (for the manifold $\mathcal{W}_x^u$). Geometrically, the unstable manifold $\mathcal{W}_x^u$ moving under Φ^s focuses at such points in some directions.

We now consider a nonfocusing (generic) point $x = (q, v)$. Then for every $dq \in J_x^u$ there is a unique $dv \in V_x^u$ such that $(dq, dv) \in \mathcal{E}_x^u$. This defines a linear operator $B_x : J_x^u \to V_x^u$ by $dv = B_x(dq)$. As it follows from (4.3), B_x is a self-adjoint operator: $(dq' \cdot B_x(dq'')) = (dq'' \cdot B_x(dq'))$ for any $dq', dq'' \in J_x^u$.

Convention. We will work with linear operators taking one linear subspace of a given Euclidean vector space to another. Such is our operator $B_x : J_x^u \to V_x^u$, where both J_x^u and V_x^u are subspaces of J_x. For such operators we define a determinant and a trace as follows. Let $A : L \to E$ be a linear operator, where L, E are linear subspaces in $\mathbb{R}^m$ for some $m \ge 1$. Let $\dim L = k$. Then $\det A$ is the volume expansion factor of the space

L under A, i.e. it is the k-dimensional volume of $A(K)$, where K is the unit cube in L. The trace is defined by $\operatorname{tr} A = \sum_{i=1}^{k}(Ae_i, e_i)$ for any orthonormal basis $(e_1, \ldots, e_k)$ in L. This is the regular trace of the operator $\Pi_L \circ A : L \to L$, where Π_L is the orthoprojector of $\mathbb{R}^m$ onto L. In addition, for two operators $A_1 : L \to E_1$ and $A_2 : L \to E_2$ we denote by $A_1 + A_2$ the linear operator on L defined by $(A_1 + A_2)w = A_1 w + A_2 w$; its image is some linear subspace in $E_1 \oplus E_2$.

According to (4.1), if the trajectory segment $\{\Phi^s x,\, 0 \le s \le t\}$ has no reflections, the operator $(I + tB_x)$ sends J_x^u onto $J_{x_t}^u$. Here I is the identity operator on J_x^u. The point $\Phi^t x$ is focusing iff the operator $I + tB_x$ is degenerate, i.e. $\det(I + tB_x) = 0$. If, on the other hand, the point $x_t = \Phi^t x$ in nonfocusing, then

$$B_{x_t} = B_x (I + tB_x)^{-1} \tag{4.4}$$

which is an operator $J_{x_t}^u \to V_{x_t}^u = V_x^u$. In particular, if the operator $B_x : J_x^u \to V_x^u$ is one-to-one, i.e. $\dim V_x^u = \dim J_x^u$ $(= \dim \mathcal{E}_x^u)$, then (4.4) can be rewritten as

$$B_{x_t} = (tI + B_x^{-1})^{-1} \tag{4.5}$$

where I is the identity operator on $V_x^u = V_{x_t}^u$.

At a point $x = (q, v)$ of reflection, the operators B_x^- and B_x^+ taken immediately before and after the reflection are related by

$$B_x^+ = UB_x^- U^{-1} + \Theta U^{-1} \tag{4.6}$$

as it follows from (4.2).

Remark. For 2-D billiard tables $\dim J_x$=1. Therefore, if there is an unstable manifold $\mathcal{W}_x^u$ at all, then B_x and other operators in the above formulas are one-dimensional, or just real numbers.

Remark. If the point x is fully hyperbolic, then $\dim \mathcal{E}_x^u = \dim \mathcal{E}_x^s = d - 1$, so that $J_x^u = V_x^u = J_x$. In that case all the above operators are defined on the entire $J_x^u = J_x$, and the determinant and the trace assume their regular values.

5 Entropy formulas for billiards

Now, assume that the point $x = (q, v)$ is on the exit from a collision with boundary, i.e. $q \in \partial Q$ and $(v \cdot n(q)) \geq 0$. Let x be a nonfocusing point and $\tau = \tau(x)$ its free path to the next collision.

In order to compute the jacobian $|DT_x^u|$ entering (3.2) we fix a metric $|| \cdot ||_*$ in E_x^u that is induced by the Euclidean metric in J_x^u. Precisely, for any vector $w \in E_x^u$ we find a unique vector $(dq, dv) \in \mathcal{E}_x^u$ such that $(D\tilde{\pi}_-)(dq, dv) = w$ and set $||w||_* = ||dq||$. This metric cannot be extended to any metric in the entire space $\mathcal{T}_x(\Omega)$, but it is a valid metric on E_x^u. This is a standard 'pseudo-metric' technique in the billiard theory, see [8] for a more detailed explanation. The advantage of using the Euclidean metric in J_x^u is that the instantaneous transformation of the space J_x^u that it undergoes at every collision with the boundary is an isometry under U, see (4.2). Thus, with this choice of metric, we have $|DT_x^u| = \det(I + \tau(x)B_x)$.

With this choice of metric in E_x^u, the formula (3.2) can be rewritten like this:

Theorem 5.1 *Assume that a.e. point $x \in \Omega$ is nonfocusing (generic). The measure-theoretic (K-S) entropy of the billiard ball map T with respect to the measure ν is given by*

$$h(T) = \int_\Omega \ln\det(I + \tau(x)B_x)\, d\nu(x) \tag{5.1}$$

In order to derive a formula for the entropy of the billiard flow Φ^t we use classical Abramov's formula

$$h(\Phi^t) = h(T)/\bar{\tau} \tag{5.2}$$

see [8] for more detail. Along with (2.4) we have

$$h(\Phi^t) = c_\mu c_\nu^{-1} h(T) = c_\mu \int_\Omega \ln\det(I + \tau(x)B_x)\, dq\, dv \tag{5.3}$$

Lemma 5.2 *Let L, E be linear subspaces of the Eclidean vector space $\mathbb{R}^m$, $m \geq 1$. For any linear operator $B:\ L \to E$ and $t > 0$ we have*

$$\frac{d}{dt} \ln\det(I + tB) = \operatorname{tr} B(I + tB)^{-1} \tag{5.4}$$

provided the determinant is not zero. Here I is the identity operator on L.

The lemma is proved in Appendix.

Nonfocusing assumption. For almost every point $x \in \Omega$ the trajectory segment $\{\Phi^s x,\ 0 \leq s \leq \tau(x)\}$ has no focusing points. Equivalently, for a.e. $x \in \Omega$ and every $0 \leq t \leq \tau(x)$ we have $\det\,(I + tB_x) \neq 0$.

Under this assumption, we can combine Eqs. (5.3) and (5.4) as follows:

$$h(\Phi^t) = c_\mu \int_\Omega \int_0^{\tau(x)} \mathrm{tr} B_x (I + tB_x)^{-1}\, dt\, dq\, dv$$

We now recall (4.4) and (1.2) and arrive at the following theorem.

Theorem 5.3 *Assume the nonfocusing condition stated above. Then the measure-theoretic (K-S) entropy of the billiard flow Φ^t with respect to the measure μ is given by*

$$h(\Phi^t) = \int_M \mathrm{tr}\, B_x\, d\mu(x) \tag{5.5}$$

On the contrary, if the nonfocusing assumption fails, the integral in (5.5) diverges and this formula makes no sense.

The formula (5.5) was first established for 2-D dispersing billiards in [27]. It was later proved in [28, 8] for semidispersing billiards in any dimension. The formula (5.1) was proven in [8] for semidispersing billiards and Bunimovich-type planar billiards bounded by circular arcs, see Sect. 3. It was later proved in [9] for all planar hyperbolic billiards bounded by absolutely focusing arcs.

As we have just shown, Theorems 5.1 and 5.3 hold for generic (not necessarily hyperbolic) billiard tables in any dimension. In such a generality, these results have never been published before.

Remark. For 2-D billiard tables our nonfocusing condition is equivalent to the semidispersing property. This can be verified by constructing a set of trajectories of positive measure with focusing points on each. To this end, one can take trajectories that make long series of nearly grazing reflections along a smooth convex component of ∂Q. We omit details. As a conclusion, (5.5) does not hold for billiards of Bunimovich, Wojtkowski or Markarian types (even though (5.1) still holds).

Open question. Is the nonfocusing assumption equivalent to the semidispersing property in any dimension?

6 Operator-valued continued fraction

For certain classes of billiards, there is an explicit formula for the linear operator B_x that looks like an infinite continued fraction.

For any $x \in \Omega$ with an infinite past trajectory let $0 > t_1 > t_2 > \cdots$ be all the negative moments of reflection. Denote by U_i and Θ_i for $i = 0, 1, \ldots$ the operators associated with those reflections, see Sect. 4. Let $\tau_i = t_i - t_{i+1} > 0$, $i \geq 0$, be the intercollision times. Then

$$B_x = \Theta_0 U_0^{-1} + U_0 \frac{I}{\tau_0 I + \frac{I}{\Theta_1 U_1^{-1} + U_1 \frac{I}{\tau_1 I + \frac{I}{\cdots}} U_1^{-1}}} U_0^{-1} \tag{6.1}$$

where $\frac{I}{A}$ means A^{-1}. Here the terms $\Theta_i U_i$ and $\tau_i I$ alternate. They describe the contribution of reflections and free paths in between to the formation of unstable manifolds.

It readily follows from (4.5) and (4.6) that

$$B_x = \Theta_0 U_0^{-1} + U_0 \frac{I}{\tau_0 I + \frac{I}{B_{T^{-1}x}}} U_0^{-1}$$

where I following τ_0 is the identity operator in $V^u_{T^{-1}x}$. A recursive application of this formula gives (6.1). This is, however, a superficial argument. In order to prove (6.1) mathematically, one has to verify the convergence of the continued fraction (6.1). There is no proof of the convergence working for generic billiard tables. One of the most general results in this direction may be found in [6]. For fully hyperbolic billiards the invariant cone techniques by Wojtkowski [34, 35, 22] normally gives not only the hyperbolicity but also the convergence of (6.1). On the other hand, one can possibly find a table Q and a phase point $x \in \Omega$ for which the fraction (6.1) diverges. We cite known convergence theorems for two specific classes of billiard tables.

Proposition 6.1 *Let Q be a semidispersing billiard table ($d \geq 2$). Then the operator-valued continued fraction (6.1) converges at every point $x \in \Omega$ with an infinite past trajectory. Moreover, if $B_{x,n}$ is a finite continued fraction obtained from (6.1) by truncation at the n-th reflection, we get*

$$||B_x - B_{x,n}|| \leq 1/|t_n|$$

The proof is based on the fact that all the operators in (6.1) are selfadjoint positive semidefinite, i.e. $\tau_i > 0$ and $\Theta_i \geq 0$. The first proof was published in [30], see also [22]. In a weaker form the statement was given without proof earlier in [29]. For 2-D billiard tables the statement was proved in [27].

Remark. If Q is a polyhedron of any dimension, then the wall ∂Q is flat at all its regular points, and so all Θ_i in (6.1) are zero, hence $B_x = 0$ for all x. Therefore, all Lyapunov exponents are zero everywhere, and $h(T) = h(\Phi^t) = 0$. For 2-D polygons, this fact was first proved in [19] by showing that the topological entropy of the map T vanishes.

Proposition 6.2 (see [9]) *Let Q be a 2-D billiard table of Bunimovich, Wojtkowski or Markarian type. Then the continued fraction (6.1) converges at every point $x \in \Omega$ with an infinite past trajectory.*

Unlike the previous proposition, now the values of Θ_i in (6.1) corresponding to reflections at focusing components of the boundary are negative. This makes the proof of convergence in (6.1) more difficult. In [9], the convergence of (6.1) was proved by using a general theorem on convergent continued fractions by Bunimovich [6].

7 Entropy of the periodic Lorentz gas

The Lorentz gas is a dynamical system where a pointlike particle moves freely in space and bounces off some fixed, immovable obstacles (scatterers). It is a classical model of electrons in metals. If the scatters are periodically situated in space, the Lorentz gas is said to be periodic. In this case one can find a fundamental domain in space and project the trajectory of the particle onto that domain. In this way one gets a billiard dynamical system on a torus with a finite number of obstacles. We will consider only disjoint convex obstacles. A popular simple example is a torus with just one ball-like obstacle.

The simplicity of the periodic Lorentz gas has stimulated numerous computer simulations and theoretical studies of this model.

A full hyperbolicity, ergodicity and K-mixing property of the periodic Lorentz gas have been proved in [27] in the 2-D case and [31] in any dimension. The Bernoulli property has been established in [15] in the 2-D case and in [10] in any dimensions.

Numerical researches on periodic Lorentz gases have been focused on the entropy, Lyapunov exponents, the rate of the decay of correlations and the diffusion coefficients. We briefly recall here the numerical results on the Lyapunov exponents and the entropy.

For a 2-D periodic Lorentz gas with a single circular scatterer of radius $r > 0$ on a unit torus the entropy was estimated [14] to be

$$h(T) \approx -2 \ln r \tag{7.1}$$

as $r \to 0$, which was later proved in [8]. It was also conjectured in [14] that for d-dimensional periodic Lorentz gas with a spherical scatterer of radius $r > 0$ it should be $h(T) \approx -d \ln r$, which turned out to be wrong, see below. It was also estimated there that in 2-D the difference

$$\ln \int_\Omega \tau(x)\, d\nu(x) \; - \; \int_\Omega \ln \tau(x)\, d\nu(x) \tag{7.2}$$

remains bounded and has a positive limit ($\approx 0.44 \pm 0.01$) as $r \to 0$. The first part of this conjecture (boundedness) was later rigorously proved in [8], see below. The convergence is still an open problem.

Lyapunov exponents for the billiard ball map T for multi-dimensional periodic Lorentz gases with a single spherical scatterer of radius r have been studied in [3]. It was estimated that every positive Lyapunov exponent $\chi_i > 0$, as a function of r, increases like const$\cdot|\ln r|$, as $r \to 0$. Moreover, every positive exponent but the maximal one was conjectured to be $\approx -1/4\ln(r/2)$. The maximal Lyapunov exponent was conjectured to be $\approx -(3d+2)/4\ln r$. The last two conjectures turned out to be wrong, see (7.7) and (7.8) below. The first one is proved below by our (7.8).

Baldwin [1] gave a theoretical argument supporting the following sharpening of the formula (7.1):

$$h(T) = -2\ln r + \text{const} + O(r) \tag{7.3}$$

His argument was not a mathematical proof, and so his prediction still remains an open problem.

The following theorem was rigorously proved in [8].

Theorem 7.1 ([8]) *The entropy of the d-dimensional periodic Lorentz gas ($d \geq 2$) with a single spherical scatterer of radius $r > 0$ in a unit torus is given by*

$$h(T) = -d(d-1)\,\ln r + O(1) \tag{7.4}$$

and

$$h(\Phi^t) = -d(d-1)\,|B^{d-1}|\,r^{d-1}\,\ln r + O(r^{d-1})$$

as $r \to 0$. The mean free path is

$$\bar{\tau} = \frac{1-|B^d|\,r^d}{|B^{d-1}|\,r^{d-1}} = \frac{1}{|B^{d-1}|\,r^{d-1}} + O(r) \tag{7.5}$$

The difference (7.2) is always positive and uniformly bounded in r for every d.

The proof in [8] is based on the approximation of the operator B_x in (5.1) by $\Theta_0 U_0^{-1}$, see (6.1). The norm of the error is bounded

$$||B_x - \Theta_0 U_0^{-1}|| \leq 1/\tau_0 \leq \text{const}$$

cf. Proposition 6.1. Therefore, the substitution of $\Theta_0 U_0^{-1}$ for B_x in (5.1) can only change the integral in (5.1) by a uniformly bounded amount.

Next, for small r the operator Θ_0 has eigenvalues of order r^{-1}, which can be computed explicitly for spherical scatterers. The details may be found in [8]. As a result, the integration in (5.1) gives

$$h(T) = (d-1)\left(-\ln r + \int_\Omega \ln \tau(x)\, d\nu(x)\right) + H(d) + o(1) \tag{7.6}$$

The value of $H(d)$ here comes from the substitution of $\Theta_0 U_0^{-1}$ for B_x in (5.1). Moreover, it was computed explicitly in [8]: $H(2) = 2$, $H(3) = \ln 4$, and for $d \geq 4$ we have

$$H(d) = (d-1)\ln 2 - (d-3)\,|S^{d-2}| \int_0^1 t^{d-2} \ln \sqrt{1-t^2}\, dt$$

Lastly, the boundedness of (7.2) that was proved in [8] gives (7.4). The other results of Theorem 7.1 then follow from (2.4) and Abramov's formula (5.2).

It also follows from (7.6) that the existence of the limit of the difference (7.2) is equivalent to the following asymptotical formula:

$$h(T) = -d(d-1)\ln r + \text{const} + o(1)$$

Both remain, however, open questions, as well as the more refined prediction (7.3).

All the open questions involving the entropy $h(T)$ can be equivalently restated for the entropy $h(\Phi^t)$, in view of (5.2) and (7.5).

As for the Lyapunov exponents for T, it follows directly from (7.4) that the maximal one is bounded by

$$-d\ln r + O(1) \leq \chi_{\max} \leq -d(d-1)\ln r + O(1) \tag{7.7}$$

By using again the approximation of B_x by $\Theta_0 U_0^{-1}$, and the asymptotic eigenvalues of the latter, see [8] for details, it is easy to estimate *every* positive Lyapunov exponent from below: $\chi_i \geq -d\ln r + O(1)$ for all $\chi_i > 0$. Together with (7.4) this give an asymptotic formula

$$\chi_i = -d\ln r + O(1) \tag{7.8}$$

for every positive Lyapunov exponent $\chi_i > 0$.

Therefore, all positive Lyapunov exponents have the same asymptotics as $r \to 0$. It was also conjectured in [8] that, due to the geometrical symmetry of spherical scatterers, all the positive Lyapunov exponents should be actually equal. This conjecture is still open. However, it was shown recently [21], both analytically and numerically, that in a 3-D *random* Lorentz gas (with a random configuration of scatterers) the two positive Lyapunov exponents are distinct!

Two more general results were proved in [8].

Consider a periodic Lorentz gas with m disjoint spherical scatterers with radii $r_1, \ldots, r_m$ in a unit torus. Put

$$Z_0 = r_1^{d-1} + \cdots + r_m^{d-1}$$

and

$$Z_1 = r_1^{d-1} \ln r_1 + \cdots + r_m^{d-1} \ln r_m$$

The entropy of such a Lorentz gas was proved [8] to be

$$h(T) = -(d-1)[\ln Z_0 + Z_1/Z_0] + O(1) \tag{7.9}$$

and

$$h(\Phi^t) = -(d-1)\,|B^{d-1}|\,[Z_0 \ln Z_0 + Z_1] + O(Z_0)$$

as $r_1, \ldots, r_m \to 0$, while the distances between the scatterers remain bounded away from 0. The mean free path is

$$\bar{\tau} = \frac{1}{|B^{d-1}|\,Z_0} + O(\max r_i)$$

Lastly, consider a periodic Lorentz gas with m disjoint convex scatterers in a unit torus, which are homotetically shrinking with a common scaling factor $\varepsilon > 0$. Let S_1 be the total surface area and V_1 the total volume of the scatterers when $\varepsilon = 1$. Then we have, see [8],

$$h(T) = -d(d-1)\,\ln \varepsilon + O(1)$$

and

$$h(\Phi^t) = -d(d-1)\,|B^{d-1}|\,|S^{d-1}|^{-1} S_1 \varepsilon^{d-1} \ln \varepsilon + O(\varepsilon^{d-1})$$

as $\varepsilon \to 0$.

8 Entropy of stadia and alike

A stadium is a planar convex billiard table bounded by two parallel line segments of length $2a$ and two semicircles of radius r that are tangent to the segments at points of contact. Its boundary is C^1 but not C^2.

Bunimovich showed [5] that billiards in stadia are hyperbolic, ergodic and K-mixing. This produced one of the very first examples of convex tables with completely chaotic billiard dynamics. This example was simple and pictorial enough to encourage its further study and numerical experiments on it.

In particular, the asymptotics of the entropy have been studied under the conditions that a stadium is deformed approaching either a circle, which happens as $a/r \to 0$, or a straight segment, as $r/a \to 0$. In both cases the entropy of the billiard ball map T approaches zero, and its asymptotics has been estimated numerically and heuristically, see, e.g., [2, 37].

The only available rigorous estimate for the entropy of the stadium approaching a circle belongs to Wojtkowski [35].

Theorem 8.1 (see [35]) *There is a constant $c = c(r) > 0$ such that the entropy $h(T)$ of the billiard ball map in the stadium obeys $h(T) \geq c(r) \cdot \sqrt{a}$ as $a \to 0$ and $r > 0$ fixed.*

This is in agreement with an earlier numerical experiment [2] that showed that $h(T) \approx \text{const} \cdot \sqrt{a}$.

As the stadium approaches a segment ($r/a \to 0$), the following asymptotic formulas for the entropy were proved in [8].

Theorem 8.2 (see [8]) *Let $r/a \to 0$. Then the entropy of the billiard ball map in the stadium obeys*

$$h(T) = (r/a)\ln(a/r) + O(r/a) \tag{8.1}$$

and the entropy of the billiard flow obeys

$$h(\Phi^t) = (\pi a)^{-1}\ln(a/r) + O(1/a)$$

The mean free path is

$$\bar{\tau} = \frac{\pi r(4a + \pi r)}{4a + 2\pi r} = \pi r + O(r^2/a) \tag{8.2}$$

The deformation of the stadium so that it approaches a segment may seem physically meaningless. However, it can be transformed into a pictorial model as follows. Take $N \to \infty$ copies of a stadium with parameters $a > 0$ (fixed) and $r \to 0$, so that $N \cdot r$ approaches a constant $b > 0$. Put them together side by side thus making a nearly rectangular billiard table, Q_r, with linear dimensions $2Nr \approx 2b$ and $\approx 2a$. Two sides of this big table are straight, and two others are "scalloped", made up of a large number of tiny convex semicircles. It then follows from Theorem 8.2, as it was shown in [8], that the entropy of the billiard ball map in Q_r is

$$h(T) = \frac{2b}{2a + \pi b}\ln(a/r) + O(1)$$

and the entropy of the billiard flow is

$$h(\Phi^t) = (\pi a)^{-1}\ln(a/r) + O(1)$$

Note that both the entropy of the billiards ball map and that of the billiard flow in Q_r grow to infinity as $r \to 0$, while the table Q_r approaches the rectangular billiard table, Q_0, where the entropy is zero, cf. Sect. 6 or [19]. To explain this 'mystery', we point out that the trajectories in Q_r do not approach those in Q_0 as $r \to 0$. In particular, parallel close trajectories remain parallel after reflections at the boundary in Q_0 but such trajectories diverge drastically in Q_r.

The above construction can be generalized as follows. Let Q be an arbitrary domain with piecewise smooth boundary. Every piece $\Gamma \subset \partial Q$ of the boundary of Q is then replaced with a chain of circular arcs of nearly 180^o with the same small radius $r > 0$ facing outward and stretching along the curve Γ. We thus get another domain, Q_r^+, with "scalloped" boundary, see Fig. 1. The details of this construction are not so important, but in order to be specific, we can take a chain of circles of radius r whose centers all belong to ∂Q such that every circle is tangent to the neighboring two. Then we erase the "inner" arc of every circle (the one that faces the domain Q), and the remaining arcs will form the boundary of Q_r^+. Less formally, we take a glue and attach identical semicircles to the boundary of the given domain Q.

Possible location of Figure 1

.

The billiard in Q_r^+ satisfies Bunimovich's conditions [4, 5], and so it is completely hyperbolic, ergodic and K-mixing. The entropy of the billiard ball map in Q_r^+ is then [8]

$$h(T) = -\frac{2}{\pi} \ln \frac{r}{\operatorname{diam} Q} + O(1) \tag{8.3}$$

and the entropy of the billiard flow is

$$h(\Phi^t) = -\frac{|\partial Q|}{\pi |Q|} \ln \frac{r}{\operatorname{diam} Q} + O(1) \tag{8.4}$$

where $|Q|$ stands for the area of Q, and $|\partial Q|$ for the perimeter of Q. The above formulas were derived in [8] for polygonal domains Q, but it is easy to check that the proofs work for arbitrary piecewise smooth domains as well, so we leave out details. Note that $h(T)$ does not depend on the domain Q at all. This is so because the divergence of trajectories in Q_r^+ is determined by the high curvature of the small semicircles making ∂Q_r^+ rather than by the shape of the original boundary ∂Q.

In a recent computer experiment [20], the logarithmic dependence of $h(T)$ on r was observed in the case where Q was a fixed circle.

Another twist of the above construction occurs if, instead of erasing the "inner" arc of every circle, one erases its "outer" arc, the one facing outward. Then the remaining (inner) arcs will bound another domain, $Q_r^- \subset Q_r^+$, which is piecewise smooth and *concave* at every regular point, see Fig. 1. Less formally, one takes scissors (instead of a glue) and cuts semicircular cavities (makes "cogs") along the boundary of the given table Q. Obviously, Q_r^- is a Sinai-type (dispersing) billiard table, so it is completely hyperbolic, ergodic and K-mixing. It was also shown in [8] that the entropy of the billiard in Q_r^-, to much surprise, satisfies absolutely the same asymptotic formulas (8.3) and (8.4).

This means that the exponential rate of divergence of trajectories in Sinai's (dispersing) billiard table Q_r^- and Bunimovich's (focusing) billiard table Q_r^+ is basically the same despite the seemingly opposite mechanism of divergence, cf. [4, 5, 6]. This points out a universality in the transition from regular dynamics to chaos as one perturbs the boundary of any piecewise smooth domain by convex circular "scallops" or concave circular "cogs".

Yet another modification of the stadium was studied by Zaslavski [37]. Let $Q_{a,r,b}$ be a convex billiard table bounded by two parallel segments of length $2a$ and two circular arcs of radius r and height b, see Fig. 2. Let $b \ll r \ll a$. This billiard table satisfies Bunimovich's conditions, and so it is hyperbolic, ergodic and K-mixing. Zaslavski [37] provided heuristic calculation of the entropy in $Q_{a,r,b}$ which was later confirmed by a rigorous argument in [8]. It was shown there that

$$h(T) = (p/a)\ln(a/r) + O(p/a)$$

and

$$h(\Phi^t) = (\pi a)^{-1}\ln(a/r) + O(1/a)$$

where p is the chord of the arc bounding $Q_{a,r,b}$.

Possible location of Figure 2

.

Lastly, in [9] we modified the above "scalloped" tables Q_r^+ as follows. Let Γ be an arbitrary C^4 convex absolutely focusing curve, see [6, 9]. In particular, it may be a

Wojtkowski type [35] or a Markarian type [23] or a Bunimovich type [6] focusing arc. We shrink Γ homotetically by a small factor $\varepsilon > 0$ and attach identical copies of it to the sides of a given polygon Q so that they have common points along ∂Q. We proved [9] that the entropy of the billiard ball map in the resulting table is $h(T) = -D \ln \varepsilon + O(1)$, where $D = D(\Gamma) > 0$ is a constant.

9 Mean free path for hard ball gases

Here we apply the formulas for the mean free path in Section 2 to study the mean intercollision time in systems of hard balls.

We consider a system of N hard balls of diameter σ and unit mass in the k-dimensional torus T_L^k whose linear dimension is $L > 0$. The k-dimensional volume of the torus T_L^k is L^k. The balls move freely and collide with each other elastically. Let $q_{i,1}, \dots, q_{i,k}$ and $p_{i,1}, \dots, p_{i,k}$ be the coordinates of the position and velocity vector, respectively, of the i-th ball. The configuration space Q of the system is a subset of the kN-dimensional torus T_L^{kN}, which correspond to all feasible (nonoverlapping) positions of the balls. The total kinetic energy of the system is preserved in time, and we fix it: $p_{1,1}^2 + \cdots + p_{N,k}^2 = 2EN$, where the constant $E > 0$ is the mean kinetic energy per particle. The phase space is then $M = Q \times S_1^{kN-1}$ where S_1^{kN-1} is the $(kN-1)$-dimensional sphere of radius $(2EN)^{1/2}$.

The dynamics of the hard balls with elastic collisions correspond to the billiard dynamics in the configuration space Q with specular reflections at the boundary ∂Q. The billiard particle in Q will move at the speed $(2EN)^{1/2}$ rather than the conventional unit speed, and we will take this into account later. The boundary ∂Q consists of $N(N-1)/2$ cylindrical surfaces corresponding to the pairwise collisions of the balls. We denote by $C_{i,j}$ the open solid cylinder corresponding to overlapping positions of the balls $i \neq j$. It is given by the inequality

$$\sum_{r=1}^{k}(q_{i,r} - q_{j,r})^2 < \sigma^2 \pmod{L}$$

The configuration space is then $Q = \mathrm{T}_L^{kN} \setminus \cup_{i\neq j} C_{i,j}$, and its boundary is $\partial Q = Q \cap (\cup_{i\neq j}\partial C_{i,j})$.

In order to estimate the mean free path by using Eq. (2.4) we need to compute the volume of the space Q and the surface area of its boundary ∂Q. This is a difficult problem, very hard to solve exactly, since the cylinders $C_{i,j}$ have plenty of pairwise and multiple intersections. We will simplify the matter and find the asymptotic values of both $|Q|$ and $|\partial Q|$ for the gases of hard balls with very low densities.

¿From now on we assume that our gas of hard balls is dilute, i.e. its density

$$\rho = \frac{|B^k| \cdot \sigma^k N}{(2L)^k}$$

is low, $\rho \to 0$. (Here again $|B^k|$ is the volume of the unit ball in $\mathbb{R}^k$.) The quantity ρ measures the fraction of volume of T_L^k occupied by all the balls together. Technically, our further calculations will be valid under either of the following regimes:

Regime A. The number of balls N is fixed and $\rho \to 0$;

Regime B. $N \to \infty$ and $\rho \to 0$ in such a way that $\rho N \to 0$;

For the kN-dimensional volume of Q, we have then

$$|Q| = L^{kN}(1 - O(\rho N)) = L^{kN}(1 - o(1))$$

For the $(kN-1)$-dimensional volume of ∂Q we have

$$|\partial Q| = \frac{N(N-1)}{2} \cdot |\partial C_{1,2}| \cdot (1 - o(1))$$

To compute the area of the cylindrical surface $\partial C_{1,2}$ we use an orthogonal change of variables: $q'_r = (q_{1,r} - q_{2,r})/\sqrt{2}$ and $q''_r = (q_{1,r} + q_{2,r})/\sqrt{2}$ for $1 \le r \le k$, leaving the other coordinates $q_{i,r}$, with $i \ge 3$, unchanged. Then the equation of $\partial C_{1,2}$ becomes

$$\sum_{r=1}^{k} (q'_r)^2 = \sigma^2/2 \pmod{L/\sqrt{2}}$$

This shows that the base of the cylindrical surface $\partial C_{1,2}$ is a $(k-1)$-dimensional sphere of radius $\sigma/\sqrt{2}$. The other coordinates vary as follows: $0 \le q''_r \le \sqrt{2}L$ and $0 \le q_{i,r} \le L$ for $i \ge 3$ and all $1 \le r \le k$. Therefore,

$$\begin{aligned} |\partial C_{1,2}| &= (\sigma/\sqrt{2})^{k-1} \cdot |S^{k-1}| \cdot (\sqrt{2}L)^k \, L^{(N-2)k} \, (1 + o(1)) \\ &= \sqrt{2}\, \sigma^{k-1} \cdot |S^{k-1}| \cdot L^{kN-k} \, (1 + o(1)) \end{aligned}$$

This gives the following:

$$\begin{aligned} |\partial Q| &= \frac{N(N-1)}{\sqrt{2}} \cdot |S^{k-1}| \cdot \sigma^{k-1} \, L^{kN-k} \, (1 + o(1)) \\ &= \frac{N-1}{\sqrt{2}} \cdot \frac{2^k \, k\rho}{\sigma} \cdot L^{kN} \, (1 + o(1)) \end{aligned}$$

The mean free path of the billiard particle in the domain Q is then

$$\begin{aligned} \bar{\tau} &= \frac{|Q| \cdot |S^{kN-1}| \cdot (kN-1)}{|\partial Q| \cdot |S^{kN-2}|} \\ &= \frac{\sqrt{2}\, \sigma (kN-1) \cdot |S^{kN-1}|}{2^k \, k\rho (N-1) \cdot |S^{kN-2}|} \cdot (1 + o(1)) \qquad (9.1) \end{aligned}$$

This formula for the mean free path is correct but not good enough, however, because the billiard system in Q is not ergodic. Indeed, the total momentum $\mathbf{P} = (P_1, \ldots, P_k)$, where $P_r = \sum_i p_{i,r}$, is invariant under the dynamics. Those phase trajectories whose total momentum $\mathbf{P}$ is large will display slow relative motion of the balls, and thus the mean free path between reflections in ∂Q along such trajectories will be larger than $\bar{\tau}$ in (9.1). On the contrary, the mean free path along trajectories with zero or small $\mathbf{P}$ will be below $\bar{\tau}$. The value of $\bar{\tau}$ in (9.1) only gives the phase space average of the mean free paths taken over individual trajectories.

We focus on the case of a particular physical interest, that of zero total momentum, $\mathbf{P} = \mathbf{0}$, where the gas is "at equilibrium". In this case, the ergodicity of the gas of hard balls is known as Boltzmann-Sinai ergodic hypothesis. It has been proven in many particular cases, see a survey [32], and believed to be true in general. If so, the mean free path along all typical trajectories with $\mathbf{P} = \mathbf{0}$ will be the same. We denote it by $\bar{\tau}_0$ and will compute it next (without assuming ergodicity).

Pick any point $q' \in Q$ and consider

$$Q_0(q') = \left\{ q \in Q : \sum_{i=1}^{N} (q_{i,r} - q'_{i,r}) = 0 \pmod{L} \quad \text{for all} \quad r = 1, \ldots, k \right\}$$

The hard ball dynamics with $\mathbf{P} = \mathbf{0}$ and initial configuration point q' corresponds to billiard dynamics in the $(kN - k)$-dimensional domain $Q_0(q')$ with specular reflections at its boundary $\partial Q_0(q')$. Therefore,

$$\bar{\tau}_0 = \frac{|Q_0(q')| \cdot |S^{kN-k-1}| \cdot (kN - k - 1)}{|\partial Q_0(q')| \cdot |S^{kN-k-2}|}$$

Note that the domains $Q_0(q') \subset Q$ are isomorphic for all $q' \in Q$, and so $|Q_0(q')|/|\partial Q_0(q')| = |Q|/|\partial Q|$. Combining this with (9.1) gives

$$\begin{aligned}\bar{\tau}_0 &= \frac{\sqrt{2}\,\sigma\,(kN-k-1)\cdot|S^{kN-k-1}|}{2^k\,k\,\rho\,(N-1)\cdot|S^{kN-k-2}|}\cdot(1+o(1))\\ &= \frac{\sqrt{2\pi}\,\sigma\cdot\Gamma\left(\frac{kN-k+1}{2}\right)}{2^k\,\rho\cdot\Gamma\left(\frac{kN-k+2}{2}\right)}\cdot(1+o(1)) \qquad (9.2)\end{aligned}$$

One can 'translate' this result into physically sensible terms as follows. The speed of the billiard particle in Q is $(2EN)^{1/2}$, and so the mean intercollision time (in the whole system) is $\bar{t}_{\rm sys} = \bar{\tau}_0\,(2EN)^{-1/2}$. The mean intercollision time for every individual particle is simply $\bar{t}_{\rm par} = \bar{t}_{\rm sys}\cdot N/2$, since every collision involves two particles. This gives

$$\bar{t}_{\rm par} = \frac{\pi^{1/2}\cdot\Gamma\left(\frac{kN-k+1}{2}\right)\cdot N\sigma}{2^{k+1}\cdot\Gamma\left(\frac{kN-k+2}{2}\right)\cdot(EN)^{1/2}\,\rho}\cdot(1+o(1)) \qquad (9.3)$$

We now take the limit in (9.3) as $N\to\infty$ by using a handy formula $\Gamma(N)/\Gamma(N-1/2) = \sqrt{N}(1+o(1))$:

$$\bar{t}_{\rm par}(N\to\infty) = \frac{\pi^{1/2}\,\sigma}{2^{k+1}\,(Ek/2)^{1/2}\,\rho}\cdot(1+o(1))$$

In particular, for $k=2$ and $k=3$ we recover the so-called Boltzmann mean free time for hard disks and hard balls in the dilute mode, see, e.g., [7, 13]:

$$\bar{t}_{\rm Boltz}(k=2) = \frac{\pi^{1/2}\,\sigma}{8\,E^{1/2}\,\rho} = \frac{1}{2\sigma\,n\,\sqrt{\pi k_B T}} \qquad (9.4)$$

and

$$\bar{t}_{\rm Boltz}(k=3) = \frac{\pi^{1/2}\,\sigma}{8\,(6E)^{1/2}\,\rho} = \frac{1}{(2\sigma)^2\,n\,\sqrt{\pi k_B T}} \qquad (9.5)$$

Here $n = N/L^k$ is the number density of the gas, k_B is the Boltzmann constant and T is the temperature of the gas related to E by classical formulas: $E = k_B T$ for 2-D disks and

$E = \frac{3}{2} k_B T$ for 3-D balls. To our best knowledge, this is the first mathematically exact derivation of the Boltzmann free time formulas based solely on the Liouville equilibrium distribution for finite systems of hard balls.

Lastly, a little numerical experiment reported below in Table 1 shows that the above formulas are fairly accurate for hard disks at low densities. The first column shows the value of the product $\bar{t}_{\rm par} \cdot \rho$ computed according to (9.3) for $k = 2$ and some finite N. The other columns show experimentally estimated mean free times per particle for three particular values of ρ. The last row of the table shows the Boltzmann mean free time (9.4) and the so-called Enskog mean free times for hard disk fluids. The latter take into account the non-zero density ρ of the fluid, which is incorporated into the Enskog scaling factor χ. Precisely,

$$\bar{t}_{\rm Enskog}(k=2) = \frac{\pi^{1/2}\,\sigma}{8\,E^{1/2}\,\rho\,\chi} = \frac{1}{2\sigma\,n\,\chi\,\sqrt{\pi k_B T}} \tag{9.6}$$

see, e.g., [16], with

$$\chi \approx 1 + 0.782 \cdot 2\rho + 0.5327 \cdot (2\rho)^2$$

see, e.g., [11].

Table 1 actually illustrates two phenomena. First, our theoretical formula (9.3) works well as $\rho \to 0$ for *every* particular value of N. Second, the Enskog formula (9.6) approximates $\bar{t}_{\rm par}$ as $N \to \infty$ for every particular value of ρ.

Our experiment was performed on the SPARC workstation at the University of Alabama at Birmingham. In every run, molecular dynamics have been simulated up to 10^7 interparticle collisions, with a random choice of the initial state. We have chosen

$\sigma = 1$ (this sets the unit of length) and $E = 1/2$ (this simply sets the unit of time). To ensure that the total kinetic energy ($= 2EN = N$) and total momentum ($= \mathbf{0}$) do not deteriorate due to round-off errors, our program resets these values periodically, after every 100 collisions between particles.

Possible location of Table 1.

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Acknowledgements. The author was partially supported by NSF grant DMS-9622547. It is also a pleasure to thank R. Markarian for helping with the references to the mean free path formula (2.4) and R. Dorfman for a helpful discussion of problems studied in [21].

Appendix

Here we prove Lemma 5.2. We will need another lemma.

Lemma A.1 *Let L, E be linear subspaces of the Euclidean vector space $\mathbb{R}^m$, $m \geq 1$. For any linear operator $A: L \to E$ and $s > 0$ we have*

$$\frac{d}{ds} \left|_{s=0} \det(I + sA) = \operatorname{tr} A \right. \tag{A.1}$$

where $d/ds \,|_{s=0}$ means the value of the derivative at $s = 0$. Here I is the identity operator on L.

In the case $L = E = \mathbb{R}^m$, this lemma is an easy consequence of the fact that $\operatorname{tr} A$ is the second leading coefficient of the characteristic polynomial of the matrix A.

In the general case, we pick an orthonormal basis $e_1, \ldots, e_k$ in L, where $k = \dim L$. Then the determinant in (A.1) equals the volume of the k-dimensional parallelepiped K_s spanned by the vectors $f_i = e_i + sAe_i$, $1 \leq i \leq k$. It is clear that $f_i = [1 + s(e_i \cdot Ae_i)]e_i + sg_i$, where g_i is some vector perpendicular to e_i. For small s, the component sg_i of f_i contributes to the volume of K_s a quantity of order s^2. Therefore,

$$\operatorname{vol} K_s = \prod_{i=1}^{k} [1 + s(e_i \cdot Ae_i)] \, + \, O(s^2)$$

Now Lemma A.1 follows, see our convention in Section 4.

The proof of Lemma 5.2 consists in the following calculation:

$$\begin{aligned}
\frac{\frac{d}{dt} \det(I + tB)}{\det(I + tB)} &= \frac{\frac{d}{ds}\,|_{s=0} \det(I + tB + sB)}{\det(I + tB)} \\
&= \frac{d}{ds}\,|_{s=0}\, \frac{\det(I + tB + sB)}{\det(I + tB)} \\
&= \frac{d}{ds}\,|_{s=0} \det\Big((I + tB + sB)(I + tB)^{-1}\Big) \\
&= \frac{d}{ds}\,|_{s=0} \det\Big(I_1 + sB(I + tB)^{-1}\Big) \\
&= \operatorname{tr} B(I + tB)^{-1}
\end{aligned}$$

Here I_1 is the identity operator on the linear space $(I + tB)L$, i.e. on the image of L under the operator $I + tB$.

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	theory	experiment		
	by (9.3)	$\rho = 0.001$	$\rho = 0.01$	$\rho = 0.1$
$N = 3$	0.3607	0.3600	0.3540	0.2955
$N = 5$	0.3396	0.3391	0.3329	0.2821
$N = 10$	0.3257	0.3255	0.3197	0.2736
$N = 50$	0.3157	0.3151	0.3109	0.2671
$N = 100$	0.3145	0.3142	0.3091	0.2660
$N = \infty$	0.3133	0.3128	0.3084	0.2661
	(Boltz.)	(Enskog)	(Enskog)	(Enskog)

Table 1. Theoretical and experimental values of $\bar{t}_{\mathrm{par}} \cdot \rho$. Here $k = 2$, $\sigma = 1$ and $E = 1/2$.