Nonergodicity of the motion in three-dimensional steep repelling dispersing potentials

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It is demonstrated numerically that smooth three degrees of freedom Hamiltonian systems that are arbitrarily close to three-dimensional strictly dispersing billiards (Sinai billiards) have islands of effective stability, and hence are nonergodic. The mechanism for creating the islands is corners of the billiards domain. © 2006 American Institute of Physics. [DOI: 10.1063/1.2357331]

The motion of a point particle traveling with a constant speed inside a region \(D \in \mathbb{R}^N, N \gg 2\), undergoing elastic collisions at the region’s boundary, is known as the billiard problem. Since the days of Boltzmann, scientists have been using various billiard models to approximate the classical and semiclassical motion in systems with steep potentials (e.g., for studying classical molecular dynamics, a cold atom’s motion in dark optical traps, and microwave dynamics). The invalidity of this approximation near certain types of trajectories is the main issue of this paper. Indeed, we examine this approximation in the most robust case of a scattering Sinai billiard (all the boundary components of the billiard are smooth, dispersing, and their intersections are all oblique). Such billiards are known to be ergodic, hyperbolic, and strongly mixing, thus small smooth deformations of the billiard boundaries do not change these properties. Nonetheless, it had been long conjectured that by introducing smooth steep potentials that are close to the billiards, hyperbolicity may be destroyed. In the two-dimensional settings, it had been proven analytically that tangent periodic orbits and certain corners produce stability islands for arbitrarily steep potentials, with precise estimates of the scaling of the islands size with the steepness parameter. Direct generalization of these results to higher dimensions may produce nonhyperbolic behavior, but one would intuitively suspect that in the scattering case there will always be some unstable directions that will destroy stability. Here, we provide a mechanism for the creation of islands of effective stability (destroying both hyperbolicity and ergodicity) in the higher-dimensional setting. We demonstrate numerically that the islands of stability are created for an arbitrarily steep potential in \textit{both two- and three-dimensional billiards}. Furthermore, we show that the islands are created for an interval of steepness parameters, hence, for a fixed geometry, one may destroy an island by either making the potential steeper or softer.

I. INTRODUCTION

Sinai billiards are known to be ergodic and strongly mixing.\textsuperscript{1–3} In many applications,\textsuperscript{4–7} the billiard’s flow is a simplified model that imitates the conservative motion in a steep potential,

\[ H = \sum_{i=1}^{N} p_i^2/2 + W(q;\varepsilon), \quad W(q;\varepsilon) \rightarrow \begin{cases} 0 & q \in D \setminus \partial D \\ \infty & q \in \partial D \end{cases}, \tag{1} \]

where \(c\) may be infinite. Here we always take the particle’s energy, \(h\), to be smaller than \(c\) so that the particle is confined to \(D\). An important question is whether the billiard and the smooth flows are similar for sufficiently small \(\varepsilon\), and in particular whether the billiard’s ergodicity property is preserved. A definite answer to such a question requires a well-defined limiting procedure.\textsuperscript{8,9} For finite-range axis-symmetric potentials, it was shown that some configurations remain ergodic\textsuperscript{10–13} while other configurations may possess stability islands.\textsuperscript{14,15} Recently, it was established that in the most general two-dimensional settings of dispersing billiards (not necessarily axis-symmetric or of finite range), the answer is definitely negative; it was proven that there are two mechanisms for the creation of stability islands for arbitrarily small \(\varepsilon\). One mechanism is tangency-periodic orbits or homoclinic orbits that are tangent to the billiard’s boundary produce islands.\textsuperscript{9} Another mechanism is corners: a sequence of regular reflections that begins and ends in a corner (termed a \textit{corner polygon}) may, under some prescribed conditions, produce stable periodic orbits.\textsuperscript{8} In both cases, it was shown that a two-parameter family of potentials \(W(q;\varepsilon, \alpha)\) (\(\varepsilon\) is the softness parameter and \(\alpha\) is responsible for a regular continuous change of the billiard’s geometry) possesses a wedge in the \((\varepsilon, \alpha)\) plane, at which the Hamiltonian flow has an elliptic periodic orbit. This orbit limits the tangent billiard orbit/ corner polygon as \(\varepsilon \rightarrow 0\). Furthermore, a method for estimating the width of the stability wedge in the parameter space and of the area of the elliptic islands in the phase space was developed; for typical potentials both quantities have a power-law dependence on \(\varepsilon\).\textsuperscript{9,16} These findings were realized experimentally using cold atoms in atom-optics billiards.\textsuperscript{6} In the experiments, a mixing billiard domain is drawn by a fast-moving laser beam that encloses cold atoms. A small gap is opened after an initial run time, and the fact that the decay rate of the remaining atoms depends on the gap location demonstrates that the dynamics is not mixing and that some of the particles are trapped in stability islands. The
numerical simulations of the experiments show that islands are indeed produced by corner polygons.\textsuperscript{6}

Much less is known on the dynamics in multidimensional billiards ($N \geqslant 3$). Motivated by the Boltzmann hypothesis regarding the ergodicity of hard sphere gas, the ergodicity property of hard-wall semidispersing billiards was studied extensively (see Refs. 17–19 and reference therein). Nondispersing ergodic billiards in $R^N$ with $N \geqslant 3$ were constructed in Refs. 20–23. In these papers and in Ref. 24, examples of three-dimensional semifocusing billiards with mixed phase space were presented as well. Conditions under which multidimensional billiards with finite range spherically symmetric potentials are hyperbolic were found in Ref. 25. A semiclassical study of three-dimensional Sinai billiards was presented in Ref. 26. Recently, the asymptotic expansion of regular (nontangent, away from corners) motion in steep multidimensional potentials by integrals along an auxiliary multidimensional billiard was developed.\textsuperscript{27} In this work, the geometry is arbitrary, and error bounds on the billiard approximation are found.

Here, we demonstrate numerically, for the first time, that islands of stability are created for arbitrarily small $\epsilon$ in three-dimensional soft billiards. The ability to locate small islands of stability in the six-dimensional phase space of the highly chaotic nearly billiard three-degrees-of-freedom flow may appear to be hopeless. Three technical innovations enable us to establish these results numerically. The first idea is to construct a simple symmetric billiard, so that instead of looking for islands of stability in arbitrary places, we may concentrate on the properties of a simple periodic trajectory that exists for all small $\epsilon$ values by symmetry. We examine its stability properties by computing the monodromy matrix of the local return map near this orbit. Inspired by Refs. 6 and 16, we chose a trajectory that limits, as $\epsilon \to 0$, to the simplest possible corner polygon—a cord that enters a corner (see the bold lines in Figs. 1–3). Furthermore, in the three-dimensional case, by the symmetry of the constructed billiard, the two nontrivial pairs of eigenvalues of the monodromy matrix are identical, and are thus controlled by a single parameter. The second idea is that by using proper rescaling, it is possible to integrate numerically the equations of motion for arbitrarily small $\epsilon$. Indeed, if we fix the geometry and take small $\epsilon$ values, we encounter the usual problem of stiffness near the boundary. On the other hand, the equivalent increase of the billiard’s domain by a similarity factor does not introduce a serious numerical problem since $\nabla W$ is small in the domain’s interior. The third idea is that the boundaries of the wedges of stability in the parameter space may be found numerically by a continuation scheme on the critical eigenvalues value. Thus the stability regions may be found effectively and efficiently.

II. BILLIARD GEOMETRY

To construct concrete examples, we define the billiard’s domains as the region exterior to several spheres $\Gamma_k$ with centers at $A^k$ and radii $r^k$, $\Gamma_k(A^k,r^k) \equiv \{q \in R^N|\sum_{i=1}^{N}(q_i-A_i)^2=(r^k)^2\}$, $N=2$ or 3. For the two-dimensional case, we take three circles (Fig. 1). The first two circles $(A^{1,2},r^{1,2})=(a, \pm b, r)$ intersect at the point $q_c=(d,0)$, where $d(a,b,r)=a-\sqrt{r^2-b^2}$, and the third circle, which has a larger radius, has $(A^3,r^3)=(-R-d(a,b,r),0,0)$ with $R \gg r \gg b$. The angle between the tangents to the two circles at $q_c$ is given by

\[ \theta = \arctan \left( \frac{d}{\sqrt{r^2-b^2}} \right) \]

FIG. 1. (Color online) The billiard geometry in the 2D case. A cord $\gamma$ is denoted by the bold line.

FIG. 2. (Color online) The billiard geometry in the 3D case. The cord $\gamma$ is denoted by the bold line.

FIG. 3. (Color online) The billiard geometry in the 3D case, at the cross section $y=0$. The cord $\gamma$ is denoted by the bold line.
in finite angles, or by a large box, so that for all \( 0 < \alpha < \pi/2 \)
the billiard’s reflection law \( \phi_{in} = \phi_{out} = \pi/2 \) and at \((x, y) = (d, 0)\) it enters a corner. We will study the behavior of the smooth system near this corner polygon, thus the closing of the billiard domain away from this line is irrelevant here. It may be achieved by a union of a finite number of dispersing smooth boundaries that meet at nonzero angles, or by enclosing the whole system in a large box. For all \( \alpha > 0 \), the family of billiard tables thus defined belongs to the class of Sinai billiards—they are mixing dynamical systems, having one ergodic component and a positive Lyapunov exponent for almost all initial conditions.

Similarly, in the three-dimensional case, we take four spheres (Figs. 2–4). Three spheres have equal radii \( r \) and have equidistant centers, \((A^1, r^1) = (a, b, \pm \sqrt{3}b, r), (A^2, r^2) = (a, -2b, 0, r)\). These three spheres intersect, for \( r \geq 2b \), at \( q_0 = (d, 0, 0) \), where \( d(a, b, r) = a - \sqrt{r^2 - 4b^2} \). The fourth sphere, of radius \( R \gg r \), is located at a distance \( 2d \) from the corner point, \((A^3, r^3) = (-R - d(a, b, r), 0, 0, R)\). The angle between the pairs of tangent lines to the circles of intersections of pairs of spheres is

\[
\alpha_{3D} = \alpha \cos \left( 1 - 2 \frac{b^2}{r^2} \right),
\]

so that when \( r = b \) these circles are tangent and \( \alpha_{3D} = 0 \). The cord \( \gamma = \{(x, y) \mid x \in (-d, d), y = 0 \} \) is a corner polygon. Here again we can close the billiard domain by adding a finite number of dispersing surfaces that intersect each other in finite angles, or by a large box, so that for all \( \alpha > 0 \) the resulting billiard domain is compact and dispersing. Note that if we rescale all the spheres and the distances between them by a fixed scale \( L \), the billiards geometry will not change and the corresponding corner angles remain unchanged.

### III. Equations of Motion for the Smooth Flow

Consider the smooth motion in this region, which is induced by the potential \( W(q; w_0) = \sum_{k=1}^{N} V_k(q; w_0) \); \( V_k(q; w_0) \) may be taken as the Gaussian potential associated with the boundary component \( \Gamma_k \); \( V_k(q; w_0) = \exp(-Q_k^2(q)/w_0^2) \), where \( Q_k(q) \) is the distance between \( q \) and the circle \( \Gamma_k \); \( Q_k(q) = \sqrt{\sum_{i=1}^{N} (q_i - A_i^k)^2} - r_k \), and \( w_0 \) is the softness parameter. In the cold atom experiment, \( w_0 \) corresponds to the width of the laser beam, and \( V(Q_k(q); w_0) \) corresponds to the averaged effective Gaussian potential that bounds the atoms. Previously, we established that as this potential tends to a hard-wall potential (\( w_0 \rightarrow 0 \)), regular reflections of the smooth flow tend to those of the billiard.\(^9\)\(^,\)\(^27\) By the symmetric placement of the spheres, it is clear that for any \( w_0 < w_0^0 \) [where \( \min_{x} W(q; w_0^0) = h \), there exists a periodic solution \( y(t, w_0) = (x(t, w_0), 0) \) that limits, as \( w_0 \rightarrow 0 \), to the corner polygon \( \gamma \). Notice that studying this system for a fixed \( w_0 \) and a billiard domain that is increased proportionally by a factor \( L \) [so \((A^k, r^k) \rightarrow (L A^k, L r^k)\)] is equivalent to studying it in a fixed geometry with \( w_0 \) replaced by \( \epsilon = w_0/L \). Thus, by increasing the domain size, we may approach the limit \( \epsilon \rightarrow 0 \) without the numerical problems associated with the stiff limit \( w_0 \rightarrow 0 \).

### IV. Numerical Computations

From the analysis of Ref. 16, we expect that the stability of \( \gamma(t, \epsilon, \alpha) \) will depend nontrivially on both \( \epsilon \) and the geometrical parameter of the billiard \( \alpha \) and that near \( \alpha_k = \pi/k \) islands will appear (the limit \( \alpha \rightarrow 0 \) at which the billiard is not a Sinai billiard, and thus billiard orbits may be trapped for an arbitrarily large number of reflections near the corner, has not been studied in Ref. 16). We find that all the regions in the \((\alpha, \epsilon)\) plane at which islands of stability associated with \( \gamma(t, \epsilon, \alpha) \) exist (other islands of stability may coexist) emerge from \( \alpha = 0 \) at some finite \( \epsilon_k^* \) values, and converge toward \((\alpha, \epsilon) \rightarrow (\pi/k, 0)\). Hence, we first find the stability of \( \gamma(t, \epsilon, \alpha = 0) \) by computing the eigenvalues of the monodromy matrix of the return map to the local cross section at \( x = 0 \) for a range of \( \epsilon \) values. Since there is always a pair of neutral eigenvalues corresponding to the flow direction, for the 2D case the monodromy matrix has the eigenvalues \( \{1, 1, \lambda, 1/\lambda\} \), where \( \lambda \) is the largest eigenvalue, which is different from 1. In the 3D case, due to the symmetric form of the geometry, the spectrum is of the form \( \{1, 1, \lambda, 1/\lambda, 1/\lambda\} \) (i.e., saddle foci do not appear). In Fig. 5, the real part of \( \lambda \) is shown for a range of \( \epsilon \) values for the 2D and 3D cases. The large oscillations from positive to negative values guarantee the existence of intervals of \( \epsilon \) at which Re\(\{\lambda\} \in (-1, 1)\); on these intervals, \( \lambda \) is imaginary and belongs to the unit circle. In the left panels of Figs. 6 and 7, we present an enlarged segment of Fig. 5 with a regular \( \epsilon \) scale. These calculations are used to find the values of \( \epsilon = \epsilon_k^* \) at which Re\(\{\lambda\} = \pm 1 \), where a saddle center and period-doubling bifurcations occur, respectively (in the three-

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FIG. 4. (Color online) The billiard geometry in the 3D case: at the cross section \( x = x_f \) the radius of the circles is \( r_f = \sqrt{r^2 - (x_f - a)^2} \). Dotted line: \( x_f = a \), solid line: \( x_f = d \), dashed line: \( d < x_f < a + r \).
dimensional case these are double-bifurcation points due to the symmetry. Then, starting at \((\alpha, \epsilon) = (0, \epsilon_0^2)\), we use a continuation method for finding the bifurcation curves for \(\alpha > 0\), as shown in the right panels of Figs. 6 and 7. In the 

In the three-dimensional case, for all \(\omega\) values, the multipliers are in 1:1 resonance due to the symmetry. For generic systems, for almost all \(\omega\) values [values that are nonresonant with the frequency of \(\gamma(t, \epsilon, \alpha)\)], we expect to have non-linear stability (see, e.g., Ref. 28). Indeed, projections of the four-dimensional symplectic return map to \(x=0\) for several \((\alpha, \epsilon)\) values are shown in Fig. 8. It is demonstrated that indeed inside the wedge region \(\gamma(t, \epsilon, \alpha)\) is non-linearly stable for the full integration time (approximately 4000 periods). Moreover, if we add a sufficiently small, asymmetric perturbation to the potential \([e.g., V=V+\delta \cos(y+\eta)\cos(z+\mu)]\) with \(\delta, \eta, \mu = O(0.0001)\), we find that the effective stability region still persists. For the phase-space simulations, we use a symplectic integrator (Gniscodes\textsuperscript{29}), which keeps \(h\) up to an accuracy of \(10^{-11}\). Thus, we can confidently detect islands with transversal kinetic energy of up to \(10^{-8}\) [so \((p_y, p_z) = O(10^{-8})\)]. This limits our phase-space calculations to \(\epsilon = 0.04\)—smaller values of \(\epsilon\) produce smaller islands and their detection via phase-space plots requires a higher accuracy in the integration. We stress, however, that the calculations of the bifurcation curves are accurate for much smaller \(\epsilon\) values; in these calculations, only a single return map is computed and there exists a sharp transition between large positive and large negative values of the eigenvalues (see the left panels of Figs. 6 and 7), so the existence of elliptic regimes is guaranteed. Comparing the 2D and 3D wedges of stability, it appears that the 3D wedges are indeed narrower.

V. CONCLUDING REMARKS

While the appearance of islands in two-degrees-of-freedom steep Hamiltonian systems is somewhat expected, the mechanisms for their appearance in the higher-dimensional settings are not as well understood (see Refs. 30 and 28 for some generic possibilities). Furthermore, their appearance guarantees only effective stability due to the possible existence of Arnold diffusion\textsuperscript{31}. Nonetheless, by KAM theory, in the nondegenerate case, a large set of initial conditions belongs to KAM tori and thus stays forever near the stable periodic orbit. Thus, the existence of islands in the higher-dimensional setting implies that ergodicity is de-
stroked independently of the possible leakage out of the effective stability zone after an exponentially long time. This latter possibility suggests that stickiness may be an interesting event also in this higher-dimensional setting.

Here, we propose for the first time a mechanism for the creation of stability islands for smooth systems that are arbitrarily close to strictly dispersing three-dimensional billiards; we showed that potentials $V(q; \epsilon, \alpha)$ that become arbitrarily steep as $\epsilon \to 0$ possess wedges in the $(\epsilon, \alpha)$ plane at which a periodic orbit is elliptic. Thus, on the one hand, there exist one-parameter families of potentials $V(q; \epsilon, \alpha(\epsilon))$ that have a stable periodic orbit for arbitrarily small $\epsilon$. Since we showed that in the wedges $\alpha(\epsilon) \to \alpha(0) > 0$ as $\epsilon \to 0$, it follows that these potentials have islands of stability even when they are arbitrarily close to hard-wall dispersing (Sinai) billiards. On the other hand, for any fixed $\alpha \in (0, \pi/2)$ there exists an interval of positive $\epsilon$ values for which islands of stability exist. Thus, these islands may be destroyed by either making the potential steeper or softer—a somewhat nonintuitive result.

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20L. A. Bunimovich and J. Rehacek, “Nowhere dispersing 3D billiards with