

Approximating Multi-Dimensional Hamiltonian Flows by Billiards

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Abstract: The behavior of a point particle traveling with a constant speed in a region $D \subset \mathbb{R}^N$, undergoing elastic collisions at the region's boundary, is known as the billiard problem. Various billiard models serve as approximation to the classical and semi-classical motion in systems with steep potentials (e.g. for studying classical molecular dynamics, cold atom's motion in dark optical traps and microwave dynamics). Here we develop methodologies for examining the validity and accuracy of this approximation. We consider families of smooth potentials V_ϵ , that, in the limit $\epsilon \rightarrow 0$, become singular hard-wall potentials of multi-dimensional billiards. We define auxiliary billiard domains that asymptote, as $\epsilon \rightarrow 0$ to the original billiards, and provide, for regular trajectories, asymptotic expansion of the smooth Hamiltonian solution in terms of these billiard approximations. The asymptotic expansion includes error estimates in the C^r norm and an iteration scheme for improving this approximation. Applying this theory to smooth potentials that limit to the multi-dimensional close to ellipsoidal billiards, we predict when the billiard's separatrix splitting (which appears, for example, in the nearly flat and nearly oblate ellipsoids) persists for various types of potentials.

1. Introduction

Imagine a point particle travelling freely (without friction) on a table, undergoing elastic collisions with the edges of the table. This model resembles a game of billiards, but it looks much simpler - we have only one ball, which is a dimensionless point particle. There is no friction and the table has no pockets. The shape of the table determines the nature of the motion (see [26] and references therein) – it can be ordered (integrable, e.g. in ellipsoidal tables), ergodic (e.g. in generic polygons), mixing and possessing K and B-properties (in dispersing-Sinai [50] tables or focusing-Bunimovich tables [7]), or of a mixed nature (most billiard shapes). While the above dynamical classification of two-dimensional billiards is well established, the statistical properties of such systems

(e.g. the rate of the decay of correlations) is still widely open and is non-trivial even for mixing systems, like Sinai and Bunimovich billiards, see [36, 60] and references therein.

While two-dimensional billiards had been extensively studied, much less is known regarding the dynamics in higher dimensional billiards; motivated by Boltzmann ergodic hypothesis, the geometrical and dynamical properties of a hard sphere gas had been the focus of a series of works; indeed the motion of N rigid d -dimensional balls in a d -dimensional box ($d = 2$ or 3) corresponds to a billiard problem in an n -dimensional domain, where $n = N \times d$ and the domain's boundary is formed by a union of cylinders [13, 31, 49]. The corresponding billiards are called semi-dispersing, and their ergodic properties had been extensively studied [27–30, 45–48]. On the other extreme, there exist several studies of integrable billiards in ellipsoids and their perturbations (see below), and several studies of ergodic and/or hyperbolic multi-dimensional billiards [8–11, 39, 59] (the nature of the singularity set in the higher dimensional case is a delicate issue [2]). Multi-dimensional billiards with mixed phase space were also studied in [11, 59] and in [61]. In [40] a semiclassical study of the three-dimensional Sinai billiard had been conducted. Recently, the hyperbolicity of certain finite range multi-dimensional spherically symmetric billiard potentials was proved [4] (see below).

In the context of Physics, the billiard description is usually used to model a more complicated system for which a particle is moving approximately inertially, and then is reflected by a steep potential. The reduction to the billiard problem simplifies the analysis tremendously, often allowing to describe completely the dynamics in a given geometry. Numerous applications of this idea appear in the physics literature; it works as an idealized model for the motion of charged particles in a steep potential, a model which is often used to examine the relation between classical and quantized systems (see [22, 52] and references therein); this approximation was utilized to describe the dynamics of the motion of cold atoms in dark optical traps (see [24] and references therein); this model has been suggested as a first step for substantiating the basic assumption of statistical mechanics – the ergodic hypothesis of Boltzmann ([31, 49–51, 53, 54]). The opposite point of view may be taken when one is interested in studying numerically the hard wall system in a complicated geometry (e.g. apply ideas of [37] to [38]) – then designing the “correct” limiting smooth Hamiltonian may simplify the complexity of the programming.

The first strategy for studying the effects of the soft potentials was to introduce finite range axis-symmetric potentials (potentials which identically vanish away from a set of circular scatterers and are axisymmetric at the scatterers). For the two-dimensional case [1, 3, 17, 19, 25, 32, 33, 35, 49], it was shown that a modified billiard map may be defined, and several works have utilized this modified map to prove ergodicity of some configurations [3, 19, 32, 33, 49], or to prove that other configurations may possess stability islands [1, 17]. More recently [4], it was shown that a similar strategy may be employed in arbitrary finite dimensions, and, moreover, that such an approach together with a careful study of the cone properties of the multi-dimensional modified billiard map, may be utilized to prove hyperbolicity of such a flow (under suitable conditions on the spherically symmetric finite range potentials and the spacing between the scatterers).

The more general problem of studying the limiting process of making a steep two-dimensional potential steeper up to the hard-wall limit can be approached in a variety of ways. In [37] approach based on generalized functions was proposed. In [56] we developed a different paradigm for studying this problem. We first formulated a set of conditions on general smooth steep potentials in two-dimensional domains (C^r -smooth, not necessarily of finite range, nor axis-symmetric) which are sufficient for proving that

regular reflections of the billiard flow and of the smooth flow are close in *the C^r topology*. This statement, which may appear first as a mathematical exercise, is quite powerful. It allows to prove immediately the persistence of various kinds of billiard orbits in the smooth flows (see [56] and Theorem 5 in Sect. 3.4) and to investigate the behavior near singular orbits (e.g. orbits which are tangent to the boundary) by combining several Poincaré maps, see for example [12, 43, 57]. The first part of this paper (see Theorems 1-2) is a generalization of this result to the multi-dimensional case in the most general geometrical setting.

Thus, it appears that the Physicists' approach, of approximating the smooth flow by a billiard has some mathematical justification. How good is this approximation? Can this approach be used to obtain an asymptotic expansion to the smooth solutions? The second part of this paper answers these questions. We propose an approximation scheme, with a constructive twist - we show that the best zero-order approximation should be a billiard map in a slightly distorted domain. We provide the scaling of the width of the corresponding boundary layer with the steepness parameter and with the number of derivatives one insists on approximating. Furthermore, the next order correction is explicitly found, supplying a modified billiard map (reminiscent of the shifted billiard map of [4, 17, 49]) which may be further studied. We believe this part is the most significant part of the paper as it supplies a constructive tool to study the difference between the smooth flow and the billiard flow.

In the last part of this paper we demonstrate how these tools may be used to instantly extend novel results (that were obtained for billiards) to the steep potential setting; it is well known that the billiard map is integrable inside an ellipsoid [26]. Moreover, the Birkhoff-Poritski conjecture claims that in 2 dimensions among all the convex smooth concave billiard tables only ellipses are integrable [55]. In [58] this conjecture was generalized to higher dimensions. Delshams *et al* ([15, 14] see references therein) studied the effect of small entire symmetric perturbations to the ellipsoid shape on the integrability. They proved that in some cases (nearly flat and nearly oblate) the separatrices of a simple periodic orbit split; thus, they proved a local version of the Birkhoff conjecture in the two-dimensional setting, and provided several non-integrable models in the n -dimensional case. Here, we show that a simple combination of their results with ours, extends their result to the smooth case - namely it shows that the Hamiltonian flow, in a sufficiently steep potential which asymptotically vanishes in a shape which is a small perturbation of an ellipsoid, is chaotic. Furthermore, we quantify, for a given perturbation of the ellipsoidal shape, what "sufficiently steep" means for exponential, Gaussian and power-law potentials.

These results may give the impression that the smooth flow and the billiard flow are indeed very similar, and so a Scientist's dream of greatly simplifying a complicated system is realized here. In the discussion we go back to this point - as usual dreams never materialize in full. In particular, we discuss there the possibility of having non-hyperbolic orbits and even effective stability islands in the case of steep repelling multi-dimensional potentials.

The paper is ordered as follows; in Sect. 2 we define and describe the billiard flow and billiard map. In Sect. 3 we study the smooth Hamiltonian flow; we first prove that if the potential satisfies some natural conditions, the smooth regular reflections will limit smoothly to the billiard's regular reflections (Theorems 1, 2). Then, we define a natural Poincaré section on which a generalized billiard map may be defined for the smooth flow. Next, we derive the correction term to the zeroth order billiard approximation (Theorem 3) and calculate it for three model potentials (exponential, Gaussian and power-law). We

end this section by stating its immediate implication - a persistence theorem for various types of trajectories (Theorem 5). In Sect. 4 we apply these results to the perturbed ellipsoidal billiard. We end the paper with a short summary and discussion. The appendices contain most of the proofs, whereas in the body of the paper we usually only indicate their main steps.

2. Billiards in d Dimensions

2.1. The billiard flow. Consider a billiard flow as the motion of a point mass in a compact domain $D \subset \mathbb{R}^d$ or \mathbb{T}^d . Assume that the boundary ∂D consists of a finite number of C^{r+1} smooth ($r \geq 1$) $(d - 1)$ -dimensional submanifolds:

$$\partial D = \Gamma_1 \cup \Gamma_2 \cup \dots \cup \Gamma_n, \quad i = 1 \dots n. \tag{1}$$

The boundaries of these submanifolds, when these exist, form *the corner set* of ∂D :

$$\Gamma^* = \partial\Gamma_1 \cup \partial\Gamma_2 \cup \dots \cup \partial\Gamma_n, \quad i = 1 \dots n. \tag{2}$$

The moving particle has a position $q \in D$ and a momentum vector $p \in \mathbb{R}^d$ which are functions of time. If $q \in \text{int}(D)$, then the particle moves freely with a constant velocity according to the rule¹:

$$\begin{cases} \dot{q} = p \\ \dot{p} = 0 \end{cases}. \tag{3}$$

Equation (3) is Hamiltonian with the Hamiltonian function (hereafter $p^2 = \langle p, p \rangle$)

$$H(q, p) = \frac{p^2}{2}. \tag{4}$$

The particle moves at a constant speed and bounces of ∂D according to the usual elastic reflection law : *the angle of incidence is equal to the angle of reflection*. This means that the outgoing vector p_{out} is related to the incoming vector p_{in} by

$$p_{out} = p_{in} - 2\langle p_{in}, n(q) \rangle n(q), \tag{5}$$

where $n(q)$ is the inward unit normal vector to the boundary ∂D at the point q , see [13]. To use the reflection rule (5), we need the normal vector $n(q)$ to be defined, hence the rule cannot be applied at points $q \in \Gamma^*$, where such a vector fails to exist².

Definition 1. *The domain D is called the **configuration space** of the billiard system.*

The phase space of the system is $\mathcal{P} = D \times S^{d-1}$, where S^{d-1} is a $(d - 1)$ -dimensional unit sphere (we set $H = \frac{1}{2}$) of velocity vectors. So the elements of \mathcal{P} are

$$\rho \equiv (q, p).$$

¹ We assume that the particle has mass one (otherwise one may rescale time).

² To be precise, one may define $n(q)$ by continuity at points of Γ^* , but this might give more than one normal vector $n(q)$, hence the dynamics would be multiply defined for a generic corner. We adopt the standard convention that the reflection is not defined at any $q \in \Gamma^*$.

Denote the time t map of the billiard flow as

$$b_t : \rho_0 \rightarrow \rho_t. \tag{6}$$

We do not consider reflections at the points of the corner set, so $\rho_t = b_t \rho_0$ implies here that the distance between any point on the trajectory connecting q_0 with q_t and the set Γ^* is bounded away from zero. A point $\rho \in \mathcal{P}$ is called an *inner point* if $q \notin \partial D$ and a *collision point* if $q \in \partial D \setminus \Gamma^*$. Obviously, if ρ_0 and $\rho_t = b_t \rho_0$ are inner points, then ρ_t depends continuously on ρ_0 and t . If ρ_t is a (non-tangent) collision point then the velocity vector undergoes a jump. Thus, in this case both b_{t-0} and b_{t+0} are defined. The map $R_o = b_{t+0} b_{t-0}^{-1}$ is the reflection law (5) (augmented by $q_{out} = q_{in}$).

If the piece of the trajectory which connects q_0 with q_t does not have tangencies with the boundary, then ρ_t depends C^r -smoothly on ρ_0 . It is well-known [50, 56] that the map b_t loses smoothness at any point q_0 whose trajectory is tangent to the boundary at least once on the interval $(0, t)$. Clearly a tangency may occur only if the boundary is concave in the direction of motion at the point of tangency. Consider hereafter only *non-degenerate tangencies*, namely assume that the curvature in the direction of motion does not vanish. Choose local coordinates $q = (x, y)$ in such a way that the origin corresponds to the collision point, the y -axis is normal to the boundary and looking inside the billiard region D , and the x -coordinates ($x \in \mathbb{R}^{d-1}$) correspond to the directions tangent to the boundary. If $Q(x, y) = 0$ is the equation of the boundary in these coordinates, then $Q_y(0, 0) \neq 0$ and $Q_x(0, 0) = 0$. We choose the convention that $Q_y(0, 0) > 0$. Obviously, the tangent trajectory is characterized by the condition $p_y = 0$, where (p_x, p_y) are the components of the momentum p . The vector $p_x = \dot{x}$ indicates the direction of motion of the tangent trajectory. It is easy to check that the tangency is non-degenerate if and only if

$$p_x^T Q_{xx}(0, 0) p_x > 0. \tag{7}$$

If the billiard boundary is strictly concave (strictly dispersing), then all the tangencies are non-degenerate. On the other hand, if the billiard's boundary has saddle points (or if the billiard is semi-dispersing), then there always exist directions for which this non-degeneracy assumption fails. Let $x = (x_1, \dots, x_{d-1})$ with x_1 corresponding to the direction of motion (i.e. $p_x = (1, 0, \dots, 0)$). Then, the boundary surface near the point of non-degenerate tangency is described by the following equation:

$$y = -\alpha x_1^2 + O(z^2, x_1 z), \quad \alpha > 0,$$

where we denote $z = (x_2, \dots, x_{d-1})$. It is easy to see now that for a non-degenerate tangency, for a small τ the map b_τ of the line $\rho_0 = (x_0 = (-\tau/2, 0, \dots, 0), y_0 \leq 0, p_{0x} = (1, 0, \dots, 0), p_{0y} = 0)$ is given by

$$\begin{aligned} \rho_\tau = & ((\tau/2, 0, \dots, 0) + O(y_0), 2\tau\sqrt{-\alpha y_0} + O(y_0), \\ & (1, 0, \dots, 0) + O(y_0), 4\sqrt{-\alpha y_0} + O(y_0)). \end{aligned}$$

As we see, the billiard flow loses smoothness indeed (it has a square-root singularity in the limit $y \rightarrow -0$) near the tangent trajectory. See Fig. 1.

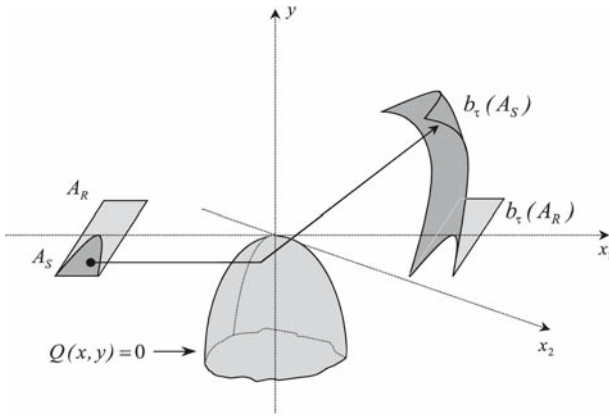


Fig. 1. Singularity near a tangent trajectory. For better visualization we present a slanted hyperplane which is divided into 2 parts: b_t has a square-root singularity on the boundary between A_R and A_S

2.2. *The billiard map.* It is standard in dynamical system theory to reduce the study of flows to maps by constructing a cross-section. The latter is a hypersurface transverse to the flow. For the flow b_t , such a hypersurface in phase space \mathcal{P} can be naturally constructed with the help of the boundary of D , i.e. the natural cross-section S corresponds exactly to the collision points of the flow with the domain’s boundary:

$$S = \{ \rho = (q, p) \in \mathcal{P} : q \in \partial D, \langle p, n(q) \rangle \geq 0 \}. \tag{8}$$

This is a $(2d - 2)$ -dimensional submanifold in \mathcal{P} . Any trajectory of the flow b_t crosses S every time it reflects at ∂D . This defines the *Poincaré map*

$$B : S \rightarrow S \text{ such that } B\rho = b_{\tau_o(\rho)+0}\rho, \tag{9}$$

where

$$\tau_o(\rho) = \min\{t > 0 : b_{t+0}\rho \in S\}.$$

Definition 2. *The map B is called the billiard map.*

We propose to represent the billiard map as a composition of a free-flight and a reflection:

$$B = R_o \circ F_o,$$

where the free-flight map is given by

$$F_o(q, p) = b_{\tau_o(\rho)-0}(q, p), \tag{10}$$

and the reflection law is given by

$$R_o(q, p) = (q, p - 2\langle p, n(q) \rangle n(q)).$$

The billiard map B is a C^r -diffeomorphism at all points $\rho \in S \setminus \Sigma$ such that $B\rho \in S \setminus \Sigma$, where Σ is the *singular set*

$$\Sigma = \Sigma_{tangencies} \cup \Sigma_{corners} = \{(q, p) \in S : \langle p, n(q) \rangle = 0\} \cup \{(q, p) \in S : q \in \Gamma^*\}, \tag{11}$$

and B is C^0 at the non-degenerate tangent trajectories.

3. Smooth Hamiltonian Approximation

3.1. *Setup and conditions on the potential.* Consider the family of Hamiltonian systems associated with:

$$H = \frac{p^2}{2} + V(q; \epsilon), \tag{12}$$

where the C^{r+1} -smooth potential $V(q; \epsilon)$ tends to zero inside a region D as $\epsilon \rightarrow 0$, and it tends to infinity (or to a constant larger than the fixed considered energy level, say $H = \frac{1}{2}$) outside. Formally, the billiard flow in D may be expressed as a limiting Hamiltonian system of the form:

$$H_b = \frac{p^2}{2} + V_b(q), \tag{13}$$

where

$$V_b(q) = \begin{cases} 0 & q \in \text{int}(D) \\ +\infty & q \notin D \end{cases}. \tag{14}$$

Let us formulate conditions under which this simplified billiard motion approximates the smooth Hamiltonian flow. In the two-dimensional case these conditions were introduced in [56].

Condition I. For any fixed (independent of ϵ) compact region $K \subset \text{int}(D)$ the potential $V(q; \epsilon)$ diminishes along with all its derivatives as $\epsilon \rightarrow 0$:

$$\lim_{\epsilon \rightarrow 0} \|V(q; \epsilon)|_{q \in K}\|_{C^{r+1}} = 0. \tag{15}$$

The growth of the potential near the boundary for sufficiently small ϵ values needs to be treated more carefully. We assume that the level sets of V may be realized by some finite function near the boundary. Namely, let $N(\Gamma^*)$ denote the fixed (independent of ϵ) neighborhood of the corner set and $N(\Gamma_i)$ denote the fixed neighborhood of the boundary component Γ_i (in the R^d topology); define $\tilde{N}_i = N(\Gamma_i) \setminus N(\Gamma^*)$ (we assume that $\tilde{N}_i \cap \tilde{N}_j = \emptyset$ when $i \neq j$). Assume that for all small $\epsilon \geq 0$ there exists a pattern function

$$Q(q; \epsilon) : \bigcup_i \tilde{N}_i \rightarrow \mathbb{R}^1$$

which is C^{r+1} with respect to q in each of the neighborhoods \tilde{N}_i and it depends continuously on ϵ (in the C^{r+1} -topology, so it has, along with all derivatives, a proper limit as $\epsilon \rightarrow 0$). See Fig. 2. Further assume that in each of the neighborhoods \tilde{N}_i the following is fulfilled.

Condition IIa. The billiard boundary is composed of level surfaces of $Q(q; 0)$ ³:

$$Q(q; \epsilon = 0)|_{q \in \Gamma_i \cap \tilde{N}_i} \equiv Q_i = \text{constant}. \tag{16}$$

In the neighborhood \tilde{N}_i of the boundary component Γ_i (so $Q(q; \epsilon)$ is close to Q_i), define a barrier function $W_i(Q; \epsilon)$, which is C^{r+1} in Q , continuous in ϵ and does not depend explicitly on q , and assume that there exists ϵ_0 such that

³ This is the $Q(x, y; 0)$ defined in Sect. 2.1.

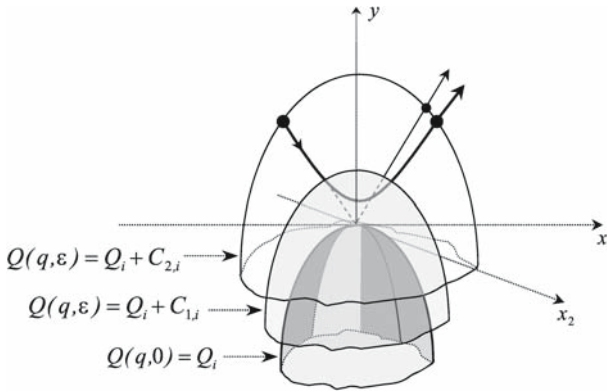


Fig. 2. Level sets of a pattern function $Q(q; \epsilon)$. A bold line is a trajectory of the Hamiltonian flow near the boundary; a solid is a billiard trajectory

Condition IIb. For all $\epsilon \in (0, \epsilon_0]$ the potential level sets in \tilde{N}_i are identical to the pattern function level sets and thus:

$$V(q; \epsilon)|_{q \in \tilde{N}_i} \equiv W_i(Q(q; \epsilon) - Q_i; \epsilon), \tag{17}$$

and

Condition IIc. For all $\epsilon \in (0, \epsilon_0]$, ∇V does not vanish in the finite neighborhoods of the boundary surfaces, \tilde{N}_i , thus:

$$\nabla Q|_{q \in \tilde{N}_i} \neq 0 \tag{18}$$

and for all $Q(q; \epsilon)|_{q \in \tilde{N}_i}$

$$\frac{d}{dQ} W_i(Q - Q_i; \epsilon) \neq 0. \tag{19}$$

Now, the rapid growth of the potential across the boundary may be described in terms of the barrier functions alone. Note that by (18), the pattern function Q is monotone across $\Gamma_i \cap \tilde{N}_i$, so either $Q > Q_i$ corresponds to the points near Γ_i inside D and $Q < Q_i$ corresponds to the outside, or vice versa. To fix the notation, we will adopt the first convention.

Condition III. There exists a constant (may be infinite) $\mathcal{E} > 0$ such that as $\epsilon \rightarrow +0$ the barrier function increases from zero to \mathcal{E} across the boundary Γ_i :

$$\lim_{\epsilon \rightarrow +0} W(Q; \epsilon) = \begin{cases} 0, & Q > Q_i \\ \mathcal{E}, & Q < Q_i \end{cases}. \tag{20}$$

By (19), for small ϵ , Q could be considered as a function of W and ϵ near the boundary: $Q = Q_i + \mathcal{Q}_i(W; \epsilon)$. Condition IV states that for small ϵ a finite change in W corresponds to a small change in Q :

Condition IV. As $\epsilon \rightarrow +0$, for any fixed W_1 and W_2 such that $0 < W_1 < W_2 < \mathcal{E}$, for each boundary component Γ_i , the function $\mathcal{Q}_i(W; \epsilon)$ tends to zero uniformly on the interval $[W_1, W_2]$ along with all its $(r + 1)$ derivatives.

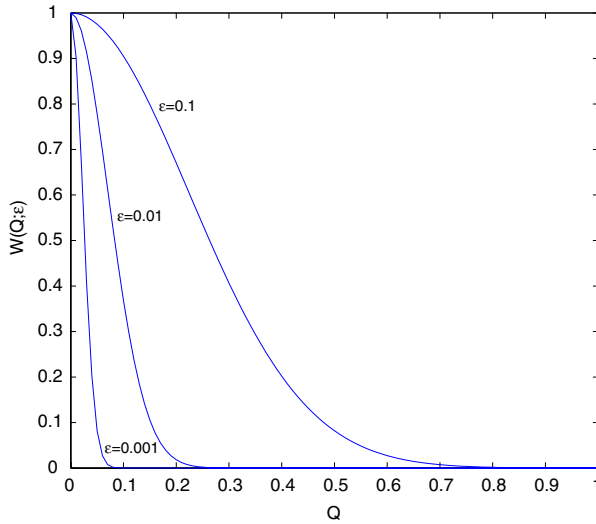


Fig. 3. Gaussian potential given near the boundary by $W(Q; \epsilon) = e^{-\frac{Q^2}{\epsilon}}$ satisfies Conditions I-IV

Figure 3 shows the geometric interpretation of the pattern function and a typical dependence of the barrier function on Q and ϵ . The use of the pattern and barrier functions essentially reduces the d -dimensional Hamiltonian dynamics in arbitrary geometry to a one-dimensional dynamics, thus allowing direct asymptotic integration of the smooth problem. This is the main tool, introduced first in [56] for the two-dimensional case, which enables us to deal with arbitrary geometry and dimension.

3.2. C^0 and C^r - closeness theorems.

Theorem 1. *Let the potential $V(q; \epsilon)$ in (12) satisfy Conditions I-IV. Let h_t^ϵ be the Hamiltonian flow defined by (12) on an energy surface $H = H^* < \mathcal{E}$ (with positive H^*), and b_t be the billiard flow in D . Let ρ_0 and $\rho_T = b_T \rho_0$ be two inner phase points. Assume that on the time interval $[0, T]$ the billiard trajectory of ρ_0 has a finite number of collisions, and all of them are either regular reflections or non-degenerate tangencies. Then $h_t^\epsilon \rho \xrightarrow{\epsilon \rightarrow 0} b_t \rho$, uniformly for all ρ close to ρ_0 and all t close to T .*

Theorem 2. *In addition to the conditions of Theorem 1, assume that the billiard trajectory of ρ_0 has no tangencies to the boundary on the time interval $[0, T]$. Then $h_t^\epsilon \rho \xrightarrow{\epsilon \rightarrow 0} b_t \rho$ in the C^r -topology in a small neighborhood of ρ_0 , and for all t close to T .*

Recall that we speak here about trajectories which do not visit corner points, i.e. all the collisions are on $\cup_i \Gamma_i \cap \tilde{N}_i$.

The proof of the theorems follows closely their proof for the two-dimensional case in [56]. However, as minor corrections needed to be introduced, we presented the proof in the supplement [42]. Most of it deals with the analysis of the equations of motion in the boundary layers \tilde{N}_i . Informally, the logic behind Conditions I-IV is as follows. Condition I implies that the particle moves with almost constant velocity (along a straight line) in the interior of D until it reaches a thin layer near the boundary where V runs

from zero to large values (a smaller ϵ corresponds to a thinner boundary layer). Note that the boundary layer can not be fully penetrated by the particle. Indeed, as in all mechanical Hamiltonians, the energy level defines the region of allowed motion: for a fixed energy level $H = H^* < \mathcal{E}$, all trajectories stay in the region $V(q; \epsilon) \leq H^*$. It follows from Condition III that for any such H^* , the region of allowed motion approaches D as $\epsilon \rightarrow 0$. Thus, by Condition III, if the particle enters the layer near a boundary surface (note that points from Γ^* are not considered in this paper), it has, in principle, two possibilities. First, it may be reflected and then exit the boundary layer near the point it entered. The other possibility, which we want to avoid, is that the particle sticks to the boundary and travels along it far from the entrance point. It is shown in the proof of Theorem 1 that Condition IV guarantees that if the reflection is regular, or if it is tangent and the tangency is non-degenerate, then the travel distance along the boundary vanishes asymptotically with ϵ . The case of degenerate tangencies is important but it is not studied here; notice that degenerate tangencies cannot occur in the strictly dispersing case, yet these are unavoidable if the boundary has directional curvatures of opposite signs (saddle points) or in the semi-dispersing case.

Once we know that the time spent by the particle near the boundary is small, we can see that Condition II guarantees that the reflection will be of the right character, namely the smooth reflection is C^0 -close to that of the billiard. Indeed, Condition II implies that the reaction force is normal to the boundary, hence, as the time of collision is small and the position of the particle does not change much during this time, the direction of the force stays nearly constant during the collision. Thus, only the normal component of the momentum is changing sign while the tangent components are nearly preserved. Computations along these lines provide a proof of Theorem 1.

Proving Theorem 2, i.e. the C^r -closeness, makes a substantial use of Condition IV. Let us explain in more detail the difference between the C^0 and C^r topologies in this context. Take the same initial condition (q_0, p_0) for a billiard orbit and for an orbit of the Hamiltonian system (12) (the Hamiltonian orbit will be called *the smooth orbit*). Consider a time interval t for which the billiard orbit collides with the boundary only once. In these notations φ_{in} is the angle between p_0 (the momentum at the point q_0) and the normal to the boundary at the collision point, φ_{out} is the angle between p_t (the velocity vector at the point q_t) and the normal. Define the incidence and reflection angles ($\varphi_{in}(\epsilon)$ and $\varphi_{out}(\epsilon)$) for the smooth trajectory in the same way. Theorem 1 implies the correct reflection law for smooth trajectories:

$$\varphi_{in}(\epsilon) + \varphi_{out}(\epsilon) \approx 0 \tag{21}$$

for sufficiently small ϵ . However, $\varphi_{in} + \varphi_{out}$ is a function of the initial conditions, so a non-trivial question is when it is close to zero along with all its derivatives. In Theorem 2 we prove that Condition IV is sufficient for guaranteeing the correct reflection law in the C^r -topology in the case of non-tangent collision (near tangent trajectories the derivatives of the smooth flow cannot converge to those of the billiard because the billiard flow is singular there, see Fig. 1).

Hereafter, we will fix the energy level of the Hamiltonian flow to $H^* = \frac{1}{2}$. Notice that the analysis may be applied to systems with steep potentials which do not depend explicitly on ϵ (or do not degenerate as $\epsilon \rightarrow 0$) in the limit of sufficiently high energy: the reduction to the setting (12) which we consider here may be achieved by a scaling of time.

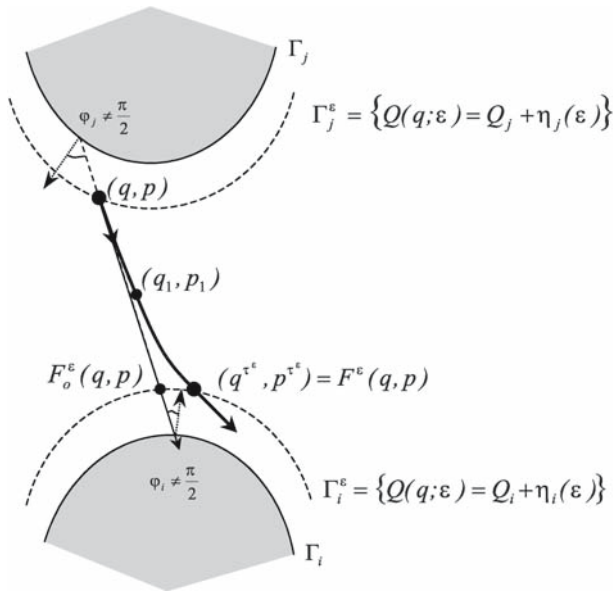


Fig. 4. Free flight between boundaries Γ_i^ϵ and Γ_j^ϵ . A smooth trajectory is marked by a bold line and an auxiliary billiard trajectory is marked by a solid line

3.3. *Asymptotic expansion for regular reflections.* It follows from the proof of Theorem 2 that the behavior of smooth trajectories close to billiard trajectories of regular reflections can be described by an analogue of the billiard map. More precisely, one can construct a cross-section S_ϵ in the phase space of the Hamiltonian flow, close to the “natural” cross-section S where the billiard map B is defined; the trajectories of the Hamiltonian flow which are close to regular billiard trajectories define the Poincaré map on S_ϵ , and this map is C^r -close to B . Let us explain this in more details. It is convenient to consider an auxiliary billiard in the modified domain D^ϵ , defined as follows. For each i , take any $\nu_i(\epsilon) \rightarrow +0$ such that the function (inverse barrier) $\mathcal{Q}_i(W; \epsilon)$ tends to zero along with all its derivatives, uniformly for $\frac{1}{2} \geq W \geq \nu_i$. We will use the notation

$$M_i^{(r)}(\nu; \epsilon) = \sup_{\substack{\nu \leq W \leq \frac{1}{2} \\ 0 \leq l \leq r+1}} |\mathcal{Q}_i^{(l)}(W; \epsilon)|. \tag{22}$$

Condition IV implies that M approaches zero as $\epsilon \rightarrow 0$ for any fixed $\nu > 0$, hence the same holds true for any sufficiently slowly tending to zero $\nu(\epsilon)$, i.e. the required $\nu_i(\epsilon)$ exist. Let $\eta_i(\epsilon) = \mathcal{Q}_i(\nu_i; \epsilon)$ and consider the billiard in the domain D^ϵ which is bounded by the surfaces $\Gamma_i^\epsilon : \mathcal{Q}(q; \epsilon)|_{q \in \tilde{N}_i} = Q_i + \eta_i(\epsilon)$ (see Fig. 4). For sufficiently small ϵ , the surface Γ_i^ϵ is a smooth surface which is close to Γ_i and is completely contained in \tilde{N}_i (its boundaries belong to $N(\Gamma^*)$). Indeed, recall that the boundaries Γ_i of the original billiard table D are given by the level sets $Q(q; 0) = Q_i$ and that $\eta_i(\epsilon)$ is small, so the new billiard is close to the original one. In particular, for regular reflections, the billiard map B^ϵ of the auxiliary billiard tends to the original billiard map B along with all its derivatives. It is established in the proof of Theorem 2 that for any choice of ν_i 's tending to zero, the condition $q \in \partial D^\epsilon$ defines a cross-section in the phase space of

the smooth Hamiltonian flow; trajectories which are close to the billiard trajectories of regular reflection, i.e. those which intersect ∂D^ϵ at an angle bounded away from zero, define the map

$$F^\epsilon : (q \in \partial D^\epsilon, p \text{ looking inwards } D^\epsilon) \rightarrow (q \in \partial D^\epsilon, p \text{ looking outwards } D^\epsilon),$$

namely

$$F^\epsilon(q, p) = h_{\tau^\epsilon}^\epsilon(q, p) \tag{23}$$

and this map is close to the free-flight map F_\circ^ϵ (see Sect. 2.2) of the billiard in D^ϵ :

$$F_\circ^\epsilon(q, p) = b_{\tau_\circ^\epsilon - 0}(q, p), \tag{24}$$

where $\tau^\epsilon(q, p)$ is the time the smooth Hamiltonian orbit of (q, p) needs to reach ∂D^ϵ , and $\tau_\circ^\epsilon(q, p)$ denotes the same for the billiard orbit. Note that we cannot claim the closeness of the time τ maps for the smooth Hamiltonian and billiard flows everywhere in D^ϵ , still we claim that the maps (23) and (24) are close; we will return to this later.

Outside D^ϵ , the overall effect of the motion of smooth orbits is close to that of a billiard reflection. Namely, as it is proved in Theorem 2, once v_i is chosen such that $M_i^{(r)}(v_i, \epsilon) \rightarrow 0$, the smooth trajectories which enter the region $W_i(Q; \epsilon) \geq v_i$ at a bounded away from zero angle to the boundary, spend in this region a small interval of time (denoted by $\tau_c^\epsilon(q_{in}, p_{in})$) after which they return to the boundary $W_i(Q; \epsilon) = v_i$ (namely to $Q(q; \epsilon) = Q_i + \eta_i(\epsilon)$). Thus, these orbits define the map

$$R^\epsilon : (q_{in} \in \partial D^\epsilon, p_{in} \text{ looking outwards } D^\epsilon) \rightarrow (q_{out} \in \partial D^\epsilon, p_{out} \text{ looking inwards } D^\epsilon).$$

It follows from the proof of Theorem 2 that the map R^ϵ is close to the standard reflection law R_\circ^ϵ from the boundary ∂D^ϵ :

$$R_\circ^\epsilon(q, p) = (q, p - 2n(q) \langle n(q), p \rangle), \tag{25}$$

where $n(q)$ is the unit normal vector to the boundary ∂D^ϵ at the point q . See Fig. 5. Note that the smooth reflection law R^ϵ corresponds to a non-zero (though small) collision time $\tau_c^\epsilon(q, p)$, unlike the billiard reflection R_\circ^ϵ which happens instantaneously.

Summarizing, from the proof of Theorem 2 we extract that on the cross-section

$$S_\epsilon = \{\rho = (q, p) : q \in \partial D^\epsilon, \langle p, n(q) \rangle > 0\} \tag{26}$$

the Poincaré map

$$\Phi^\epsilon = R^\epsilon \circ F^\epsilon \tag{27}$$

is defined for the smooth Hamiltonian flow (for regular orbits - orbits which intersect ∂D^ϵ at an angle bounded away from zero), and this map is C^r -close to the billiard map $B^\epsilon = R_\circ^\epsilon \circ F_\circ^\epsilon$. As the billiard map B^ϵ is close to the original billiard map B , we obtain the closeness of the Poincaré map Φ^ϵ to B as well. However, when developing asymptotic expansions for Φ^ϵ , it is convenient to use the map B^ϵ (rather than B) as the zeroth order approximation for Φ^ϵ . Then, the next term in the asymptotic may be explicitly found (see below) and the whole asymptotic expansion may be similarly developed.

We start with the estimates for the “free flight” segment of the motion, i.e. for the smooth Hamiltonian trajectories inside D^ϵ . For every boundary surface Γ_i , choose some $\delta_i(\epsilon) \rightarrow 0$ such that the surfaces $Q(q; \epsilon)|_{q \in \tilde{N}_i} = Q_i + \delta_i(\epsilon)$ together with $\partial N(\Gamma^*)$ bound

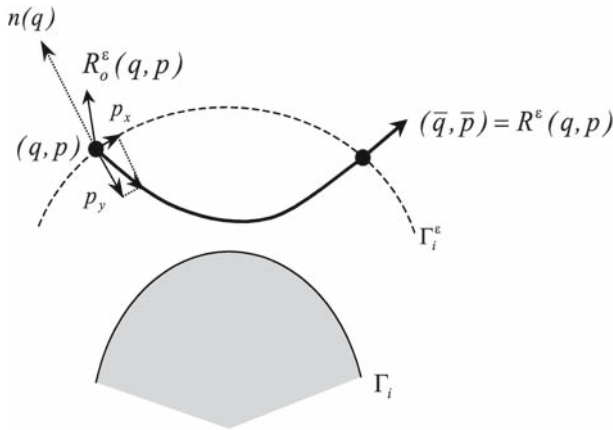


Fig. 5. Reflection from the boundary Γ_i . A smooth trajectory is marked by a bold line. An auxiliary billiard trajectory only changes its direction according to the law (25)

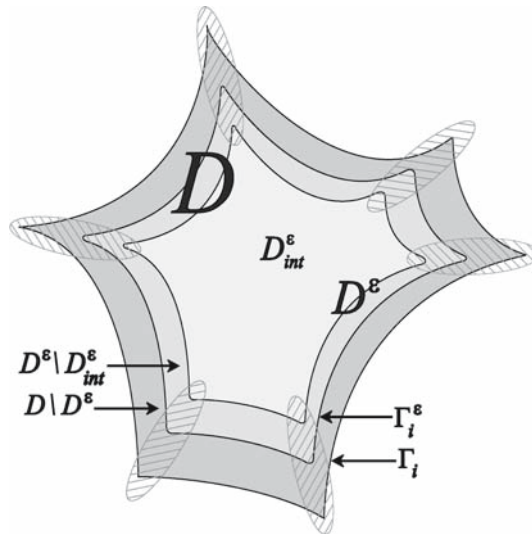


Fig. 6. The partition of the domain D into regions: $D^{\epsilon}_{int} \subset D^{\epsilon}$

the region D^{ϵ}_{int} inside D^{ϵ} in which the potential V tends to zero uniformly along with all its derivatives. See Fig. 6. Let

$$m^{(r)}(\delta; \epsilon) = \sup_{\substack{q \in D^{\epsilon}_{int} \\ 1 \leq l \leq r+1}} \|\partial^l V(q; \epsilon)\|. \tag{28}$$

According to Condition I, $m^{(r)}$ approaches zero as $\epsilon \rightarrow 0$ for any fixed δ of the appropriate signs, therefore the same holds true for any choice of sufficiently slowly tending to zero $\delta_i(\epsilon)$. As $m^{(r)} \rightarrow 0$, it follows that within D^{ϵ}_{int} the flow of the smooth Hamiltonian trajectories is C^r -close to the free flight, i.e. to the billiard flow. In other words, the time

τ map $h_\tau^\epsilon(q, p) = (q_\tau, p_\tau)$ of the smooth flow in D_{int}^ϵ is $O_{C^r}(m^{(r)})$ -close to the time τ map of the billiard flow

$$b_\tau(q, p) = \begin{pmatrix} q + p\tau \\ p \end{pmatrix}. \tag{29}$$

Note that on the boundary of D^ϵ we have, by construction, $Q'_i(W; \epsilon) \rightarrow 0$, i.e. $W'_i(Q; \epsilon) \rightarrow \infty$, while on the boundary of D_{int}^ϵ we have $W'_i(Q; \epsilon) \rightarrow 0$. Thus, we have a boundary layer $D^\epsilon \setminus D_{int}^\epsilon$ of a non-zero width $|\delta_i(\epsilon) - \eta_i(\epsilon)|$ in which the gradient of the potential rapidly decreases. The speed with which the value of $Q(q(t); \epsilon)$ changes within this boundary layer is bounded away from zero (see the proof of Theorem 2), so the time the orbit needs to penetrate it is $O(\delta_i)$. Within this boundary layer the time τ map $(q, p) \mapsto (q_\tau, p_\tau)$ of the smooth flow is not necessarily close to the time τ map of the billiard flow (29). However, it is shown in the proof of Theorem 2, that the maps from one surface $Q = const$ to any other such surface within the boundary layer are C^r -close for the two flows. This, obviously, implies the closeness of the maps F^ϵ and F_\circ^ϵ (because the corresponding cross-section is the surface of the kind $Q = const$ indeed).

In Appendix 7.1 we show that by an appropriate change of coordinates in each of the three regions we consider (inside D_{int}^ϵ , in $D^\epsilon \setminus D_{int}^\epsilon$, and outside D^ϵ), the equations of motion may be written as differential equations integrated over a finite interval with a right-hand side which tends to zero in the C^r -topology as $\epsilon \rightarrow 0$. Thus, not only do we obtain error estimates for the zeroth order approximation, we also find a method for obtaining higher order corrections using Picard iterations; the asymptotic behavior of the right-hand side of the equations leads to a contractivity constant which asymptotically vanishes and thus the Picard iteration scheme provides asymptotic for the solutions (each new iteration provides a better asymptotic). In this way we prove in Appendix 7.2 the following

Lemma 1. *Let q be an inner point of D , and p be such that the first hit of the billiard orbit of (q, p) with the boundary is at $\Gamma_i \setminus N(\Gamma^*)$ and is non-tangent. Let the potential $V(q; \epsilon)$ satisfy Conditions **I-IV**, and choose δ_i 's and v_i 's such that $\delta_i(\epsilon), v_i(\epsilon), m^{(r)}(\epsilon), M_i^{(r)}(\epsilon) \rightarrow 0$ as $\epsilon \rightarrow 0$. Then, for sufficiently small $\epsilon \leq \epsilon_0$, the orbit of the smooth flow hits the cross-section $\{q \in \Gamma_i^\epsilon\} = \{Q(q; \epsilon) = Q_i + \eta_i(\epsilon)\}$ at the point (q_τ, p_τ) such that*

$$\begin{aligned} q_\tau &= q + p\tau + O_{C^r}(m^{(r)} + v_i) \\ &= q + p\tau + \int_0^\tau \nabla V(q + ps; \epsilon)(s - \tau)ds + O_{C^{r-1}}((m^{(r)} + v_i)^2), \\ p_\tau &= p + O_{C^r}(m^{(r)} + v_i) \\ &= p - \int_0^\tau \nabla V(q + ps; \epsilon)ds + O_{C^{r-1}}((m^{(r)} + v_i)^2), \end{aligned} \tag{30}$$

where $\tau = \tau^\epsilon(q, p)$ denotes the travel time to the boundary of D^ϵ (so $Q(q_\tau; \epsilon) = Q_i + \eta_i(\epsilon)$):

$$\begin{aligned} \tau^\epsilon(q, p) &= \tau_\circ^\epsilon(q, p) + O_{C^r}(m^{(r)} + v_i) \\ &= \tau_\circ^\epsilon(q, p) + \frac{\langle \nabla Q, \int_0^{\tau_\circ^\epsilon} \nabla V(q + ps; \epsilon)(\tau_\circ^\epsilon - s)ds \rangle}{\langle \nabla Q, p \rangle} + O_{C^{r-1}}((m^{(r)} + v_i)^2), \end{aligned} \tag{31}$$

∇Q is evaluated at the (auxiliary) billiard collision point $q + p\tau_\circ^\epsilon(p, q)$, and $\tau_\circ^\epsilon(p, q)$ is the time the billiard orbit of (q, p) needs to reach Γ_i^ϵ .

Now, let us estimate the free-flight map F^ϵ of the Hamiltonian flow. If $q \in \Gamma_j^\epsilon$ and $\langle p, n(q) \rangle$ is positive and bounded away from zero, and if the straight line issued from q in the direction of p first intersects ∂D^ϵ (say, the surface Γ_i^ϵ) transversely as well (in our notations this can be expressed as the condition that $\langle p, n(q + p\tau_\circ^\epsilon(q, p)) \rangle$ is negative and bounded away from zero), then the orbits of the Hamiltonian flow define the map F^ϵ from a small neighborhood of (q, p) on the cross-section $\{q \in \Gamma_j^\epsilon\}$ in phase space into a small neighborhood of the point $(q + p\tau_\circ^\epsilon(q, p), p)$ on the cross-section $\{q \in \Gamma_i^\epsilon\}$, see Fig. 4. Take an inner point (q_1, p_1) on the smooth Hamiltonian trajectory of (q, p) . By construction (see (23)),

$$\begin{aligned} \tau^\epsilon(q, p) &= \tau^\epsilon(q_1, -p_1) + \tau^\epsilon(q_1, p_1), \\ (q, p) &= h_{-\tau^\epsilon(q_1, -p_1)}^\epsilon(q_1, p_1) \end{aligned}$$

and

$$F^\epsilon(q, p) = h_{\tau^\epsilon(q_1, p_1)}^\epsilon(q_1, p_1).$$

As q_1 is bounded away from the billiard boundary, we can plug (30) and (31) in these relations, which gives us the following

Lemma 2. *Let the potential $V(q; \epsilon)$ satisfy Conditions **I-IV**, and choose δ_i 's and v_i 's such that $\delta_i(\epsilon), v_i(\epsilon), m^{(r)}(\epsilon), M_i^{(r)}(\epsilon) \rightarrow 0$ as $\epsilon \rightarrow 0$. Given a $c > 0$ and sufficiently small $\epsilon \leq \epsilon_0$, consider the set of initial condition (q, p) such that $q \in \Gamma_j^\epsilon$ for some j , the segment $q + p\tau$ with $\tau \in [0, \tau_\circ^\epsilon(p, q)]$ connects Γ_j^ϵ with Γ_i^ϵ for some i and lies inside D^ϵ so that $q + p\tau_\circ^\epsilon(q, p) \in \Gamma_i^\epsilon$, $\langle p, n(q) \rangle > c$ and $\langle p, n(q + p\tau_\circ^\epsilon(q, p)) \rangle < -c$. Then, the free flight map $F^\epsilon : (q, p) \mapsto (q_{\tau^\epsilon}, p_{\tau^\epsilon})$ for the smooth Hamiltonian flow is $O_{Cr}(m^{(r)} + v_i + v_j)$ -close to the free flight map F_\circ^ϵ of the billiard in D^ϵ and is given by*

$$\begin{aligned} q_{\tau^\epsilon} &= q + p\tau^\epsilon + \int_0^{\tau^\epsilon} \nabla V(q + ps; \epsilon)(s - \tau^\epsilon)ds + O_{Cr-1}((m^{(r)} + v_i + v_j)^2), \\ p_{\tau^\epsilon} &= p - \int_0^{\tau^\epsilon} \nabla V(q + ps; \epsilon)ds + O_{Cr-1}((m^{(r)} + v_i + v_j)^2). \end{aligned} \tag{32}$$

The flight time $\tau^\epsilon(q, p)$ is $O_{Cr}(m^{(r)} + v_i + v_j)$ -close to $\tau_\circ^\epsilon(p, q)$ and is uniquely defined by the condition $Q(q_{\tau^\epsilon}; \epsilon) = Q_i + \eta_i(\epsilon)$ (cf.(31)):

$$\tau^\epsilon(q, p) = \tau_\circ^\epsilon(q, p) + \frac{\langle \nabla Q, \int_0^{\tau_\circ^\epsilon} \nabla V(q + ps; \epsilon)(\tau_\circ^\epsilon - s)ds \rangle}{\langle \nabla Q, p \rangle} + O_{Cr-1}((m^{(r)} + v_i + v_j)^2), \tag{33}$$

where ∇Q is taken at the billiard collision point $q + p\tau_\circ^\epsilon(p, q)$, where $Q_i(q + p\tau_\circ^\epsilon(p, q); \epsilon) = Q_i + \eta_i(\epsilon)$.

This could be written as

$$F^\epsilon = F_\circ^\epsilon + O_{Cr}(m^{(r)} + v_i + v_j) = F_\circ^\epsilon + F_1^\epsilon + O_{Cr-1}((m^{(r)} + v_i + v_j)^2),$$

where $F_1^\epsilon = O_{Cr}(m^{(r)} + v_i + v_j)$ and F_\circ^ϵ is defined by (24). Note that the above estimates hold true for any choice of δ_i 's such that $m^{(r)} \rightarrow 0$. Therefore, one may take δ_i 's tending to zero as slow as needed in order to ensure as good estimates as possible for the error terms in (32),(33).

Next we estimate the reflection law R^ϵ for the smooth orbit. Consider a point $q \in \Gamma_i^\epsilon$ and let the momentum p be directed outside D^ϵ (i.e. towards the boundary) at a bounded from zero angle with Γ_i^ϵ . As we explained, the smooth trajectory of (q, p) spends a small time $\tau_c^\epsilon(q, p)$ outside D^ϵ and then returns to Γ_i^ϵ with the momentum directed strictly inside D^ϵ . Let p_y and p_x denote the components of momentum, respectively, normal and tangential to the boundary Γ_i^ϵ at the point q :

$$p_y = \langle n(q), p \rangle, \quad p_x = p - p_y n(q). \tag{34}$$

We assume that the unit normal to Γ_i^ϵ at the point $q, n(q)$, is oriented inside D^ϵ , so $p_y < 0$ at the initial point. Denote by $Q_y(q; \epsilon)$ the derivative of Q in the direction of $n(q)$:

$$Q_y(q; \epsilon) := \langle \nabla Q(q; \epsilon), n(q) \rangle.$$

Recall that the surface Γ_i^ϵ is a level set of the pattern function $Q(q; \epsilon)$, and thus we may study how the normal $n(q)$ changes as one moves along the level set Γ_i^ϵ (in the tangential plane) and as one moves to nearby level sets (in the normal direction). Let $K(q; \epsilon)$ denote the derivative of $n(q)$ in the directions tangent to Γ_i^ϵ , and let $l(q; \epsilon)$ denote the derivative of $n(q)$ in the direction of $n(q)$. Obviously, Q_y is a scalar, K is a matrix, and l is a vector tangent to Γ_i^ϵ at the point q . Note that $Q_y \neq 0$ by virtue of Condition IIc. Define the integrals:

$$\begin{aligned} I_1 &= I_1(q, p) = 2 \int_0^{-p_y} Q'_i \left(\frac{1-p_x^2-s^2}{2}; \epsilon \right) ds, \\ I_2 &= I_2(q, p) = 2 \int_0^{-p_y} Q'_i \left(\frac{1-p_x^2-s^2}{2}; \epsilon \right) s^2 ds, \end{aligned} \tag{35}$$

and the vector J :

$$J(q, p) = \left[-\frac{I_2(q, p)}{p_y} l(q; \epsilon) + I_1(q, p) K(q; \epsilon) p_x \right] / Q_y(q; \epsilon). \tag{36}$$

Notice that J is a vector tangent to Γ_i^ϵ at the point q and that by (22),

$$I_{1,2} = O_{Cr}(M_i^{(r)}), \quad J = O_{Cr-1}(M_i^{(r)}). \tag{37}$$

In Appendix 7.3 we prove the following

Lemma 3. *Let the potential $V(q; \epsilon)$ satisfy Conditions I-IV, and choose δ_i 's and v_i 's such that $\delta_i(\epsilon), v_i(\epsilon), m^{(r)}(\epsilon), M_i^{(r)}(\epsilon) \rightarrow 0$ as $\epsilon \rightarrow 0$. Consider a point $q \in \Gamma_i^\epsilon$ and assume $\langle p, n(q) \rangle < -c < 0$. Then, for sufficiently small $\epsilon \leq \epsilon_0$ the collision time of the smooth Hamiltonian flow is estimated by*

$$\tau_c^\epsilon(q, p) = O_{Cr}(M_i^{(r)}) = -\frac{1}{Q_y(q; \epsilon)} I_1(q, p) + O_{Cr-1}((M_i^{(r)})^2). \tag{38}$$

The reflection map $R^\epsilon : (q, p) \mapsto (\bar{q}, \bar{p})$ is given by:

$$\begin{aligned} \bar{q} &= q + O_{Cr}(M_i^{(r)}) = q + p_x \tau_c^\epsilon(q, p) + O_{Cr-1}((M_i^{(r)})^2), \\ \bar{p} &= p - 2n(q)p_y + O_{Cr}(M_i^{(r)}) = p - 2n(q)p_y - p_y J(q, p) - n(q)\langle p_x, J(q, p) \rangle \\ &\quad + O_{Cr-1}((M_i^{(r)})^2). \end{aligned} \tag{39}$$

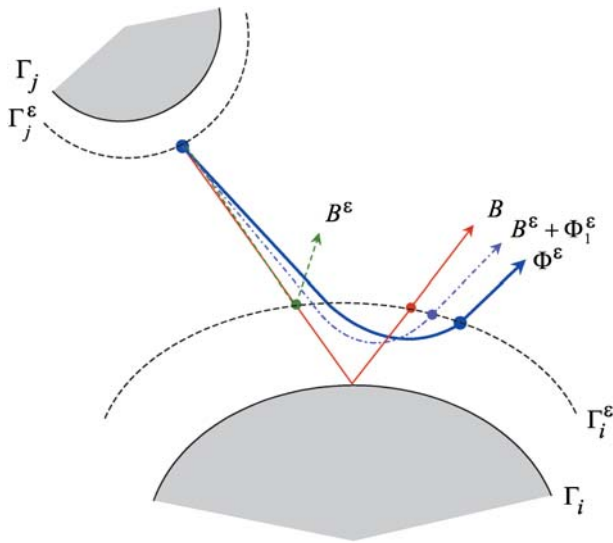


Fig. 7. Billiard map B (solid). Billiard map of the auxiliary billiard B^ϵ (dashed). Poincaré map for the smooth Hamiltonian flow Φ^ϵ (bold). The first approximation of $\Phi^\epsilon B^\epsilon + \Phi_1^\epsilon$ (dash-dotted)

As we see from this lemma (see also (37)),

$$R^\epsilon = R_\circ^\epsilon + O_{C^r}(M_i^{(r)}) = R_\circ^\epsilon + R_1^\epsilon + O_{C^{r-1}}((M_i^{(r)})^2),$$

where $R_1^\epsilon = O_{C^{r-1}}(M_i^{(r)})$ and R_\circ^ϵ is defined by (25). Thus, the smooth reflection law is $O_{C^r}(M_i^{(r)})$ -close to the billiard reflection law (25) and we have obtained explicit expression to the next order correction term. These estimates are obviously non-uniform in c - they must break when the collision is nearly tangent. Combining the above lemmas we establish:

Theorem 3. *Let the potential $V(q; \epsilon)$ satisfy Conditions **I-IV**, and choose δ_i 's and v_i 's such that $\delta_i(\epsilon), v_i(\epsilon), m^{(r)}(\epsilon), M_i^{(r)}(\epsilon) \rightarrow 0$ as $\epsilon \rightarrow 0$. Then, on the cross-section S_ϵ (see (26)) near orbits of regular reflections⁴, for all sufficiently small $\epsilon \leq \epsilon_0$ the Poincaré map Φ^ϵ of the smooth Hamiltonian flow is defined, and it is $O(m^{(r)} + v + M^{(r)})$ -close in the C^r -topology to the billiard map $B^\epsilon = R_\circ^\epsilon \circ F_\circ^\epsilon$ in the auxiliary billiard table D^ϵ (see Fig. 7). Furthermore,*

$$\begin{aligned} \Phi^\epsilon &= R^\epsilon \circ F^\epsilon = B^\epsilon + O_{C^r}(m^{(r)} + v + M^{(r)}) = (R_\circ^\epsilon + R_1^\epsilon) \circ (F_\circ^\epsilon + F_1^\epsilon) + O_{C^{r-1}}((m^{(r)} + v + M^{(r)})^2) \\ &=: B^\epsilon + \Phi_1^\epsilon + O_{C^{r-1}}((m^{(r)} + v + M^{(r)})^2) \quad (40) \end{aligned}$$

(where $v = \max_i v_i, M^{(r)} = \max_i M_i^{(r)}, \Phi_1^\epsilon = O_{C^{r-1}}(m^{(r)} + v + M^{(r)})$, and the first order corrections F_1^ϵ and R_1^ϵ are explicitly calculated in Lemmas 2 and 3).

⁴ That is, given any constant $C > 0$, near the points $(q, p) \in S_\epsilon$ such that $\langle n(q), p \rangle \geq C$ and $|\langle n(\bar{q}), \bar{p} \rangle| \geq C$ where $(\bar{q}, \bar{p}) = B^\epsilon(q, p)$.

Theorem 4. *Under the same conditions as in Theorem 3, given a finite T and a regular billiard trajectory in $[0, T]$, the time t map of the smooth Hamiltonian flow and of the corresponding auxiliary billiard are $O(v + m^{(r)} + M^{(r)})$ -close in the C^r -topology for all $t \in T \setminus T_R$, where T_R is the finite collection of impact intervals each of them of length $O(|\delta| + M^{(r)})$.*

3.3.1. Error estimates for some model potentials. Now we can estimate the deviation of the smooth Hamiltonian trajectories from the regular (non-tangent, non-corner) billiard ones for various concrete potentials $V(q; \epsilon)$. To make a general estimate possible, we assume that the behavior of the potential near the boundary dominates the estimate; we say that $V(q; \epsilon)$ is *boundary dominated*, if $V(q; \epsilon)$ and its derivatives are smaller in the interior of D_{int}^ϵ (i.e. in the region bounded by the surfaces $Q(q; \epsilon) = Q_i + \delta_i(\epsilon)$) than on the boundary of this domain. This means that for boundary dominated potentials

$$m^{(r)}(\delta; \epsilon) = \sup_{\substack{q \in D_{int}^\epsilon \\ 1 \leq l \leq r+1}} \|\partial^l V(q; \epsilon)\| = \sup_{\substack{q \in \partial D_{int}^\epsilon \\ 1 \leq l \leq r+1}} \|\partial^l V(q; \epsilon)\|. \tag{41}$$

By the definition of the pattern function Q , near a given boundary Γ_i ,

$$V(q; \epsilon) \Big|_{q \in \partial D_{int}^\epsilon} \equiv W_i(Q(q; \epsilon) - Q_i; \epsilon) \Big|_{Q=Q_i+\delta_i} = W_i(\delta_i; \epsilon).$$

Since $Q(q; \epsilon)$ is bounded with its derivatives, we conclude that there exists a constant C such that

$$m^{(r)}(\delta; \epsilon) = C \max_i \max_{1 \leq l \leq r+1} |W_i^{(l)}(\delta_i; \epsilon)|. \tag{42}$$

Thus, for boundary dominated potentials, one can estimate the differences $h_t^\epsilon - b_t$ and $\Phi^\epsilon - B^\epsilon$ in terms of the barrier functions alone.

Remark 1. The boundary dominance condition is a natural condition which is introduced as a matter of convenience. Its introduction allows to explicitly estimate the errors for general geometries with given potential growth near the boundaries, without the need of specifying the potentials in the full domain. When it is not satisfied (e.g. if in a specific application the potential becomes mildly rougher in the domain's interior as ϵ is decreased), one needs to compute $m^{(r)}(\delta; \epsilon)$ explicitly and then proceed as below.

The corresponding estimates given by Theorems 4 and 3 hold true for every choice of v and δ such that $\delta(\epsilon), v(\epsilon), m_r(\delta(\epsilon); \epsilon), M_r(v(\epsilon); \epsilon) \rightarrow 0$ as $\epsilon \rightarrow 0$ (for simplicity of notation we assume hereafter that the barrier function W is the same for all boundary surfaces Γ_i , and thus suppress the dependence on i). To obtain the best estimates, we have to find $v(\epsilon)$ and $\delta(\epsilon)$ which minimize the expression $v + M^{(r)}(v; \epsilon) + m^{(r)}(\delta; \epsilon)$. In this way, we first find $v(\epsilon)$ which minimizes $v + M^{(r)}(v; \epsilon)$. Since $M^{(r)}$ is a decreasing function of v (see (22)), the sought $v(\epsilon)$ solves the equation

$$v = M^{(r)}(v; \epsilon). \tag{43}$$

After v is determined, we may try to make $\delta(\epsilon)$ go to zero so slow that the corresponding value of $m^{(r)}$ (see (42)) will be asymptotically equal to $v(\epsilon)$. Then, this $v(\epsilon)$ (given by (43)) estimates the deviation between regular billiard and smooth trajectories.

Notice that the significance of $\nu(\epsilon)$ is three-fold. First, it determines the optimal auxiliary billiard which supplies the best approximation to the smooth Hamiltonian flow (see Lemma 3). Second, it estimates the accuracy of this approximation. Third, it determines, via the relation $m^{(r)}(\delta) = \nu$, the width $|\delta(\epsilon)| + \nu(\epsilon)$ of the boundary layer in which the billiard and the Hamiltonian flows are not close (Theorem 4). Let us proceed to examples.

Proposition 1. *Consider the boundary dominated potential $V(q; \epsilon)$ corresponding to the barrier function $W(Q) = e^{-\frac{Q}{\epsilon}}$ for small Q . Then, $\delta(\epsilon) = -(r + 1 + \frac{1}{r+2})\epsilon \ln \epsilon$ and $\nu(\epsilon), m^{(r)}(\epsilon), M^{(r)}(\epsilon) = O(\epsilon^{\frac{r+2}{\sqrt{\epsilon}}})$ supply adequate bounds for Theorem 3 to apply near regular billiard trajectories. Hence, the smooth Hamiltonian flow is $O(\epsilon^{\frac{r+2}{\sqrt{\epsilon}}})$ -close in the C^r -topology to the billiard flow within the auxiliary billiard defined by the level set $Q(q; \epsilon) = Q_i + \eta(\epsilon) = Q_i + O(\epsilon \ln \epsilon)$. The corresponding Poincaré map Φ^ϵ is $O_{C^r}(\epsilon^{\frac{r+2}{\sqrt{\epsilon}}})$ -close to the auxiliary billiard map B^ϵ . The impact intervals lengths are $O(\epsilon^{\frac{r+2}{\sqrt{\epsilon}}})$.*

Proof. Since $W^{(l)}(Q; \epsilon) = (-\epsilon)^{-l} e^{-\frac{Q}{\epsilon}}$, we obtain that $m^{(r)}(\delta; \epsilon) = O(\epsilon^{-(r+1)} e^{-\frac{\delta}{\epsilon}})$ (since the potential is boundary dominated, we may use (42)). The inverse to $W(Q; \epsilon)$ is given by $Q(W; \epsilon) = -\epsilon \ln W$, so $Q^{(l)}(W; \epsilon) = (-1)^l (l - 1)! \epsilon W^{-l}$, and $M^{(r)}(\nu, \epsilon) = O(\epsilon \nu^{-(r+1)})$ (see (22)). Plugging this in (43), we find

$$\nu(\epsilon) = \epsilon^{\frac{r+2}{\sqrt{\epsilon}}}. \tag{44}$$

By choosing $\delta(\epsilon) = -(r + 1 + \frac{1}{r+2})\epsilon \ln \epsilon$, we obtain $m^{(r)}(\delta, \epsilon) \sim \nu(\epsilon)$, so for ν given by (44) we have that $\nu + M^{(r)} + m^{(r)} = O(\nu)$, and the proposition now follows immediately from Theorems 3 and 4 (the value of $\eta(\epsilon) = O(\epsilon \ln \epsilon)$ is given by $\eta = Q(\nu; \epsilon)$). \square

Proposition 2. *Let the boundary dominated potential $V(q; \epsilon)$ correspond to the barrier function $W(Q) = e^{-\frac{Q^2}{\epsilon}}$ for small Q . Then, $\delta(\epsilon) = \sqrt{-\frac{1}{2}(r + 1 + \frac{1}{r+2})\epsilon \ln \epsilon}$ and $\nu(\epsilon), m^{(r)}(\epsilon), M^{(r)}(\epsilon) = O(\epsilon^{2(r+2)\sqrt{\frac{\epsilon}{|\ln \epsilon|}}})$ supply adequate bounds for Theorem 3 to apply near regular billiard trajectories. Hence, near the regular billiard trajectories, the smooth Hamiltonian flow is $O(\nu(\epsilon)) = O(\epsilon^{2(r+2)\sqrt{\frac{\epsilon}{|\ln \epsilon|}}})$ -close in the C^r -topology to the billiard flow within the auxiliary billiard defined by the level set $Q(q; \epsilon) = Q_i + \eta(\epsilon) = Q_i + O(\sqrt{\epsilon |\ln \epsilon|})$. The corresponding Poincaré map Φ^ϵ is $O_{C^r}(\nu(\epsilon))$ -close to the auxiliary billiard map B^ϵ . The impact intervals are of the length $O(\nu(\epsilon))$.*

Proof. It is easy to see that $W^{(l)}(Q; \epsilon) = O((\frac{Q}{\epsilon})^l e^{-\frac{Q^2}{\epsilon}})$ for $Q \gg \sqrt{\epsilon}$, hence $m^{(r)}(\delta; \epsilon) = O((\frac{\delta}{\epsilon})^{r+1} e^{-\frac{\delta^2}{\epsilon}})$. From $Q(W; \epsilon) = \sqrt{-\epsilon \ln W}$ we obtain $M^{(r)}(\nu; \epsilon) = O(\sqrt{\frac{\epsilon}{|\ln \nu|}} \nu^{-(r+1)})$. Plugging this in (43), we indeed find

$$\nu(\epsilon) = M^{(r)}(\nu; \epsilon) = O(\epsilon^{2(r+2)\sqrt{\frac{\epsilon}{|\ln \epsilon|}}}),$$

as required. By choosing $\delta(\epsilon) \sim \sqrt{-\frac{1}{2}(r + 1 + \frac{1}{r+2})\epsilon \ln \epsilon}$, we obtain $m^{(r)}(\delta; \epsilon) \sim \nu(\epsilon)$, so the rest follows directly from Theorems 3 and 4. \square

Proposition 3. *Let the boundary dominated potential $V(q; \epsilon)$ correspond to the barrier function $W(Q) = (\frac{\epsilon}{Q})^\alpha$. Then, $v(\epsilon), m^{(r)}(\epsilon), M^{(r)}(\epsilon) = O(\epsilon^{r+2+\frac{1}{\sqrt[r]{\epsilon}}})$ and $\delta(\epsilon) = v^{\frac{\alpha(r+2)+1}{r+1+\alpha}}$ supply adequate bounds for Theorem 3 to apply near regular billiard trajectories. Hence, near the regular billiard trajectories, the smooth Hamiltonian flow is $O(v(\epsilon)) = O(\epsilon^{r+2+\frac{1}{\sqrt[r]{\epsilon}}})$ -close in the C^r -topology to the billiard flow within the auxiliary billiard defined by the level set $Q(q; \epsilon) = Q_i + \eta(\epsilon) = Q_i + O(v^{r+2})$. The corresponding Poincaré map Φ^ϵ is $O_{C^r}(v(\epsilon))$ -close to the auxiliary billiard map B^ϵ . The impact intervals are $O(v(\epsilon))$ when $\alpha \geq 1$, and $O(v(\epsilon)^{\frac{\alpha(r+2)}{\alpha+r+1}})$ when $\alpha \leq 1$.*

Proof. As above, using $W^{(l)}(Q; \epsilon) = O(\frac{\epsilon^\alpha}{Q^{l+\alpha}})$ we obtain that $m^{(r)}(\delta; \epsilon) = O(\frac{\epsilon^\alpha}{\delta^{r+1+\alpha}})$, and since $Q(W; \epsilon) = \frac{\epsilon}{W^{1/\alpha}}$, we find $Q^{(l)}(W; \epsilon) = O(\frac{\epsilon}{W^{l+1/\alpha}})$ and thus $M^{(r)}(v; \epsilon) = O(\frac{\epsilon}{v^{r+1+1/\alpha}})$. It follows that $v(\epsilon) = O(\epsilon^{r+2+\frac{1}{\sqrt[r]{\epsilon}}})$ solves $v = M^{(r)}(v; \epsilon)$. Now $\eta(\epsilon) = Q(v) = \frac{\epsilon}{v^{1/\alpha}} = O(v^{r+2})$. By taking $\delta(\epsilon) = v^{\frac{\alpha(r+2)}{r+1+\alpha}}$, we ensure that $m^{(r)}(\delta, \epsilon) \sim v(\epsilon)$. The length of the impact intervals is now given by $O(v + \delta)$. \square

These three propositions are summarized by the following table (see the next section for the interpretation of the last column):

Table 3.3.1.

Potential	Boundary layer width	Approximation error	Length of impact intervals	Transverse homoclinics
$W(Q; \epsilon)$	$\eta(\epsilon)$	$m^{(r)} + v + M^{(r)}$	$T_R = O(\delta + M^{(r)})$	$\epsilon_\gamma(\gamma)$
$e^{-\frac{Q}{\epsilon}}$	$O(\epsilon \ln \epsilon)$	$O(\epsilon^{r+2\sqrt[r]{\epsilon}})$	$O(\epsilon^{r+2\sqrt[r]{\epsilon}})$	$\gamma^{3+\varkappa}, \varkappa > 0$
$e^{-\frac{Q^2}{\epsilon}}$	$O(\sqrt{\epsilon} \ln \epsilon)$	$O(\epsilon^{2(r+2)\sqrt[r]{\frac{\epsilon}{ \ln \epsilon }}})$	$O(\epsilon^{2(r+2)\sqrt[r]{\frac{\epsilon}{ \ln \epsilon }}})$	$\gamma^{6+\varkappa}, \varkappa > 0$
$(\frac{\epsilon}{Q})^\alpha$	$\epsilon^{\frac{r+2}{r+2+1/\alpha}}$	$O(\epsilon^{r+2+\frac{1}{\sqrt[r]{\epsilon}}})$	$O(\epsilon^{r+2+\frac{1}{\sqrt[r]{\epsilon}}})$ $\alpha \geq 1$ $\frac{\alpha(r+2)}{\epsilon^{(r+1+\alpha)(r+2+\frac{1}{\alpha})}}$ $\alpha \leq 1$	$\gamma^{3+\frac{1}{\alpha}+\varkappa}, \varkappa > 0$

Note that the asymptotic for the deviation of the smooth trajectories from the billiard ones and for the length of the impact intervals depend strongly on r , i.e. on the number of derivatives (with respect to initial conditions) which we want to control.

3.4. Persistence of periodic and homoclinic orbits. The closeness of the billiard and smooth flows after one reflection leads, using standard results, to persistence of regular periodic and homoclinic orbits. For completeness we state these results explicitly:

Theorem 5. *Consider a Hamiltonian system with a potential $V(q, \epsilon)$ satisfying Conditions I-IV in a billiard table D . Let $P^b(t)$ denote a non-parabolic, non-singular periodic orbit of a period T for the billiard flow. Then, for any choice of $v(\epsilon), \delta(\epsilon)$ such that $v(\epsilon), \delta(\epsilon), m^{(1)}(\epsilon), M^{(1)}(\epsilon) \rightarrow 0$ as $\epsilon \rightarrow 0$, for sufficiently small ϵ , the smooth Hamiltonian flow has a uniquely defined periodic orbit $P^\epsilon(t)$ of period $T^\epsilon = T + O(v + m^{(1)} + M^{(1)})$, which stays $O(v + m^{(1)} + M^{(1)})$ -close to P^b for all t outside of collision intervals (finitely many of them in a period) of length $O(|\delta| + M^{(1)})$. Away from the collision intervals, the local Poincaré map near P^ϵ is $O_{C^r}(v + m^{(r)} + M^{(r)})$ -close to the local*

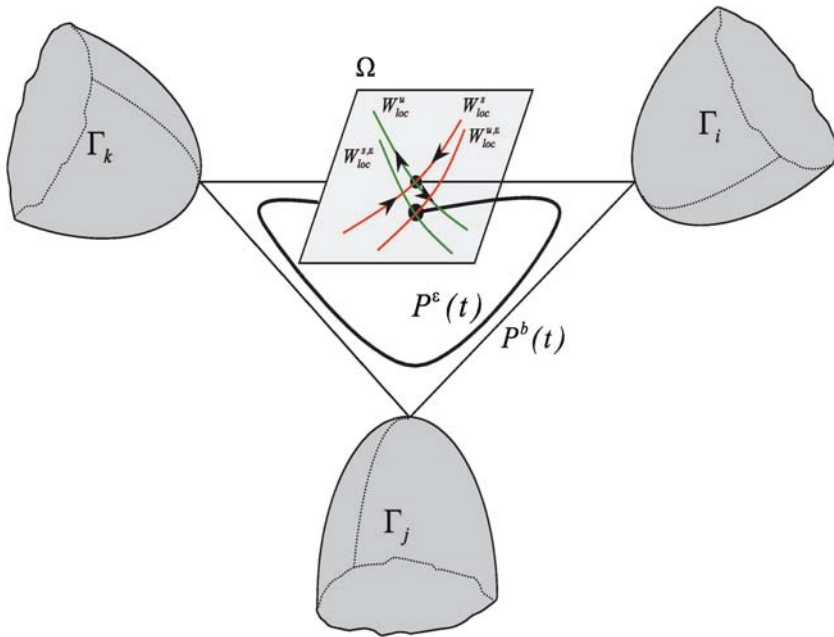


Fig. 8. P^b is a billiard periodic orbit (solid). P^ϵ is a periodic orbit of the smooth Hamiltonian flow (bold)

Poincaré map near P^b . In particular, if P^b is hyperbolic, then P^ϵ is also hyperbolic and, inside D^ϵ , the stable and unstable manifolds of P^ϵ approximate $O_{cr}(\nu + m^{(r)} + M^{(r)})$ -closely the stable and unstable manifolds of P^b on any compact, forward-invariant or, respectively, backward-invariant piece bounded away from the singularity set in the billiard’s phase space; furthermore, any transverse regular homoclinic orbit to P^b is, for sufficiently small ϵ , inherited by P^ϵ as well.

Proof. As P^b is a regular periodic orbit, i.e. it makes only regular reflections from the boundary (a finite number of them on the period), it follows from Theorem 3 that a Poincaré map for the smooth Hamiltonian flow near P^b is $O(\nu + m^{(1)} + M^{(1)})$ -close in C^1 topology to the Poincaré map of the auxiliary billiard D^ϵ , while the latter is $O(\eta(\epsilon))$ -close to the Poincaré map for the original billiard D . Moreover, from (22) it follows that $\eta(\epsilon) \leq M^{(0)} \leq M^{(1)}$ and we can conclude that a Poincaré map for the smooth Hamiltonian flow near P^b is $O(\nu + m^{(1)} + M^{(1)})$ -close in C^1 topology to the Poincaré map for the original billiard D . Since, by assumption, $P^b(t)$ is non-parabolic, the corresponding fixed point of the Poincaré map persists for sufficiently small ϵ by virtue of the implicit function theorem (the closeness of the corresponding continuous-time orbits is given by Theorem 4). The continuous dependence of the invariant manifolds on ϵ in the hyperbolic case follows from the continuous dependence of the Poincaré map Φ^ϵ on ϵ at all $\epsilon \geq 0$ (Theorem 3), and implies the persistence of transverse homoclinics immediately. Indeed, the formulation regarding the closeness of compact pieces of the *global* stable and unstable manifolds may be easily verified by applying finite time extensions of the local stable and unstable manifolds. Note that a similar persistence result holds true for topologically transverse homoclinic orbits. \square

More generally, one may claim (by the shadowing lemma) the persistence of compact uniformly hyperbolic sets composed of regular billiard orbits. Note that the accuracy of the approximation of smooth orbits (periodic and aperiodic) by the billiard ones, does not depend on the orbit (e.g. is independent of its period) and is given by the maximal deviation for each reflection (times a constant). This holds true for any compact set of regular orbits of a strictly dispersing billiard flow (since such billiards are uniformly hyperbolic); see for example a nice application by Chen [12]. In some cases, to establish the existence of transverse or topologically transverse homoclinic orbits in a family of billiard flows $b_r(\gamma)$ in D_γ , one uses higher dimensional generalizations of the Poincaré-Melnikov integral (see Sect. 4). In particular, with the near integrable setting, the “splitting distance” between the manifolds near the transverse homoclinic orbit may be proportional to an unfolding parameter γ . The above theorem implies that if $\epsilon_g = \epsilon_g(\gamma)$ is chosen so that $\nu(\epsilon_g, \gamma) + m^{(1)}(\delta(\epsilon_g, \gamma); \epsilon_g, \gamma) + M^{(1)}(\nu(\epsilon_g, \gamma); \epsilon_g, \gamma) = o(\gamma)$ and $\epsilon_g(\gamma) \rightarrow 0$ as $\gamma \rightarrow 0$ then, for sufficiently small γ , transverse homoclinic orbits appear in the smooth flow for all $\epsilon \in (0, \epsilon_g(\gamma))$. The value of $\epsilon_g(\gamma)$ for the three types of potentials considered here are listed in the last column of Table 3.3.1. In the next section we use this remark and [14] to establish that transverse homoclinic orbits appear in families of smooth billiard potentials that limit to the ellipsoidal billiard.

4. Application to Ellipsoidal Billiards with Potential

Consider the billiard motion in an ellipsoid

$$D = \{q \in \mathbb{R}^n : \langle q, A^{-2}q \rangle \leq 1\}, \quad (45)$$

$$A = \text{diag}(d_1, \dots, d_n) \quad d_1 \geq \dots \geq d_n \geq 0.$$

The ellipsoid is called *generic* if all the above inequalities are strict. A well known result of Birkhoff [5] is that the billiard motion in an ellipsoid is integrable, and the mathematical theory which may be invoked to describe and generalize this result is still under development - see [20] and references therein. Delshams *et al* [14] and recently Bolotin *et al* [6] (see also references therein) investigate when small non-quadratic symmetric perturbations to the ellipsoidal shape change the integrability property. In this series of works the authors prove the persistence of some symmetric homoclinic orbits, and for specific cases they prove that these orbits are transverse homoclinic orbits of the perturbed billiard, thus proving that integrability is destroyed. Here, we show that using the machinery we developed we can immediately extend their work to the smooth billiard-potential case (notice that in [6] some results are extended to billiards with a C^2 -small Hamiltonian perturbation in the domain's interior, however the billiard potentials which we consider do not fall into this category - near the boundary they correspond to a large perturbation even in the C^1 -norm). We will first explain the relevant main results of Delshams *et al*, then supply the corresponding proposition for the smooth case (consequences of Theorem 2, or more specifically of Theorem 5) and then the corresponding quantitative estimates for specific potentials (which follows from Propositions 1-3 and are summarized in Table 3.3.1).

4.1. The billiard in a perturbed ellipsoid. Consider the simplest unstable periodic orbit in an ellipsoidal billiard - the orbit along the diameter of the ellipsoid joining the vertices $(-d_1, 0, \dots, 0)$ and $(d_1, 0, \dots, 0)$. Denote the set formed by the two-periodic points

associated with the diameter by

$$P^b = \{\rho_+, \rho_-\} \quad \rho_\pm = \{q_\pm, p_\mp\} \quad q_\pm = (\pm d_1, 0, \dots, 0) \quad p_\pm = (\pm 1, 0, \dots, 0). \quad (46)$$

These points correspond to isolated two-periodic hyperbolic orbits of the Billiard map B and the corresponding periodic orbit $P_t^b = b_t(\rho_+)$ of the billiard flow. The $(n - 1)$ -dimensional (n -dimensional for the flow) stable and unstable manifolds of this periodic orbit coincide; in 2-dimensions there are 4 separatrices connecting $\{\rho_+, \rho_-\}$ whereas the topology of the separatrices in the higher dimensional case is non-trivial - it is well described by CW complexes for the 3 dimensional case and by hierarchal structure of separatrix submanifolds in the higher dimensional case (see [14]). Of specific interest are the symmetric homoclinic orbits - it is established in [14] that in the generic 2 dimensional case there are exactly 4 homoclinic orbits which are x -symmetric (symmetric, in the configuration space, to reflections about the x -axis) and 4 which are y -symmetric. In the generic 3 dimensional case, in addition to the 16 planar symmetric orbits (8 in each of the symmetry planes- xy and xz) there are 16 additional symmetric spatial orbits - 8 are symmetric with respect to reflection about the xz plane and 8 are y axial. In the n dimensional case there are 2^{n+1} spatial symmetric orbits. Denote by $P^{b\text{-hom}} = \left\{ P_i^{b\text{-hom}} \right\}_{i=-\infty}^{\infty}$ one of these symmetric homoclinic orbits of the billiard map in the ellipsoid, so $P_{i+1}^{b\text{-hom}} = B P_i^{b\text{-hom}}$ and $P_i^{b\text{-hom}} = b_t(P_0^{b\text{-hom}})$ denotes the corresponding continuous orbit of the billiard flow. Given a ζ such that $0 < \zeta \ll d_n$, define the local cross-sections of the billiard map by:

$$\begin{aligned} \Sigma^- &= \{(q, p) | q \in \partial D, q_1 + d_1 < \zeta, 1 - p_1 < \zeta\}, \\ \Sigma^+ &= \{(q, p) | q \in \partial D, d_1 - q_1 < \zeta, p_1 + 1 < \zeta\}, \end{aligned}$$

so, in particular, $\rho_\pm \in \Sigma^\pm$ and $\Sigma^\pm \subset S$, where S is the natural cross-section on which the billiard map is defined (see Sect. 2.2). It follows that only a finite number of points in $P^{b\text{-hom}}$ do not fall into Σ^\pm , and that for any given geometry there exist a finite ζ such that $P^{b\text{-hom}} \setminus \{P^{b\text{-hom}} \cap \Sigma^\pm\} \neq \emptyset$ for all the symmetric orbits. See Fig. 9. Thus, it is possible to choose $P_0^{b\text{-hom}}$ and a local cross-section Σ^0 such that $P_0^{b\text{-hom}} \in \Sigma^0 \subset \{S \setminus \{\Sigma^+ \cup \Sigma^-\}\}$. Notice that for the ellipsoid all the reflections are regular, and furthermore, for the symmetric homoclinic orbits, if d_1 is finite and d_n is positive then all the reflection angles of $P^{b\text{-hom}}$ are strictly bounded away from $\pi/2$.

Now, consider a **symmetric** perturbation of the ellipsoid Q of the form:

$$D_\gamma = \{q \in \mathbb{R}^n : \langle q, A^{-2}q \rangle \leq 1 + \gamma \Xi\left(\frac{q_1^2}{d_1^2}, \dots, \frac{q_n^2}{d_n^2}\right)\}, \quad (47)$$

where the hypersurface $D_\gamma \subset \mathbb{R}^n$ is symmetric with regard to all the coordinate axis of \mathbb{R}^n and the function $\Xi : \mathbb{R}^n \rightarrow \mathbb{R}$ is either a general *entire* function, such that $\Xi(0, \dots, 0) = 0$ or of a specific form (e.g. quadratic). By using symmetry arguments, Delshams *et al* [14] prove that for a generic billiard the above mentioned symmetric homoclinic orbits persist under such symmetric perturbations. Furthermore, analyzing the asymptotic properties of the symplectic discrete version of the Poincaré-Melnikov potential (the high-dimensional analog [14, 16] of the planar Poincaré-Melnikov integral [21, 15]), they prove that for sufficiently small perturbations (small γ) the n -dimensional symmetric homoclinic orbits are transverse in the following four cases:

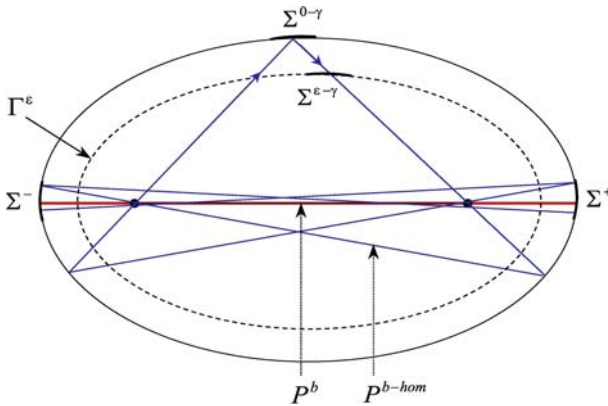


Fig. 9. Billiard trajectory giving rise to a y-symmetric homoclinic orbit (solid)

1. In two-dimensions, for narrow ellipses ($\beta_1 = \frac{d_2^2}{d_1^2} \ll 1$), for any analytic small enough symmetric perturbation.
2. In two-dimensions, in the non-circular case ($\beta_1 \neq 1$), for $\Xi(\frac{x^2}{d_1^2}, \frac{y^2}{d_2^2}) = \frac{y^4}{d_2^4}$.
3. In the three-dimensional case, for nearly flat ellipses ($\beta_2 = \frac{d_3^2}{d_1^2} \ll 1$), for perturbations of the form: $\Xi(\frac{x^2}{d_1^2}, \frac{y^2}{d_2^2}, \frac{z^2}{d_3^2}) = \frac{z^2}{d_3^2} R(\frac{y^2}{d_2^2}, \frac{z^2}{d_3^2})$, where R is a generic polynomial (or of some specific list).
4. In the three-dimensional case, for nearly oblate ellipses ($\beta_1 = \frac{d_2^2}{d_1^2} \simeq 1$), for the perturbation $\Xi(\frac{x^2}{d_1^2}, \frac{y^2}{d_2^2}, \frac{z^2}{d_3^2}) = \frac{z^2}{d_3^2} \frac{y^2}{d_2^2}$.

To establish these results, the Poincaré-Melnikov potential is calculated for each of these cases, and it is shown that it has non-degenerate critical points at the corresponding symmetric trajectories. It follows that $P^{b-hom-\gamma}$ persists and the change in the splitting distance between the separatrices \mathcal{W}^u and \mathcal{W}^s near $P_0^{b-hom-\gamma}$ is proportional to γ , the perturbation amplitude, so that near $P_0^{b-hom-\gamma}$ at the local cross-section $\Sigma^{0-\gamma}$,

$$d(W_\gamma^s, W_\gamma^u) = M(\tau)\gamma + O(\gamma^2), \tag{48}$$

where $\tau \in R^{n-1}$ denotes some parametrization along \mathcal{W} and $M(\tau)$ (the gradient of the Poincaré-Melnikov potential) has simple zeroes at the parameter values corresponding to any of the spatial symmetric homoclinic orbits P_0^{b-hom} .

4.2. *Smooth potential in a near ellipsoidal region.* Let us now consider a two parameter family of smooth potentials $V(q; \gamma, \epsilon)$ which limit, as $\epsilon \rightarrow 0$ to the billiard flow in the perturbed ellipsoid family D_γ ; namely, consider the family of Hamiltonian flows:

$$H(\epsilon, \gamma) = \frac{p^2}{2} + V(q; \gamma, \epsilon), \tag{49}$$

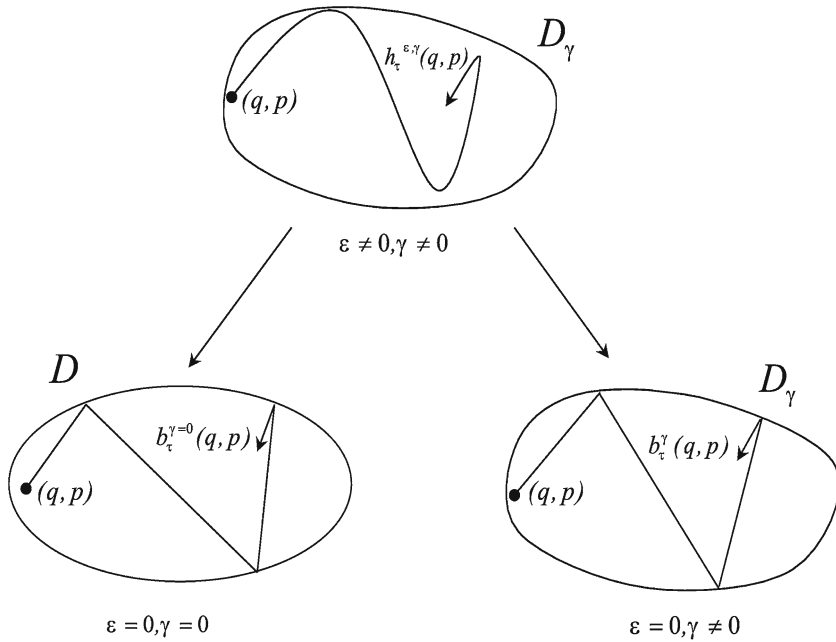


Fig. 10. Perturbation of a billiard flow inside a perturbed ellipsoid family D_γ

where $V(q; \gamma, \epsilon)$ satisfies conditions I-IV for all γ values. In the four cases mentioned above, the flow limits, as $\epsilon \rightarrow 0$, to an integrable billiard motion inside the ellipsoid D when $\gamma = 0$ and, for $\gamma \neq 0$, to a non-integrable billiard motion inside the perturbed ellipsoid D_γ . See Fig. 10. Applying Theorem 5 to an interior transverse local return map near $\Sigma^{0-\gamma}$, and noticing that all homoclinic orbits of the billiard flow in D_γ are regular orbits, we immediately establish:

Proposition 4. Consider the Hamiltonian flow (49), where $V(q; \gamma, \epsilon)$ is a billiard potential limiting to the billiard flow in D_γ ($V(q; \gamma, \epsilon)$ satisfies Conditions I-IV for all $\epsilon \in (0, \epsilon_0]$ for all γ values). Let the function $\epsilon_g(\gamma)$ satisfy

$$v(\epsilon_g, \gamma) + m^{(1)}(\delta(\epsilon_g, \gamma); \epsilon_g, \gamma) + M^{(1)}(v(\epsilon_g, \gamma); \epsilon_g, \gamma) = o(\gamma)$$

and $\epsilon_g(\gamma) \rightarrow 0$ as $\gamma \rightarrow 0$. Then, for each of the above cases 1-4, for sufficiently small $\gamma > 0$, the smooth flow has transverse homoclinic orbits which limit the billiard's transverse homoclinic orbits for all $0 < \epsilon < \epsilon_g(\gamma)$.

Indeed, for sufficiently small $\gamma > 0$, $\epsilon_g(\gamma) < \epsilon_0$ and Eq. (48) is valid, and thus the homoclinic billiard orbit $P^{b-\text{hom}-\gamma}$ is transverse, so the above theorem follows immediately from Theorem 5 and the discussion after it. Based on this proposition and Propositions 1-3 we conclude (see Table 3.3.1):

Proposition 5. Consider the Hamiltonian flow (49), where $V(q; \gamma, \epsilon)$ is a billiard potential limiting the billiard flow in D_γ ($V(q; \gamma, \epsilon)$ satisfies Conditions I-IV for all $\epsilon \in (0, \epsilon_0]$ for all γ values). Further assume that the potential $V(q; \gamma, \epsilon)$ is boundary dominated and is given near the boundary of D_γ by $W(Q; \epsilon)$, so that (41) holds for the corresponding δ values which are specified below. Then, for each of the above cases 1-4, for

sufficiently small $\gamma > 0$, the smooth flow has transverse homoclinic orbits which limit the billiard's transverse homoclinic orbits and thus is non-integrable for all $0 < \epsilon < \epsilon_g(\gamma)$, where

- For $W(Q; \epsilon) = e^{-\frac{Q}{\epsilon}}$: $\delta = O(-\epsilon \ln \epsilon)$ and $\epsilon_g(\gamma) = \gamma^{3+\varkappa}$, $\varkappa > 0$.
- For $W(Q; \epsilon) = e^{-\frac{Q^2}{\epsilon}}$: $\delta = O(\sqrt{-\epsilon \ln \epsilon})$ and $\epsilon_g(\gamma) = \gamma^{6+\varkappa}$, $\varkappa > 0$.
- For $W(Q; \epsilon) = (\frac{\epsilon}{Q})^\alpha$: $\delta = O(\sqrt[3+\frac{1}{\alpha}]{\epsilon})$ and $\epsilon_g(\gamma) = \gamma^{3+\frac{1}{\alpha}+\varkappa}$, $\varkappa > 0$.

The existence of transverse homoclinic orbits implies non-integrability; there are regions which are mapped onto themselves in the shape of a horseshoe, and thus there are invariant sets on which the motion is chaotic (conjugate to a Bernoulli shift). In particular, it is thus established that the topological entropy of the flow is positive. Whether the metric entropy is positive is, as usual in these near-integrable settings, unknown (see for example [21]).

5. Discussion

The paper includes three main results:

- Theorems 1-2 deal with the smooth convergence of flows in steep potentials to the billiard's flow in the multi-dimensional case. These results, which are a natural extension of [56], provide a powerful theoretical tool for proving the persistence of various billiard trajectories in the smooth systems, and vice versa. Several issues are yet to be addressed in this higher dimensional setting. First, the study of corners and regular tangencies (extending [43, 57] to higher dimensions) is yet to be developed. Second, for geometries which are not strictly dispersing, the unavoidable emergence of degenerate tangencies, which is inherently a higher dimensional phenomena, is yet to be addressed.
- Theorems 3-4 provide the first order corrections for approximating the smooth flows by billiards for regular reflections. Theorem 3 proposes the appropriate zeroth order billiard geometry which best approximates the steep billiard and a simple formula for computing the first order correction terms, thus allowing to study the effect of smoothing. The smooth flow and the billiard flow do not match in a boundary layer - the width of it and the time spent in it are specified in Theorem 4. Propositions 1-3, as summarized in Table 3.3.1, supply the estimates for the boundary layer width and the accuracy of the auxiliary billiard approximation for some typical potentials (exponential, Gaussian and power-law). All these results are novel for any dimension, and propose a new approach for studying problems with relatively steep potentials. A plethora of questions regarding the differences between the smooth and hard wall systems can now be rigorously analyzed.
- Theorem 5 and Proposition 5 are two examples for applications of the above results. The C^1 estimates of the error terms lead naturally to the persistence Theorem 5. Applying these results to the billiards studied in [14], we prove that the motion in steep potentials in various deformed ellipsoids is non-integrable for an open interval of the steepness parameter, and we provide a lower bound for this interval length for the above mentioned typical potentials. While the analysis of higher dimensional Hamiltonian systems is highly non-trivial, we demonstrate here that some results which are obtained for maps may be immediately extended to the smooth steep case. We note that the same statement works in the opposite direction. Furthermore, one

may use the first order corrections developed in Theorem 3 and Propositions 1-3 to study the possible appearance of non-integrability due to the introduction of smooth potentials.

These results may give the impression that the smooth flow and the billiard flow are very similar. While in this work we emphasize the closeness of the two flows, it is important to bear in mind that this is not the case in general. This observation applies to the local behavior near solutions which are not structurally stable and is especially important when dealing with asymptotic properties such as ergodicity, as discussed below.

Let us first remark about the local behavior. As in the two-dimensional settings, we expect that singular orbits of the billiard give rise to various types of orbits in the smooth setting. The larger the dimension of the system, the larger is the variety of orbits which may emerge from these singularities. Moreover, in this higher dimensional setting, even though our theory implies that regular elliptic or partially-elliptic (non-parabolic) periodic orbits persist, the motion near them (and their stability) may change due to resonances.

Global properties of the phase space are even more sensitive to small changes. If the billiard periodic orbit is hyperbolic, while it and its local stable and unstable manifolds persist (see for example Theorem 5), their global structure in the smooth case may be quite different; first of all, integrability of one of the systems does not imply integrability of the other (for example, it may be possible to use the correction terms computed in Sect. 3.3 to establish that the smooth flow has separatrix splitting even when the billiard is integrable). Second, if the billiard flow has singularities, the global manifolds of a hyperbolic billiard orbit may have discontinuities and singularities whereas the global manifolds of the smooth orbit are smooth (see for example [56]).

Finally, the most celebrated global property one is interested in is ergodicity and mixing. In [18] it was shown that when two particles with a finite range potential move on a two-dimensional torus a stable periodic orbit may emerge. In [43, 56, 57] we proved that in the two-dimensional case (C^r -smooth potentials, not necessarily finite range, not necessarily symmetric), near singular trajectories (tangent trajectories or corner trajectories) islands of stability are born in the smooth flow for *arbitrarily steep* potentials. Furthermore, the scaling of the island's size with the steepness parameter for the general two-dimensional setting was found analytically. Thus there is a fundamental difference in the ergodic properties of hard-wall potentials as compared to smooth potentials. Although these results only apply to two-particle systems, they raise the possibility that systems with large numbers of particles interacting by smooth potentials could also be non-ergodic. Recently, we provided numerical evidence for the appearance of islands of effective stability for arbitrary steep potentials which are close to particular *strictly dispersing* billiards (*not* the N -particle case) in three dimensions [41] and in n dimensions [42]. The tools developed here may be essential for studying these and other prototype examples theoretically. In particular, one would hope that beyond an existence proof, these tools may assist in finding the scaling of the islands with the dimension n .

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7. Appendix

7.1. Picard iteration for equations with small right-hand side. Before we proceed to the proof of Lemmas 1 and 3, we recall the main tool of their proofs - the Picard iteration

scheme for equations with small right-hand side (see e.g. [23] and [44]). Consider the differential equation

$$\dot{v} = \psi(v, \mu, t, \epsilon), \tag{50}$$

where ψ is a C^r -smooth function of v and μ , continuous with respect to t and ϵ . Assume that for $t \in [0, L(\epsilon)]$ and bounded (v, μ) we have a function $J(\epsilon)$ such that $J(\epsilon)L(\epsilon) \rightarrow 0$ and

$$\|\psi\|_{C^r} \leq J(\epsilon). \tag{51}$$

Then, according to the contraction mapping principle, the Picard iterations v_n where

$$v_{n+1}(t) = v_0 + \int_0^t \psi(v_n(s), \mu, s, \epsilon) ds \tag{52}$$

converge to the solution of (50) starting at $t = 0$ with initial condition $v(0) = v_0$ on the interval $t \in [0, L(\epsilon)]$, in the C^r -norm as a function of v_0 and μ :

$$v_n(t; v_0, \mu) \rightarrow_{C^r} v(t; v_0, \mu) = v_0 + \int_0^t \psi(v(s; v_0, \mu), \mu, s, \epsilon) ds.$$

One can show by induction that $\|v_n(t) - v_0\|_{C^r} = O(L(\epsilon)J(\epsilon))$ uniformly for all n . Then it follows that

$$v(t; v_0, \mu) = v_0 + O_{C^r}(L(\epsilon)J(\epsilon)). \tag{53}$$

Furthermore, we now show that

$$v(t; v_0, \mu) = v_n(t; v_0, \mu) + O_{C^{r-1}}((L(\epsilon)J(\epsilon))^{n+1}) \tag{54}$$

(such kind of estimates are, in fact, a standard tool in the averaging theory). In order to prove (54), we will use induction in n . At $n = 0$ we have an even better result than (54) (see (53)). Now note that

$$\begin{aligned} v(t) - v_{n+1}(t) &= \int_0^t (\psi(v(s), \mu, s, \epsilon) - \psi(v_n(s), \mu, s, \epsilon)) ds \\ &= \int_0^t \left(\int_0^1 \psi'_v(v_n(s) + z(v(s) - v_n(s)), \mu, s, \epsilon) dz \right) \cdot (v(s) - v_n(s)) ds. \end{aligned}$$

It follows immediately that

$$\|v - v_{n+1}\|_{C^{r-1}} = O(L(\epsilon)\|\psi'_v\|_{C^{r-1}}) \cdot O(\|v - v_n\|_{C^{r-1}}) = O(L(\epsilon)J(\epsilon)) \cdot \|v - v_n\|_{C^{r-1}},$$

and (54) indeed holds true by induction.

7.2. *Proof of Lemma 1.* The “free flight” (the motion inside D^ϵ) is composed of motion in D_{int}^ϵ and the motion in the layer $N_< = D^\epsilon \setminus D_{int}^\epsilon$. We show that in each of these regions the equations may be brought to the form (50), (51). We will first consider the flight inside D_{int}^ϵ . Recall that the equations of motion for the smooth orbit are

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -\nabla V(q; \epsilon). \end{aligned} \tag{55}$$

Let us make the following change of coordinates

$$\tilde{q}(t) := q(t) - p(t)t. \tag{56}$$

Then (55) takes the form

$$\begin{aligned} \dot{\tilde{q}} &= \nabla V(\tilde{q} + pt; \epsilon)t, \\ \dot{p} &= -\nabla V(\tilde{q} + pt; \epsilon), \end{aligned} \tag{57}$$

with initial data $(\tilde{q}(0), p(0)) = (q_0, p_0)$. Since the time spent in D_{int}^ϵ must be finite as it is C^r -close to the billiard’s travel time in D_{int}^ϵ which is finite here, and using (28), we have

$$\|\psi\|_{C^r} = \left\| \begin{pmatrix} \nabla V(\tilde{q} + pt; \epsilon)t \\ -\nabla V(\tilde{q} + pt; \epsilon) \end{pmatrix} \right\|_{C^r} = O(m^{(r)}(\delta(\epsilon); \epsilon)).$$

Thus, system (57) does satisfy (51) with $L = O(1)$, $J = O(m^{(r)})$. It follows then from (53) that

$$p(t) = p_0 + O_{C^r}(m^{(r)}). \tag{58}$$

Furthermore, by applying one Picard iteration (52), we obtain from (54) the following estimate for $p(t)$:

$$p(t) = p_0 - \int_0^t \nabla V(q_0 + p_0s; \epsilon)ds + O_{C^{r-1}}((m^{(r)})^2). \tag{59}$$

By integrating the equation $\dot{q} = p$, we also obtain from (58) that

$$q(t) = q_0 + p_0t + O_{C^r}(m^{(r)}). \tag{60}$$

Next, we show that the equations in the layer $N_< = \{W : W(Q; \epsilon) \leq \nu\}$ can be brought to the form (50), (51) as well. Recall (see the proof of Theorem 2 in the supplement [42]) that $\dot{Q} = \langle \nabla Q, p \rangle$ is bounded away from zero in $N_<$, hence Q can be taken as a new independent variable (it changes in the interval $\eta \leq Q - Q_i \leq \delta$). Now the time t is considered as a function of Q and of the initial conditions $(q(t_\delta), p(t_\delta))$ (where t_δ is the moment the trajectory enters $N_<$). We show in the proof of Theorem 2 that t is a smooth function of the initial conditions, with all the derivatives bounded. So, in $N_<$, we rewrite (57) as

$$\begin{aligned} \frac{d\tilde{q}}{dQ} &= W'(Q; \epsilon) \frac{\nabla Q(\tilde{q} + pt; \epsilon)}{\langle \nabla Q(\tilde{q} + pt; \epsilon), p \rangle} t, \\ \frac{dp}{dQ} &= -W'(Q; \epsilon) \frac{\nabla Q(\tilde{q} + pt; \epsilon)}{\langle \nabla Q(\tilde{q} + pt; \epsilon), p \rangle}. \end{aligned}$$

As W is a monotone function of Q in this layer (i.e. $W'(Q; \epsilon) \neq 0$), we can take W as a new independent variable, so the equations of motion take the form

$$\begin{aligned} \frac{d\tilde{q}}{dW} &= \frac{\nabla Q(\tilde{q}+pt; \epsilon)}{\langle \nabla Q(\tilde{q}+pt; \epsilon), p \rangle} t, \\ \frac{dp}{dW} &= -\frac{\nabla Q(\tilde{q}+pt; \epsilon)}{\langle \nabla Q(\tilde{q}+pt; \epsilon), p \rangle}. \end{aligned} \tag{61}$$

Since all the derivatives of t with respect to the initial conditions are bounded, we may consider (61) as the system of type (50), (51) with $J = O(1)$, and $L = O(v)$ (recall that the value of W changes monotonically from $W_0 = W(\delta, \epsilon)$ to v). Thus, by applying one Picard iteration (52), we obtain from (54) that

$$p(W) = p(W_0) - \int_{W(\delta, \epsilon)}^W \frac{\nabla Q(q(\tilde{W}_0) + p(W_0)t; \epsilon)}{\langle \nabla Q(\tilde{q}(W_0) + p(W_0)t; \epsilon), p(W_0) \rangle} dW + O_{cr-1}(v^2).$$

From (53) we also obtain

$$p(W) = p(W_0) + O_{cr}(v).$$

Note that $O_{cr-1}(v^2)$ and $O_{cr}(v)$ refer here to the derivatives (with respect to the initial conditions) of p at constant W or, equivalently, at constant Q . Returning to the original time variable, these equations yield

$$p(t) = p(t_\delta) + O_{cr}(v) = p(t_\delta) - \int_{t_\delta}^t \nabla V(q(t_\delta) + p(t_\delta)(s - t_\delta); \epsilon) ds + O_{cr-1}(v^2).$$

Using expressions (58),(59) for $p(t_\delta)$ and (60) and $q(t_\delta)$, we finally obtain

$$p(t) = p_0 + O_{cr}(v + m^{(r)}) = p_0 - \int_0^t \nabla V(q_0 + p_0s; \epsilon) ds + O_{cr-1}((m^{(r)} + v)^2) \tag{62}$$

for all t such that $q(t) \in D^\epsilon$, in complete agreement with the claim of the lemma (as we mentioned, the $O_{cr-1}(\cdot)$ and $O_{cr}(\cdot)$ terms refer to the derivatives at constant Q). The corresponding expression for $q(t)$ (see (30)) is obtained by integrating the equation $\dot{q} = p$. The expression (31) for the flight time τ is immediately found from the relation $W(Q(q(\tau); \epsilon); \epsilon) = v$ or, equivalently, $Q(q(t); \epsilon) = Q_i + \eta$ (recall that \dot{Q} is bounded away from zero in the layer $N_<$).

7.3. Proof of Lemma 3. Here we compute the reflection map $R^\epsilon: (q_{in}, p_{in}) \mapsto (q_{out}, p_{out})$ defined by the smooth trajectories within the most inner layer $N_> : \{W \geq v\}$. We put the origin of the coordinate system at the point q_{in} (corresponding to q at Fig. 5) and rotate the axes with ϵ so that the y -axis coincides with the inward normal (denoted by $n(q)$ in Fig. 5) to the surface $Q(q; \epsilon) = Q(q_{in}; \epsilon)$ at the point q_{in} and the x -coordinates span the corresponding tangent plane. It is easy to see that in the notations of Lemma 3 we have (the explicit dependence on ϵ is suppressed for brevity, and the normal direction is suppressed)

$$K(q_{in}) = Q_{xx}(q_{in})/Q_y(q_{in}), \quad l(q_{in}) = Q_{xy}(q_{in})/Q_y(q_{in}). \tag{63}$$

By (12) and Condition II, near the boundary, the equations of motion have the form:

$$\dot{x} = \frac{\partial H}{\partial p_x} = p_x \quad \dot{p}_x = -\frac{\partial H}{\partial x} = -W'(Q; \epsilon) Q_x, \tag{64}$$

$$\dot{y} = \frac{\partial H}{\partial p_y} = p_y \quad \dot{p}_y = -\frac{\partial H}{\partial y} = -W'(Q; \epsilon) Q_y. \tag{65}$$

Note that $Q_y(q_{in}) \neq 0$, because the y -direction is normal to the level surface of Q at the point q_{in} . It is shown in the proof of Theorem 2 that the orbit may spend only a small time in $N_{>}$, so it stays close to q_{in} all the time it stays in $N_{>}$. It follows that $Q_y(q_{in})$ stays bounded away from zero. Hence, $\frac{dp_y}{dt}$ is bounded away from zero in (65). Therefore, we may use p_y as the new independent variable. Equations (64), (65) are then rewritten as

$$\frac{dq}{dp_y} = -Q'(W; \epsilon) \frac{p}{Q_y}, \quad \frac{dt}{dp_y} = -Q'(W; \epsilon) \frac{1}{Q_y}, \quad \frac{dp_x}{dp_y} = \frac{Q_x}{Q_y}, \tag{66}$$

where

$$W = H - \frac{1}{2}p^2. \tag{67}$$

In order to bring the equations of motion to the required form with the small right-hand side, we make the additional transformation

$$p_x \rightarrow \tilde{p} = p_x - \frac{Q_x(q)}{Q_y(q)} p_y. \tag{68}$$

Note that $Q_x(q_{in}; \epsilon) = 0$, hence (see (63))

$$\tilde{p} = p_x - K(q_{in})(x - x_{in})p_y - l(q_{in})(y - y_{in})p_y + O((q - q_{in})^2). \tag{69}$$

In particular

$$\tilde{p}(t_{in}) = p_{x,in}. \tag{70}$$

After the transformation, taking into account (67), Eqs. (66) take the form

$$\frac{dq}{dp_y} = -Q'\left(\frac{1}{2} - \frac{1}{2}p^2\right) \frac{p}{Q_y}, \tag{71}$$

$$\frac{dt}{dp_y} = -Q'\left(\frac{1}{2} - \frac{1}{2}p^2\right) \frac{1}{Q_y}, \tag{72}$$

$$\frac{d\tilde{p}}{dp_y} = Q'\left(\frac{1}{2} - \frac{1}{2}p^2\right) \frac{d}{dq} \left(\frac{Q_x}{Q_y} \right) \frac{p}{Q_y} p_y. \tag{73}$$

Since $Q'(W; \epsilon)$ is small in the inner layer, these equations belong to the class (50), (51), with $J = O(M^{(r)})$ (see (22)) and $L = O(1)$ (the change in p_y is bounded by the energy constraint). Thus, by (53), we obtain (see (70))

$$(q, t, \tilde{p}) = (q_{in}, t_{in}, p_{x,in}) + O_{Cr}(M^{(r)}). \tag{74}$$

Recall that $W(q_{out}) = W(q_{in})$. Therefore, by energy conservation,

$$p_{x,in}^2 + p_{y,in}^2 = p_{x,out}^2 + p_{y,out}^2, \tag{75}$$

so (74) implies

$$p_{y,out} = -p_{y,in} + O_{cr}(M^{(r)}). \quad (76)$$

By (74), and by using $Q_x(q_{in}, \epsilon) = 0$, Eqs. (71) may be written up to $O_{cr-1}((M^{(r)})^2)$ -terms as

$$\frac{dq}{dp_y} = -Q' \left(\frac{1}{2} (1 - p_{x,in}^2 - p_y^2) \right) \frac{(p_{x,in}, p_y)}{Q_y(q_{in})}, \quad (77)$$

$$\frac{dt}{dp_y} = -Q' \left(\frac{1}{2} (1 - p_{x,in}^2 - p_y^2) \right) \frac{1}{Q_y(q_{in})}, \quad (78)$$

$$\frac{d\tilde{p}}{dp_y} = Q' \left(\frac{1}{2} (1 - p_{x,in}^2 - p_y^2) \right) (K(q_{in})p_{x,in} + l(q_{in})p_y) \frac{p_y}{Q_y(q_{in})}. \quad (79)$$

Now, by applying to Eqs. (71) the estimate (54) with $n = 1$ (one Picard iteration), we can restore from (77) all the formulas of Lemma 3 (we use (69) to restore p_x from \tilde{p} , and use (75) to determine $p_{y,out}$; note also that, up to $O(M^{(r)})$ -terms, the interval of integration is symmetric by virtue of (74), so the integrals of odd functions of p_y in the right-hand-sides of (77) are $O((M^{(r)})^2)$).

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