Hard Balls Gas and Alexandrov Spaces of Curvature Bounded Above

Dmitri Burago[1]

Abstract. This lecture is an attempt to give a very elementary account of a circle of results (joint with S. Ferleger and A. Kononenko) in the theory of semi-dispersing billiard systems. These results heavily rely on the methods and ideology of the geometry of non-positively curved length spaces.

The purpose of this lecture is to give a very informal and elementary account of one geometric approach in the theory of billiard systems. Precise formulations of the results (joint with S. Ferleger and A. Kononenko), their proofs and a more detailed exposition can be found in the survey [B-F-K-4] and the papers [B-F-K-1],[B-F-K-2] and [B-F-K-3].

The approach is based on representing billiard trajectories as geodesics in a certain length space. This representation is similar to turning billiard trajectories in a square billiard table into straight lines in a plane tiled by copies of the square. It is important to understand that this construction by itself does not provide new information regarding the billiard system in question; it only converts a dynamical problem into a geometric one. Nevertheless, while a problem may seem rather difficult in its billiard clothing, its geometric counterpart may turn out to be relatively easy by the standards of the modern metric geometry. For the geometry of non-positively curved length spaces we refer to [Ba], [Gr] and [Re].

Apparently, one of the motivations to study semi-dispersing billiard systems comes from gas models in statistical physics. For instance, the hard ball model is a system of round balls moving freely and colliding elastically in a box or in empty space. Physical considerations naturally lead to several mathematical problems regarding the dynamics of such systems. The problem that served as the starting point for the research discussed in this lecture asks whether the number of collisions in time one can be estimated from above. Another well-known and still unsolved problem asks whether such dynamical systems are ergodic. A "physical" version of both problems goes back to Boltzman, while their first mathematical formulation is probably due to Ya. Sinai.

[1]The author greatfully acknowledges the support of the NSF and the Sloan Foundation in the form of a Sloan Research Fellowship and NSF grants DMS-95-05175 and DMS-98-03129. The author thanks MFI in Oberwolfach, ESI in Vienna, ETH in Zurich, IRMA in Strasbourg and Universities Paris-11&12 for his fruitful and unforgettable visits to these institutions.

Making a short digression here, I would mention that, in my opinion, the adequacy of these model problems for physical reality is quite questionable. In particular, these problems are extremely sensitive to slight changes of their formulations. Introducing particles that are arbitrarily close in shape to the round balls and that are allowed to rotate, one can produce unbounded number of collisions in unit time [Va]. It is plausible that introducing even a symmetrical and arbitrarily steep potential of interaction between particles instead of discontinuous collision "potential", one can destroy the ergodicity ([Do]). The result of Simanyi and Szasz ([Si-Sz])(seemingly, the best one can prove in support of the ergodicity of the hard balls model in the present state of the art) asserts that the ergodicity does take place ... for almost all combinations of radii and masses of the balls. Such a result should be less than satisfactory for a physicist, since a statement that is valid only for "balls of irrational radii" does not make any physical sense at all. Perhaps, one would rather hope that the existence of an ergodic component whose complement is negligibly small (at least for a system of very many balls) is a more stable property. On the other hand, hard balls gas (of even very many small balls) in a spherical or a cylindrical vessel is obviously very non-ergodic since it possesses a first integral coming from rotational symmetries of the system. This happens regardless of a good deal of hyperbolicity produced by the dynamics of colliding balls, and it is not at all clear what happens if the symmetrical shape of the vessel is slightly perturbed.

Regardless of this minor criticism of the physical meaning of mathematical problems involving gas models, the author believes that these problems are quite interesting on their own, and from now on we stick to their mathematical set-up. It is well known that, by passing to the configuration space, the dynamics of a N balls can be substituted by the dynamics of one (zero-size) particle moving in the complement of several cylinders in $\mathbf{R}^{3N}$ and experiencing elastic collisions with the cylinders. These cylinders correspond to the prohibited configurations where two of the balls intersect. Another gas model, the Lorentz gas, just begins with a dynamical system of one particle moving in the complement of a regular lattice of round scatterers; its dynamics can be studied on the quotient space, which is a torus with a scatterer in it. All these example fit in the following general scheme.

Let M be a complete Riemannian manifold M together with a (finite or at least locally-finite) collection of smooth convex subsets B_i. These convex sets B_i are bounded by (smooth, convex) hypersurfaces W_i, which (together with B_i's) will be referred to as *walls*. In most physical models, M is just a flat torus or Euclidean space (whose Euclidean structure given by the kinetic energy of the system). Throughout this lecture we assume that M has non-positive curvature and positive injectivity radius; however, local uniform bounds on the number of collisions remain valid without these restrictions. The dynamics takes place in the (semi-dispersing) billiard table, which is the complement of $\bigcup B_i$ in M. More precisely, the phase space is (a subset of) the unit tangent bundle to this complement. A point moves along a geodesic until it reaches one of the walls W_i, and then it gets reflected so that both the magnitude and the projection of its velocity on the plane tangent to the wall are conserved. For simplicity, we exclude the trajectories that ever experience a collision with two walls simultaneously.

Systematic mathematical study of such systems, called semi-dispersing billiards, was initiated by Ya. Sinai and continued by many other mathematicians and physicists.

Our discussion will be concentrated around the idea of gluing several copies of M together and then developing billiard trajectories into this new space. This idea is very old and its simplest versions arise even in elementary high-school mathematical puzzles. For instance, if the billiard table is a square, one can consider a tiling of Euclidean plane by such squares, and billiard trajectories turn into straight lines. Although this idea is rather naive, it already provides valuable information. For instance, if one wonders how close a non-periodic trajectory comes to vertices of the square, the answer is given in terms of rational approximations to the slope of the corresponding line. In this instance, a dynamical problem is transformed into a question in the arithmetic of real numbers. We plan to do an analogous reformulation with geometry of length spaces on the other side.

We are concerned with semi-dispersing billiard systems. In the early sixties V. Arnold "speculated" that "such systems can be considered as the limit case of geodesic flows on negatively curved manifolds (the curvature being concentrated on the collisions hypersurface)" [Ar]. Indeed, this is nowadays well known (due to the works of Sinai, Bunimovich, Chernov, Katok, Strelcyn, Szasz, Simanyi and many others) that a large portion of the results in the smooth theory of (semi-)hyperbolic systems can be generalized (with appropriate modifications) to (semi-)dispersing billiards. In spite of this, the construction suggested by Arnold has never been used. It also caused several serious objections; in particular, A. Katok pointed out that such approximations by geodesic flows on manifolds necessarily produce geodesics that bend around collision hypersurfaces and therefore have no analogs in the billiard system.

To illustrate both Arnold's suggestion and the difficulty noticed by Katok, let us consider a simple example of the billiard in the complement of a disc in a two-torus (or Euclidean plane). Taking two copies of the torus with (open) discs removed and gluing them along the boundary circles of the discs, one obtains a Riemannian manifold (a surface of genus 2) with a metric singularity along the gluing circle. This manifold is flat everywhere except at this circle. One can think of this circle as carrying singular negative curvature. Smoothing this metric by changing it in an (arbitrarily small) collar around the circle of gluing, one can obtain a non-positively curved metric, which is flat everywhere except in this collar. To every segment of a billiard trajectory, one can (canonically) assign a geodesic in this metric. Collisions with the disc would correspond to intersections with the circle of gluing, where the geodesic leaves one copy of the torus and goes to the other one.

Unfortunately, many geodesics do not correspond to billiard trajectories. They can be described as coming from "fake" trajectories hitting the disc at zero angle, following an arc of its boundary circle (possibly even making several rounds around it) and then leaving it along a tangent line. Dynamically, such geodesics carry "the main portion of entropy" and they cannot be disregarded. On the other hand, it is difficult to tell actual trajectories from the fake ones when analyzing the geodesic flow on this surface.

There is another difficulty arising in higher dimension. If one tries to repeat the same construction for a three-torus with a ball removed, then after gluing two copies of this torus the gluing locus defines a totally geodesic subspace. It carries positive curvature, and this positive curvature persists under smoothing of the metric in a small collar of the sphere. Thus, in this case we do not get a negatively curved manifold at all.

We will (partially) avoid these difficulties by substituting a non-positively curved manifold by a length space of non-positive curvature in the sense of A.D. Alexandrov. Unfortunately, a construction that would allow us to represent all billiard trajectories as geodesics in one compact space is unknown in dimensions higher than three. Attempts to do this lead to a striking open question: Is it possible to glue finitely many copies of a regular 4-simplex to obtain a (boundaryless) non-positive pseudo-manifold (cf. [B-F-Kl-K])?

We introduce a construction that represents trajectories from a certain combinatorial class, where by a combinatorial class of (a segment of) a billiard trajectory we mean a sequence of walls that it hits.

Fix such a sequence of walls $K = \{W_{n_i}, i = 1, 2, \dots N\}$. Consider a sequence $\{M_i, i = 0, 1, \dots N\}$ of isometric copies of M. For each i, glue M_i and M_{i+1} along B_{n_i}. Since each B_{n_i} is a convex set, the resulting space M_K has the same upper curvature bound as M due to Reshetnyak's theorem ([Re]).

There is an obvious projection $M_K \to M$, and M can be isometrically embedded into M_K by identifying it with one of M_i's (regarded as subsets of M_K). Thus every curve in M can be lifted to M_K in many ways. A billiard trajectory whose combinatorial class is K admits a canonical lifting to M_K: we lift its segment till the first collision to $M_0 \subset M_K$, the next segment between collisions to $M_1 \subset M_K$ and so on. Such lifting will be called developing of the trajectory. It is easy to see that a development of a trajectory is a geodesic in M_K.

Note that, in addition to several copies of the billiard table, M_K contains other redundant parts formed by identified copies of B_i's. For example, if we study a billiard in a curved triangle with concave walls, B_i's are not the boundary curves. Instead, we choose as B_i's some convex ovals bounded by extensions of these walls. (One may think of a billiard in a compact component of the complement to three discs.) In this case, these additional parts look like "fins" attached to our space (the term "fin" has been used by S. Alexander and R. Bishop in an analogous situation). In case of the billiard in the complement of a disc in a two-torus (see discussion above), the difference is that we do *not* remove the disc when we glue together two copies of the torus. Now a geodesic cannot follow an arc of the disc boundary, as the latter can be shorten by pushing inside the disc. Still, there are "fake" geodesics, which go through the disc. However, there are fewer of them than before and it is easier to separate them.

It might seem more natural to glue along the boundaries of W_{n_i} rather than along the whole B_{n_i}. For instance, one would do so thinking of this gluing as "reflecting in a mirror" or by analogy with the usual development of a polygonal billiard. However, gluing along the boundaries will not give us a non-positively curved space in any dimension higher than 2.

One may wonder how the interiors of B_i's may play any role here, as they are "behind the walls" and billiard trajectories never get there. For instance, instead of convex walls in a manifold without boundary, one could begin with a manifold with several boundary components, each with a non-negative definite second fundamental form (w.r.t. the inner normal). Even for one boundary component, this new set-up cannot be reduced to the initial formulation by "filling in" the boundary by a non-positively curved manifold. Such an example was pointed out to me by J. Hass ([Ha]), and our main dynamical result does fail for this example. Thus, it is indeed important that the walls are not only locally convex surfaces, and we essentially use the fact that they are filled by convex bodies.

Let us demonstrate how the construction of M_K can be used by first reproving (and slightly generalizing) a known result. L. Stoyanow has shown that each combinatorial class of trajectories in a strictly dispersing billiard (in Euclidean space or a flat torus) contains no more than one periodic trajectory. By a strictly dispersing property we mean that all walls have positive definite fundamental forms. For a semi-dispersing billiard, L. Stoyanov proved that all periodic trajectories in the same combinatorial class form a family of parallel trajectories of the same length. Together with local bounds on the number of collisions (which were known in dimension 2, and the general case is discussed below), these results imply exponential upper bound on the growth of the number of (parallel classes of) periodic trajectories. These estimates are analogous to the estimates on the number of periodic geodesic in non-positively curved manifolds.

Assume that we have two periodic trajectories in the same combinatorial class K. Choose a point on each trajectory and connect the points by a geodesic segment $[xy]$. Let us develop one period of each trajectory into M_K, obtaining two geodesics $[x'x'']$ and $[y'y'']$ connected by two lifts $[x'y']$ and $[x''y'']$ of the segment $[xy]$. Thus, M_K contains a geodesic quadrangle with the sum of angles equal to 2π. It is well known that, in a non-positively curved space, such a quadrangle bounds a flat totally-geodesic surface; in our case it has to be a parallelogram since it has equal opposite angles. Thus, $|x'x''| = |y'y''|$ and the family of lines parallel to $[x'x'']$ and connecting the sides $[x'y']$ and $[x''y'']$ projects to a family of periodic trajectories. Moreover, this parallelogram has to intersect the walls in segments, and thus it is degenerate if the fundamental forms of the walls are positive definite. This just means that the two periodic trajectories coincide. The same is true if the sectional curvature of M is strictly negative, as it is equal to zero for any plane tangent to the parallelogram.

This argument is ideologically very close to the proof of the following result: the topological entropy of the time-one map T of the billiard flow for a compact semi-dispersing billiard table is finite. Note that the differential of the time-one map T is unbounded, and therefore the finiteness of the topological entropy is not obvious. Moreover, it is quite plausible that the following problem has an affirmative solution: if one drops the curvature restriction for M, can the topological entropy of the time-one map be infinite? Is the topological entropy of the billiard in a smooth convex curve in Euclidean plane always finite?

To estimate the topological entropy by h, it is enough to show that, given a positive ϵ, there is a constant $C(\epsilon)$ with the following property: for each N, the space of trajectories $T^i(v), i = 0, 1, \dots, N$ can be partitioned into no more than

$C(\epsilon) \cdot \exp(hN)$ classes in such a way that every two trajectories from the same class stay ϵ-close to each other.

At first glance, such a partition seems rather evident in our situation. Indeed, first let us subdivide M into several regions of diameter less than ϵ (the number of these regions is independent of N). If M is simply connected, we can just say that two trajectories belong to the same class if they have the same combinatorial class and both trajectories start from the same region and land in the same region of the subdivision of M. If M is not simply-connected, one also requires that the trajectories have the same homotopy type (formally, lifting two corresponding segments of the flow trajectories of the same combinatorial class K to M_K and connecting their endpoints by two shortest path, one gets a rectangle; this rectangle should be contractible). Since both the number of combinatorial classes and the fundamental group of M grow at most exponentially, is rather easy to give an exponential (in N) upper bound on the number of such classes (using again the local uniform estimates on the number of collisions, see below). On the other hand, for two trajectories from the same class, their developments into the appropriate M_K have ϵ-close endpoints and the quadrangles formed by the geodesics and the shortest paths connecting their endpoints is contractible. For a non-positively curved space, this implies that these geodesics are ϵ-close everywhere between their endpoints.

There is, however, a little hidden difficulty, which the reader should be aware of. The previous argument proves the closeness between the projections of two trajectories onto M, while we need to establish this closeness in the phase space. Thus, some extra work has to be done to show that if two geodesics in M_K stay sufficiently close, then so do the directions of their tangent vectors (in some natural sense). This is a compactness-type argument, which we will not dwell upon here.

Let us come back to the example used above to illustrate Arnold's suggestion. This is 2-dimensional Lorentz gas, that is the billiard in the complement of a disc in a flat two-torus. To count the number of classes in the above sketch of the argument, one can pass to an Abelian cover of M_K (since this billiard table has just one wall, there is no ambiguity in choosing K). The latter is two copies of Euclidean plane glued together along a lattice of discs centered at integer points. A (class of) billiard trajectories naturally determines a broken line with integer vertices. While not every broken line with integer vertices arises from a billiard trajectory, the portion of such lines coming from "fake" trajectories approaches zero for small radii of scatterers. Counting such broken lines is a purely combinatorial problem, and one sees that the topological entropy of Lorentz gas converges to a number between 1 and 2 as the radius of the repeller approaches zero. This result is stable: the "limit entropy" is the same for a convex repeller of any shape. The author has no idea whether this number has any physical meaning.

Now we pass to the main problem of estimating the number of collisions. For the hard ball system, one asks whether the number of collisions that may occur in this system can be estimated from above by a bound depending only on the number of balls and their masses. If we consider the balls moving in unbounded Euclidean space, we count the total number of collisions in infinite time. For a system of balls in a box, we mean the number of collisions in unit time (for a fixed value of kinetic energy). As far as I know, these problems have been resolved only for systems of three balls ([Th-Sa], [Mu-Co]).

It is relatively easy to establish such upper bounds on the number of "essential" collisions, opposed to collisions when two balls barely touch each other. While such "non-essential" collisions indeed do not lead to a significant exchange by energy or momentum, they nevertheless cannot be disregarded from a "physical viewpoint". Indeed, they may serve as the main cause of instability in the system: the norm of differential of the flow does not admit an upper bound just at such trajectories. In a general semi-dispersing billiard it is also easier to estimate the number of collisions that occur at an angle separated from zero. Such arguments are based on introducing a bounded function on the phase space so that the function does not decrease along each trajectory and increases by an amount separated from zero after each "essential" collision. For some cases, such as 2-dimensional and polyhedral billiard tables, one can estimate the fraction of "essential collisions" among all collisions and thus get uniform bounds on the total number of collisions (see [Va], [Ga-1], [Ga-2], [Si-1]). The simplest case that is unclear how to treat by such methods is a particle shot almost along the intersection line of two convex surfaces in 3-dimensional Euclidean spaces and hitting the surfaces at very small angles.

Contrary to dynamical arguments indicated above, we use a geometric approach based on some length comparisons. Let us first prepare the necessary notation and formulations. When one wants to obtain uniform bounds on the number of collisions for a general semi-dispersing billiard table, it is clear that an additional assumption is needed. Indeed, already for a two-dimensional billiard table bounded by several concave walls, a trajectory may experience an arbitrarily large number of collisions (in time one) in a neighborhood of a vertex if two boundary curves are tangent to each other. Thus, a non-degeneracy condition is needed. For simplisity, let us introduce the following *non-degeneracy assumption* (it can be essentially weakened for non-compact billiard tables): there exists a number C such that, if a point is ϵ-close to all sets from some sub-collection of the B_i's, then it is $C\epsilon$-close to the intersection of B_i's from this sub-collection. This assumption rules out various degenerations of the arrangements of hyperplanes tangent to walls. It is not difficult to verify that the hard ball gas model does satisfy the non-degeneracy assumption.

The main local result reads as follows: if a semi-dispersing billiard table satisfies the non-degeneracy assumption, then there exists a finite number P such that every point p in the billiard table possesses a neighborhood $U(p)$ such that every trajectory segment *contained in* $U(p)$ experiences no more than P collisions.

Passing to estimating the global number of collisions (for infinite time) we want to stay away from situations such as a particle infinitely bouncing between two disjoint walls. The result for this case reads as follows: if a semi-dispersing billiard table satisfies the non-degeneracy assumption, M is simply-connected and the intersection $\bigcap B_i$ of B_i's is non-empty, then there exists a finite number P such that every trajectory experiences no more than P collisions.

Outlining the proofs of these results, we restrict ourselves to the case of two walls W_1 and W_2 bounding two convex sets B_1 and B_2. Thus we avoid inessential combinatorial complications and cumbersome indices.

We begin by discussing the local bound. Let us assume that M is simply-connected; otherwise, one can pass to its universal cover. Consider a billiard trajectory T connecting two points x and y and pick any point $z \in B_1 \bigcap B_2$. Denote by $K = \{W_1, W_2, W_1, W_2 \dots\}$ the combinatorial class of T, and consider the development T' of T in M_K. This is a geodesic between two points x' and y'. By Alexandrov's theorem, every geodesic in a simply-connected non-positively curved space is the shortest path between its endpoints. Note that z canonically lifts to M_K since all copies of z in different copies of M got identified. Denoting this lift by z', we see that $|zx| = |z'x'|$ and $|zy| = |z'y'|$. Thus we conclude that the lengths of T between x and y is less that $|xz| + |zy|$ for all $z \in B_1 \bigcap B_2$. In other words, any path in M connecting x and y and visiting the intersection $B_1 \bigcap B_2$ is longer than the segment of T between x and y.

The following argument is the core of the proof. It shows that if a trajectory made too many collisions then it can be modified into a shorter curve with the same endpoints and passing through the intersection $B_1 \bigcap B_2$. This contradicts the previous assertion and thus gives a bound on the number of collisions.

Assume that T is contained in a neighborhood $U(p)$ and it collided with W_1 at points $a_1, a_2, \dots a_N$ alternating with collisions with W_2 at $b_1, b_2, \dots b_N$. Let z_i be the point in $B_1 \bigcap B_2$ closest to b_i and h_i be the distance from b_i to the shortest geodesic $[a_i a_{i+1}]$. By the non-degeneracy assumption, $|z_i b_i| \le C \cdot dist(b_i, B_1) \le h_i$. Thus the distance H_i from z_i to the shortest geodesic $a_i a_{i+t}$ is at most $(C+1)h_i$.

Plugging this inequality between the heights of the triangles $a_i b_i a_{i+1}$ and $a_i z_i a_{i+1}$ into a routine argument which develops these triangles on both Euclidean plane and k-plane, one concludes that $d_i \le C_1 \cdot D_i$, where $d_i = |a_i b_i| + |b_i a_{i+1}| - |a_i a_{i+1}|$, $D_i = |a_i z_i| + |z_i a_{i+1}| - |a_i a_{i+1}|$. Here k is the infinum of the sectional curvature in $U(p)$, and a constant C_1 can be chosen depending on C alone provided that $U(p)$ is sufficiently small.

Let d_j be the smallest of d_i's. Let us modify the trajectory T into a curve with the same endpoints: substitute its pieces $a_i b_i a_{i+1}$ by the shortest segments $a_i a_{i+1}$ for all i's excluding $i = j$. This new curve is shorter than T by at least $(N-1)d_p$. Let us make a final modification by replacing the piece $a_j b_j a_{j+1}$ by $a_j z_j a_{j+1}$. It makes the path longer by D_j, which is at most $C_1 d_j$. Hence, $N \le C_1 + 1$ because otherwise we would have a curve with the same endpoints as T, passing through $z_j \in B_1 \bigcap B_2$ and shorter than T. This proves the local bound on the number of collisions.

Now we are ready to estimate the global number of collisions, and here geometry works in its full power. Consider a trajectory T making N collisions with the walls $K = \{1, 2, 1, \dots, 2, 1\}$. Reasoning by contradiction, assume that $N > 3P+1$, where P is the local bound on the number of collisions. Consider the space M_K and "close it up" by gluing $M_0 \in M_K$ and $M_N \in M_K$ along the copies of B_1. Denote the resulting space by $\tilde{M}$. We cannot use Reshetnyak's theorem to conclude that $\tilde{M}$ is a non-positively curved space any more, since we identify points in the same space and we do not glue two spaces along a *convex* set.

We recall that a space has non-positive curvature iff every point possesses a neighborhood such that, for every triangle contained in the neighborhood, its angles are no bigger than the corresponding angles of the comparison triangle in Euclidean plane. However, using the correspondence between geodesics and billiard trajectories, one can conclude (reasoning exactly as in the proof of the *local* estimates on the number of collisions), that each side of a small triangle cannot intersect interiors of more than P copies of the billiard table. Since $N > 3P+1$, for every small triangle for which we want to verify the angle comparison property, we can undo one of the gluings without tearing the sides of the triangle. This ungluing may only increase triangle's angles, but now we find ourselves in a non-positively curved space (which is actually just M_K), and thus we get the desired comparison for the angles of the triangle.

To conclude the proof, it remains to notice that the development of T in $\tilde{M}$ is a geodesic connecting two points in the same copy of B_1. This is a contradiction since every geodesic in a simply-connected non-positively curved space is the only shortest path between its endpoints; on the other hand, there is a shortest path between the same points going inside this copy of B_1.

Let us finish with the following remark. It would be desirable if one could begin with finitely many copies of M and glue them together along walls B_i to obtain a non-positively curved space $\hat{M}$ so that each wall participates in at least one gluing. In particular, such a construction would immediately provide an alternative proof for both local and global estimates on the number of collisions. For instance, for global estimates it is enough to notice that every billiard trajectory lifts to a shortest path and hence it cannot intersect a copy of one wall in $\hat{M}$ more than once. Hence the number of collisions is bounded by the total number of copies of walls in $\hat{M}$. As it is mentioned above, it is however unclear whether such gluing exists even for a regular 4-simplex.

ACKNOWLEDGEMENTS. The author would like to use this opportunity to thank M. Brin, M. Gromov, A. Katok and B. Kleiner for interesting discussions and valuable comments.

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Dmitri Burago
Pennsylvania State University
Deptartment of Mathematics
University Park PA-16802 USA
burago@math.psu.edu