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Flow-Invariant Hypersurfaces in Semi-Dispersing Billiards

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Abstract. This work results from our attempts to solve Boltzmann–Sinai's hypothesis about the ergodicity of hard ball gases. A crucial element in the studies of the dynamics of hard balls is the analysis of special hypersurfaces in the phase space consisting of degenerate trajectories (which lack complete hyperbolicity). We prove that if a flow-invariant hypersurface J in the phase space of a semi-dispersing billiard has a negative Lyapunov function, then the volume of the forward image of J grows at least linearly in time. Our proof is independent of the solution of the Boltzmann–Sinai hypothesis, and we provide a complete and self-contained argument here.

1. Introduction

The ergodic hypothesis for gases of hard balls was first put forward (in rather vague terms) by L. Boltzmann back in the 1880's, and then formalized by Ya. G. Sinai in 1963 [15]. It states that the gas of $N \geq 2$ identical hard balls (of small radius) on a torus Tor^d, $d \geq 2$, is ergodic, after certain necessary reductions. The latter mean that one fixes the total energy, sets the total momentum to zero, and restricts the center of mass to a certain discrete lattice within the torus. The assumption of a small radius is necessary to have the configuration space connected.

The motion of N hard balls in a d-dimensional torus naturally reduces to that of a single billiard particle in a $(dN-d)$-dimensional domain $\mathcal{D}$ with specular reflections off its boundary $\partial\mathcal{D}$. The domain $\mathcal{D}$, which is the configuration space of the system, is obtained by the removal of $N(N-1)/2$ cylinders from the torus Tor^{dN-d} (each cylinder corresponds to a pair of colliding balls). Thus the boundary $\partial\mathcal{D}$ is convex (as seen from inside the domain $\mathcal{D}$), but not strictly convex, which makes the billiard in $\mathcal{D}$ semi-dispersing. This is true, unless $N = 2$, in which case we have a single 'cylinder' that actually becomes a sphere, thus $\partial\mathcal{D}$ is strictly convex, which makes the corresponding billiard dispersing.

The system of $N = 2$ balls (disks) in dimension $d = 2$ was thoroughly investigated by Sinai [16]: he proved its hyperbolicity, ergodicity, and K-mixing. In this seminal paper Sinai also developed a general theory of planar dispersing billiards. Then Sinai and Chernov [20] extended these results to systems of $N = 2$ balls in any dimension $d > 2$, as well as to other multidimensional dispersing billiards (there was a notable oversight in [20] that was corrected later in [1]).

The dynamics of hard balls (and related billiards) is not entirely smooth– singularities occur at 'grazing' collisions of two balls and at multiple collisions of ≥ 3 balls (if they hit each other simultaneously). These events induce hypersurfaces in the phase space consisting of singular trajectories; they are called singularity manifolds and cause major troubles in the analysis. In addition, there is an issue of uniform versus nonuniform hyperbolicity. Dispersing billiards are characterized by strong hyperbolicity with uniform expansion and contraction rates. On the contrary, semi-dispersing billiards are only non-uniformly hyperbolic, so that their expansion and contraction rates may be arbitrarily slow. This constitutes a crucial difference between systems of $N = 2$ (dispersing) and $N > 2$ (semidispersing) cases, the latter are much harder to deal with.

The first major result for systems of $N > 2$ balls was the theorem on 'local' ergodicity by Sinai and Chernov [20] (a plan of its proof was earlier laid out by Sinai [17]); loosely speaking it states that for any hyperbolic phase point x there is an open neighborhood $U(x)$ that belongs to one ergodic component (mod 0). That theorem was proven under an assumption later referred to as Chernov-Sinai Ansatz [5,6]; roughly speaking it states that typical points on singularity manifolds must be hyperbolic.

A strategy for proving complete hyperbolicity and 'global' ergodicity for systems of $N > 2$ hard balls was first proposed by Sinai and Chernov in an unpublished manuscript [19] and further developed and refined by Krámli, Simányi, and Szász [5–7]. It is based on the following observations.

A phase point x fails to be hyperbolic in two possible ways. First, it may happen that along the trajectory of x the system of N balls splits into two (or more) groups (clusters) of balls that only interact within clusters. As unlikely as it seems, such an anomaly does occur, it is called *splitting*. Second, even without splitting the balls may collide in such a 'degenerate' manner that expansion and contraction of tangent vectors only occur in a tangent subspace of some lower dimension. The simplest example is obtained by letting all the N balls move along a closed geodesic in the torus (with different but parallel velocity vectors). In such examples the balls seem to 'conspire' to prevent complete hyperbolicity; in any case their positions and velocity vectors must satisfy very stringent requirements. We call this phenomenon *degeneracy*. Thus the complete hyperbolicity can only be destroyed by either splitting or degeneracy.

In order to prove the hyperbolicity for the system of N balls, it is enough to verify that splitting and degeneracy occur on subsets of zero measure. To establish ergodicity, one needs more than that – the set of 'bad' phase points (where splitting or degeneracy occur) must not separate two ergodic components. For instance, it is enough to show that the set of all bad phase points has topological codimension two or more. In addition, one needs to verify the Ansatz to utilize the local ergodic theorem. All these proofs are carried out inductively, by assuming the ergodicity of systems of n hard balls for all $n < N$.

The above strategy was successfully employed by Krámli, Simányi and Szász who proved hyperbolicity and ergodicity for $N = 3$ balls in any dimension [6] and for $N = 4$ balls in dimension $d \geq 3$, see [7]. Then Simányi [9,10] proved hyperbolicity and ergodicity whenever $N \leq d$ (this covers systems with an arbitrary number of balls, but only in spaces of high enough dimension, which is a very restrictive condition). By using the induction hypothesis mentioned above, Simányi [9, 10] also found a general argument showing that in any system of hard balls, splitting only occurred on a subset of zero measure and topological codimension two (or more) in phase space, thus splitting was no longer a problem. But degeneracies remained a key problem – in all the above papers they were handled by a direct analysis involving various cases specific for every system of hard balls. This 'case study' became overly complicated with every extra ball added to the system, and it was clearly impractical for $N > 4$ balls.

Further progress required novel ideas, and Simányi and Szász [11] employed the methods of algebraic geometry. They assumed that the balls had arbitrary masses $m_1, \dots, m_N$ (but the same radius r). Now by taking the limit $m_N \to 0$ they were able to reduce the dynamics of N balls to the motion of $N - 1$ balls, thus utilizing a natural induction on N. Then, algebraic methods allowed them to effectively analyze all possible degeneracies, but only for typical (generic) vectors of "external" parameters $(m_1, \dots, m_N, r)$; the latter needed to avoid some exceptional submanifolds of codimension one in $\mathbb{R}^{N+1}$, which remained largely unknown. This approach led to a proof [11] of complete hyperbolicity (but not yet ergodicity) for all $N \geq 2$ and $d \geq 2$, and for *generic* $(m_1, \dots, m_N, r)$. Later Simányi alone upgraded the hyperbolicity to ergodicity for all systems of $N \geq 2$ hard balls and typical (generic) values of external parameters $(m_1, \dots, m_N, r)$; this was done in two separate papers: [13] covered the case $d = 2$ and [14] dealt with $d > 2$. Both papers again use algebraic methods, thus their results are restricted to 'generic' masses. This was not quite satisfactory as the most interesting case of equal masses $m_1 = \cdots = m_N$ (it is exactly this case that motivated both Boltzmann and Sinai) remained open, as there was no guarantee that the exceptional submanifolds would avoid it.

It is clear that methods of algebraic geometry, however powerful, have to be abandoned if we are to obtain hyperbolicity and ergodicity for *all* gases of hard balls (including the case of equal masses). Recently Simányi [12] made a partial progress in this direction: he employed purely dynamical arguments to establish complete hyperbolicity (but not yet ergodicity) for all systems of hard balls (including equal masses $m_1 = \cdots = m_N$). In the course of that work, Simányi showed that degeneracies occurred on a countable union of smooth submanifolds in the phase space with codimension *at least one*. This implies, of course, that degeneracies are restricted to a subset of zero measure, which is enough for hyperbolicity, but ergodicity would require those submanifolds be of codimension *at least two*.

In an attempt to find a general dynamical argument that would rule out the existence of degeneracies on submanifolds of codimension one (hypersurfaces), here we show that if such hypersurfaces existed, then they would necessarily grow in size (volume) either in the past or in the future (depending whether the Lyapunov function on them is positive or negative). This fact turned out to be essential in a subsequent proof of ergodicity by one of us (Simányi), under certain conditions. Here we prove the volume growth of hypersurfaces, as a separate fact, in the context of general semi-dispersing billiards (which of course include all systems of hard balls).

2. Results and proofs

Let $\mathcal{D}$ be a bounded connected domain in $\mathbb{R}^d$ or in the torus Tor^d; the boundary $\partial\mathcal{D}$ is a finite union of C^3 smooth compact hypersurfaces (each, possibly, with boundary):

$$\partial\mathcal{D} = \Gamma_1 \cup \cdots \cup \Gamma_r\,.$$

A billiard system is generated by a pointwise particle; it moves freely (with a constant velocity vector) at unit speed in $\mathcal{D}$ and gets specularly reflected at the boundary $\partial\mathcal{D}$ (by the classical rule "the angle of incidence is equal to the angle of reflection").

The phase space of the billiard system is the unit tangent bundle $\Omega = \mathcal{D} \times S^{d-1}$ over $\mathcal{D}$. Thus phase points are pairs $x = (q, v)$ where $q \in \mathcal{D}$ is the position and $v \in S^{d-1}$ the unit velocity vector of the billiard particle. The billiard dynamics generates a flow $\Phi^t\colon \Omega \to \Omega$. It is a Hamiltonian flow that preserves its Liouville measure μ; the latter is a direct product of uniform measures on $\mathcal{D}$ and S^{d-1}.

At every (regular) boundary point $q \in \Gamma_i \setminus \partial\Gamma_i$, $1 \le i \le r$, we denote by $\nu(q)$ the (unique) unit normal vector to Γ_i pointing into $\mathcal{D}$. The curvature operator (the second fundamental form) $\mathcal{K}_q$ is a self-adjoint linear transformation acting on the tangent space $\mathcal{T}_q\Gamma_i$; is given (to the linear order) by

$$\nu(q + \delta q) = \nu(q) + \mathcal{K}_q(\delta q)\,.$$

The billiard in $\mathcal{D}$ is said to be dispersing (semi-dispersing) if $\mathcal{K}_q$ is positive definite (resp., positive semi-definite) at every regular point $q \in \partial\mathcal{D}$. Geometrically, this means that $\partial\mathcal{D}$ is strictly convex (resp., just convex) as seen from inside $\mathcal{D}$. For a recent detailed studies of the dynamics in semi-dispersing billiards we refer the reader to [2].

Now let $J \subset \mathcal{D}$ be a small smooth compact hypersurface (a submanifold of codimension-one with boundary), which is locally flow-invariant, i.e., for every $x \in J \setminus \partial J$ there is $\varepsilon > 0$ such that $\Phi^t x \in J$ for all $|t| < \varepsilon$. For every $x = (q, v) \in J \setminus \partial J$ we denote by $n_x = (z, w) \in \mathcal{T}_x\Omega$ a non-zero normal vector to J, i.e., such that for any tangent vector $(\delta q,\, \delta v) \in \mathcal{T}_x\Omega$ the relation $(\delta q,\, \delta v) \in \mathcal{T}_x J$ is equivalent to $\langle \delta q,\, z\rangle + \langle \delta v,\, w\rangle = 0$; here $\langle\,\cdot\,,\,\cdot\,\rangle$ denotes the Euclidean inner product in $\mathbb{R}^d$.

Observe that $\langle w, v\rangle = 0$ because $\|v\| = 1$ for all $x = (q, v) \in \Omega$. Also since J is flow-invariant, we have $(v, 0) \in \mathcal{T}_x J$, hence $\langle z, v\rangle = 0$. Thus $w, z \in v^\perp$, where $v^\perp$ denotes the hyperplane in $\mathbb{R}^d$ orthogonal to v.

The value $Q(n_x) :\, = \langle z, w\rangle$ is called the *(infinitesimal) Lyapunov function*, see [4] or part A.4 of the Appendix in [3]. For a detailed account of the relationship between the Lyapunov function Q, the symplectic geometry in Ω, and the dynamics, see [8].

Remark. Since the normal vector $n_x = (z, w)$ to J is only determined up to a nonzero scalar multiple, the value $Q(n_x)$ is only determined up to a positive multiple. However, in our considerations the sign of $Q(n_x)$ will be most important, and this sign is clearly independent of the choice of n_x.

Next, for any $t \in \mathbb{R}$ the image $J_t = \Phi^t(J)$ is also a locally flow-invariant compact hypersurface in Ω. Given a point $y_0 = (q_0, v_0) \in J \setminus \partial J$, its image $y_t = (q_t, v_t) = \Phi^t(y_0)$ is a regular point in J_t (i.e., $y_t \notin \partial J_t$), unless y_t is a reflection point. Given a normal vector n_0 to J at y_0, we define the unique normal vector n_t to J_t at y_t by

$$n_t = (D_{y_t}\Phi^{-t})^*(n_0)\,,$$

i.e.,

$$\langle D_{y_0}\Phi^t(\delta y), n_t\rangle = \langle \delta y, n_0\rangle \qquad \forall\, \delta y \in \mathcal{T}_{y_0}\Omega\,. \tag{2.1}$$

We develop explicit formulas for n_t $(t > 0)$. If there is no collisions during an interval of time $[s, t]$ on the orbit $\{y_t\}$, then the relation between $(\delta q_s,\, \delta v_s) \in \mathcal{T}_{y_s}\Omega$ and $(\delta q_t,\, \delta v_t) = D_{y_s}\Phi^{t-s}(\delta q_s,\, \delta v_s)$ is obviously

$$\begin{aligned}\delta v_t &= \delta v_s\,,\\ \delta q_t &= \delta q_s + (t-s)\delta v_s\,,\end{aligned}$$

from which we obtain that for all $\delta y_s = (\delta q_s, \delta v_s) \in \mathcal{T}_{y_s}\Omega$

$$\begin{aligned}\langle \delta y_s, n_s\rangle &= \langle \delta q_t - (t-s)\delta v_t,\, z_s\rangle + \langle \delta v_t,\, w_s\rangle\\ &= \langle \delta q_t,\, z_s\rangle + \langle \delta v_t,\, w_s - (t-s) z_s\rangle\,,\end{aligned}$$

hence

$$n_t = (z_t,\, w_t) = \big(z_s,\, w_s - (t-s) z_s\big)\,. \tag{2.2}$$

Observe that

$$Q(n_t) = Q(n_s) - (t-s)\|z_s\|^2 \le Q(n_s)\,. \tag{2.3}$$

Next let the orbit $\{y_t\}$ collide (reflect) at a boundary point $q \in \partial\mathcal{D}$ at some time $t > 0$. The velocity vector $v^- = v_{t-0}$ is transformed to $v^+ = v_{t+0}$ by the rule

$$v^+ = v^- + 2\cos\varphi\;\nu(q)\,,$$

where φ is the angle between the outgoing velocity vector v^+ and the unit normal vector $\nu(q)$ to $\partial\mathcal{D}$, i.e., $\cos\varphi = \langle v^+, \nu(q)\rangle$.

At the collision, the flow transforms tangent vectors $(\delta q^-,\, \delta v^-) \in \mathcal{T}_{y_{t-0}}\Omega$ (we can assume that both δq^- and δv^- belong in $(v^-)^\perp$, see above), according to the standard rules

$$\begin{aligned} \delta q^+ &= R(\delta q^-)\,, \\ \delta v^+ &= R(\delta v^-) + 2\cos\varphi\, RV^*\mathcal{K}V(\delta q^-)\,, \end{aligned} \tag{2.4}$$

where the operator $R\colon \mathcal{T}_q\mathcal{D} \to \mathcal{T}_q\mathcal{D}$ is the orthogonal reflection across the tangent hyperplane $\mathcal{T}_q\partial\mathcal{D}$, $V\colon (v^-)^\perp \to \mathcal{T}_q\partial\mathcal{D}$ is the v^--parallel projection of $(v^-)^\perp$ onto $\mathcal{T}_q\partial\mathcal{D}$, V^* is the adjoint of V, i.e., it is the $\nu(q)$-parallel projection of $\mathcal{T}_q\partial\mathcal{D}$ onto $(v^-)^\perp$, and $\mathcal{K}$ is the curvature operator of $\partial\mathcal{D}$ at q (see above).

The formulas (2.4) are given, e.g., in [18, Section 1] or [5, Proposition 2.3]. We can also rewrite them as

$$\begin{aligned} \delta q^- &= R(\delta q^+)\,, \\ \delta v^- &= R(\delta v^+) - 2\cos\phi\, RV_1^*\mathcal{K}V_1(\delta q^+)\,, \end{aligned}$$

where V_1 is the v^+-parallel projection of $(v^+)^\perp$ onto $\mathcal{T}_q\partial\mathcal{D}$.

Now let $n^- = (z^-, w^-)$ denote the normal vector to J_t at y_{t-0}, i.e., right before the collision, then

$$\begin{aligned} \langle(\delta q^-,\, \delta v^-), n^-\rangle &= \langle R(\delta q^+),\, z^-\rangle + \langle R(\delta v^+) - 2\cos\phi RV_1^*\mathcal{K}V_1(\delta q^+),\, w^-\rangle \\ &= \langle \delta q^+,\, R(z^-) - 2\cos\phi V_1^*\mathcal{K}V_1R(w^-)\rangle + \langle \delta v^+,\, R(w^-)\rangle\,. \end{aligned}$$

Thus the normal vector $n^+ = (w^+, z^+)$ to J_t at y_{t+0} (after the collision) is

$$n^+ = \big(R(z^-) - 2\cos\phi V_1^*\mathcal{K}V_1R(w^-),\, R(w^-)\big)\,.$$

Observe that $\|w^+\| = \|w^-\|$ and

$$\begin{aligned} Q(n^+) &= Q(n^-) - 2\cos\phi\,\langle V_1^*\mathcal{K}V_1R(w^-),\, R(w^-)\rangle \\ &= Q(n^-) - 2\cos\phi\,\langle \mathcal{K}V_1R(w^-),\, V_1R(w^-)\rangle \le Q(n^-)\,, \end{aligned}$$

because $\mathcal{K} \ge 0$ for semi-dispersing billiards.

We summarize our results:

Proposition 2.1. *The Lyapunov function $Q(n_t)$ is a monotone non-increasing function of t. The norm $\|w_t\|$ is a continuous function of t. The norm $\|z_t\|$ is a piecewise constant function of t changing only at collisions.*

Our normal vector n_t is related to the rate of expansion of the hypersurface J by the flow Φ^t:

Proposition 2.2. *The flow Φ^t expands the volume of the hypersurface J at a point $y_0 \in J$ by a factor $\|n_t\|/\|n_0\|$.*

Proof. According to (2.1), for every $\delta y_t \in \mathcal{T}_{y_t}\Omega$ we have

$$\langle \delta y_t,\, n_t\rangle = \left\langle D_{y_t}\Phi^{-t}(\delta y_t),\, n_0\right\rangle\,.$$

Substituting $\delta y_t = n_t$ gives

$$\frac{\|n_t\|}{\|n_0\|} = \frac{\langle D_{y_t}\Phi^{-t}(n_t),\, n_0\rangle}{\|n_t\|\,\|n_0\|}\,.$$

A simple geometric inspection shows that the right-hand-side is exactly the factor of linear expansion by Φ^{-t} between the points y_t and y_0 in the direction transversal to J_t, and since Φ^t preserves volume in Ω, it is the factor of volume expansion of the hypersurface J by Φ^t between the points y_0 and y_t. The proposition is proved. □

From now on we assume that $Q(n_0) < 0$. This assumption is motivated by the following considerations (which will not affect our further arguments, though). If there is a flow-invariant compact hypersurface $J \subset \Omega$, it might divide the phase space Ω into two (or more) Φ^t-invariant open subsets, thus preventing the ergodicity of the flow. One wants to show that such hypersurfaces cannot exist. There is a separate argument [13, Remark 7.9] showing that the Lyapunov function cannot stay identically zero on the entire trajectory of any non-splitting phase point, thus $Q < 0$ or $Q > 0$ on parts of J. We will show that if $Q < 0$, then the volume of J is expanded under the flow, at least linearly in time, hence J cannot be compact. Similarly, if $Q > 0$, then the volume of J is expanded in the past.

Proposition 2.3. *If $Q(n_0) < 0$, then $Q(n_t)$ is a monotone decreasing function of t, and the norm $\|w_t\|$ of the 'velocity' component of the normal vector $n_t = (z_t,\, w_t)$ is a monotone increasing function of t.*

Proof. We have $Q(n_s) = \langle z_s, w_s\rangle \le Q(n_0) < 0$ for all $s > 0$. Hence $\|z_s\| \neq 0$, and so $Q(n_t) < Q(n_s)$ for any collision-free time interval (s, t) due to (2.3). Also, by (2.2)

$$\|w_t\|^2 = \|w_s\|^2 - 2(t-s)\,Q(n_s) + (t-s)^2\|z_s\|^2 > \|w_s\|^2\,,$$

and $\|w_t\|$ does not change at collisions. □

Proposition 2.4. *If $Q(n_0) < 0$, then the function $\|w_t\|/|Q(n_t)|$ is monotone decreasing in t.*

Proof. For any $s \ge 0$ we have

$$w_s = \frac{Q(n_s)}{\|z_s\|^2}\, z_s + w_s^{\perp}\,,$$

where $w_s^{\perp}$ is a vector orthogonal to z_s, hence

$$\frac{\|w_s\|}{|Q(n_s)|} = \left[\frac{1}{\|z_s\|^2} + \frac{\|w_s^{\perp}\|^2}{|Q(n_s)|^2}\right]^{1/2}$$

Due to (2.2), for any collision-free time interval (s, t) we have $z_t = z_s$ and $w_t^{\perp} = w_s^{\perp}$, while $|Q(n_s)| < |Q(n_t)|$. At collisions, $\|w_t\|$ stays constant, while $|Q(n_t)|$ instantaneously increases, thus the required property holds. □

Proposition 2.5. *If $Q(n_0) < 0$, then for all $t \geq 0$*

$$\|w_t\| \geq \|w_0\| + \frac{|Q(n_0)|\, t}{\|w_0\|}\,.$$

Proof. For any $t > 0$, which is not a collision time,

$$\frac{d}{dt}\|w_t\|^2 = \frac{d}{dt}\langle w_t,\, w_t\rangle = -2\langle z_t,\, w_t\rangle = 2|Q(n_t)| \geq \frac{2\,|Q(n_0)|\,\|w_t\|}{\|w_0\|}\,,$$

where we used (2.2) and the previous proposition, hence

$$\frac{d}{dt}\|w_t\| \geq \frac{|Q(n_0)|}{\|w_0\|}\,.$$

Since $\|w_t\|$ does not change at collisions, the proposition follows. □

Next we assume that $Q(t) < 0$ on all of the manifold J; more specifically

$$Q(n_0) = \langle z_0,\, w_0\rangle \leq -c_0 < 0 \tag{2.5}$$

holds true uniformly across J for a unit normal vector field $n_0(y)$ $(y \in J)$ with a fixed constant $c_0 > 0$.

Theorem 2.6. *If* (2.5) *holds, then Φ^t expands the volume of the hypersurface J at any point $y \in J$ by a factor $\lambda_t \geq 1 + c_0 t$ for all $t \geq 1/c_0$.*

Proof. Combining Propositions 2.2 and 2.5 gives

$$\lambda_t = \|n_t\| \geq \|w_t\| \geq \|w_0\| + \frac{c_0 t}{\|w_0\|}\,.$$

Since $\|w_0\| \leq \|n_0\| = 1$, this lower bound is at least $1 + c_0 t$ for $t \geq 1/c_0$. □

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