

Decay of the Sinai well in D dimensions

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We study the decay law of the Sinai well in D dimensions and relate the behavior of the decay law to internal distributions that characterize the dynamics of the system. We show that the long time tail of the decay is algebraic ($1/t$), irrespective of the dimension D .

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I. INTRODUCTION

In a previous work [1] we studied the decay of quasibounded classical Hamiltonian systems in two dimensions, in particular the decay problem for the Sinai well. In this paper we extend the study to the D -dimensional case. We will briefly describe what a quasibounded system means, but for further details we refer to the original work.

A quasibounded system is a dynamical system transiently bounded to a finite region of the phase space where an infinite set of nonstable periodic orbits is included before it displays unbounded dynamics. The transition from the bounded motion to the unbounded motion is the decay process and the decay law is related to the bounded transient dynamics. The kind of system that we are interested in is fully chaotic, but not completely hyperbolic. In terms of the invariant set this means that instead of being completely hyperbolic, it has a nonhyperbolic (namely, parabolic [2]) subset. One of the main differences with the analogous system in two dimensions is that whereas in that case, the invariant set could be fully hyperbolic or have a parabolic subset depending on the value of a simple parameter; for the ($D > 2$)-dimensional system the invariant set always has a parabolic subset. In this case the global consequence on the decay law is that it always exhibits a crossover between a stretched exponential and an algebraic decay for long times. One of the main purposes of this work is to study the long time tail of the decay law in D dimensions and to relate the decay of population from equilibrium to internal distributions that characterize the dynamics.

Our work is organized as follows. In Sec. II we introduce the system that we will call the Sinai well in D dimensions because it is geometrically similar to the Sinai billiard [3] in D dimensions, but with a finite rather than infinite well. In Sec. III we review some results of the analogous model in two dimensions [1].

Section IV is the central body of the work and is devoted to the study of the temporal decay law both numerically and analytically. We show the results of the numerical study of the decay that reveal the above mentioned behavior, and using ergodic properties we relate the decay law to internal distributions that depend on the

internal dynamics. Finally, Sec. V is devoted to discussions and conclusions. We include an Appendix in which the explicit expression for the transition probability from the bounded to the free region is derived.

II. THE SINAI WELL IN D DIMENSIONS

Our system consists of a point particle of unit mass in a D - ($D > 2$) dimensional square well (hypercube) of depth $-V_0$ ($V_0 > 0$) and side a , which collides elastically with a fixed scatterer located in the center of the well. The scatterer is a D -dimensional unit sphere and as usual we take the speed of the particle to be one. In the study of the analogous system for $D = 2$ [1] we consider the total energy $E = p^2/2 - V_0$ ($0 \leq E \leq V_0$) and explain in detail how the collision with the scatterer rearranges the energy among the degrees of freedom in order that the particle could transit from the bounded region to the free one after colliding with the central barrier.

Although the extension to higher dimensions is straightforward, there are some features to remark on and we devote the remainder of this section to these results.

The bounded motion in D dimensions is characterized by the condition

$$\sqrt{1 - \left(\frac{\vec{p} \cdot \hat{n}_i}{|\vec{p}|}\right)^2} > \sin \Psi_{\text{lim}}, \quad (2.1)$$

where \hat{n}_i , $i = 1, \dots, D$, is the normal direction to face i on which the particle bounces and

$$\Psi_{\text{lim}} = \arcsin \frac{1}{\sqrt{1 + V_0/E}} \quad (2.2)$$

is the limit angle in D dimensions. The inequality (2.1) is the condition to have an internal reflection when the particle reaches the boundary of the hypercube. This result has been explained in detail for $D = 2$ in Appendix A of [1] and for $D > 2$ the derivation is similar. As we mentioned before, the collision with the scatterer changes the value of the components of the momentum and this enables the transition to the free region, or, in other words,

the decay process. In the D -dimensional problem the limit angle Ψ_{lim} can be related to the probability $\omega_D < 1$ that the particle transits from the bounded to the free region after one collision with the scatterer. The space of momenta is a D -dimensional unit sphere in which

$$\omega_D = \frac{d\Psi_{\text{lim}}(D)}{\Omega(D)}, \quad (2.3)$$

where $d\Psi_{\text{lim}}(D)$ and $\Omega(D)$ are, respectively, the solid angle subtended by Ψ_{lim} and the total solid angle in D dimensions. In the Appendix we derive an explicit expression for (2.3) in terms of Ψ_{lim} . Here we give the result

$$\omega_D \sim \Psi_{\text{lim}}^{D-1}, \quad (2.4)$$

which shows that the transition probability decreases with the dimensions D when $\Psi_{\text{lim}} \ll 1$ for a given (fixed) energy E .

III. PRELIMINARY REMARKS

In this section we review some results of the analogous problem in two dimensions [1]. The decay of population $N(t)$ inside the well is characterized by two distributions specific to the internal dynamics. The first one $g(t)dt$ is the fraction of particles for which the first collision with the circular scatterer occurs between t and $t + dt$; the second one $f(t)dt$ is the fraction of particles for which the time between two successive collisions with the central scatterer lies between t and $t + dt$. In the decay process from the equilibrium population these distributions are not independent, but related by

$$dg/dt = -g(0)f(t), \quad (3.1)$$

In [1] (referred to, in the following, as I) we conclude that distributions $g(t)dt$ that decrease exponentially or faster lead to an exponential decay law, while an algebraic decay of $g(t)$ gives rise to an exponential decay law that changes into a power law decay for long times. Our model is closely related to the periodic Lorentz gas in two dimensions, in which the problem of the asymptotic behavior of the velocity autocorrelation function has been studied extensively over the past several years both theoretically and numerically (see [4] and references cited therein). In that model we can distinguish two kinds of behaviors depending on the “finite” or “infinite” nature of the horizon. By definition a periodic configuration of scatterers has an infinite horizon if the length of the free motion of the particle is unbounded. Actually if the horizon is infinite, then there exist trajectories that never reflect from the scatterers. These trajectories define the so-called corridors that are characterized by the directions of the velocity such that $v_y/v_x = z_1/z_2$ (here z_1 and z_2 are coprime integer numbers). The number of open corridors increases when the radii of the scatterers R decrease. Following the notation of Ref. [5] for the square Lorentz model, there are at least two of such open channels corresponding to the x direction and the y di-

rection and we call these channels α and β , respectively. When $\sqrt{5}/10 < R < \sqrt{2}/4$ we have other open channels γ that correspond to $v_y/v_x = \pm 1$. In I we explained in detail the connection between the open corridors and the parabolic periodic orbits that appear in our system when the radius of the central scatterer decreases. For the Sinai well a finite horizon, which means $g(t)dt$ decreasing exponentially or faster, is compatible with the existence of periodic orbits of hyperbolic type (with no open corridor in the extended Lorentz version), whereas an infinite horizon, $g(t)dt$ with algebraic tail, implies the existence of parabolic nonisolated periodic orbits that appear for $R \leq R_{c1}$, and determine the corresponding corridors. In the former case the decay law is exponential and in the latter the decay law shows a crossover between an exponential and a power law decay ($\sim 1/t$) for long times.

IV. THE DECAY LAW IN D DIMENSIONS

A. Numerical study of the decay

In this subsection we show the results of the numerical study of the decay. It is a well known fact that for short times, the behavior of the decay law in D dimensions is of exponential type [6].

Our main purpose is to understand the behavior for long times. In other words, we study the long time tail of the decay law in D dimensions. As we will see in the following subsection, in order to extract information about the long time tail of the decay it is enough to study the function $g(t)dt$, the fraction of initial conditions for which the first collision with the scatterer occurs between t and $t + dt$, for the D -dimensional system [to be more precise we will compute the integral of $g(t)$, $G = \int_{t'=0}^{t'=t} g(t') dt'$]. From the numerical point of view, the study of G as a function of t instead of the decay law $N(t)/N_0$ has a great advantage because it requires less CPU time and we can get better statistics with more initial conditions. We begin with $N_0 = 10^7$ particles with random initial conditions in the phase space and the ratio $V_0/E = 20$. Figure 1(a) shows the results of the numerical study of G for $D = 2, 3, 4$ and radius of the D -dimensional scatterer $R = 0.23$. The behavior is exponential for short times and becomes algebraic for long times ($1/t^\delta$). Figure 1(b) shows the tails of G for $D = 2, 3, 4$ together with the best fit that predicts for all the curves an exponent $\delta = 1$. Figure 2(a) is the same as Fig. 1(a), but for $R = 0.4$. For $D = 2$, G is of exponential type. This agrees with the result of paper I. For the two-dimensional system $R > R_{c1} = \sqrt{2}/4$ is compatible with a $g(t)$ of finite horizon and the decay is exponential for all times. For $D = 3, 4$ again the best fit of the long time tail predicts an exponent $\delta = 1$. Figure 2(b) shows this fit together with the numerical results of the long time tails for $D = 3, 4$. These results suggest that for $D > 2$ there does not exist a critical value of the radius that changes the behavior of the decay for long times as happens for $D = 2$ (see I). In terms of the invariant trapped set, we can stress that for $D > 2$ there are always periodic orbits of parabolic type and the initial conditions asymptotic to

them are the ones that contribute to the long time tail of the decay.

B. Theoretical study of the decay

One of the main results of the present paper is that for the Sinai well in D dimensions, the long time tail of the decay law is $(\sim 1/t)$, independent of the dimension D . To our knowledge this is the first report in which this result is stated analytically and confirmed by numerical

simulations. All the previous works only study the model in two dimensions [7,8] or conjecture for the $D > 2$ system an exponential decay of the velocity autocorrelation function for long times [6]. To begin the theoretical study, we extend to the D -dimensional case some results of the previous paper I that allow us to relate the decay law to the internal dynamics:

$$\hat{Q}(s) = \frac{\omega_D \hat{g}(s)/s}{1 - (1 - \omega_D)\hat{f}(s)}, \quad (4.1)$$

where $\hat{Q}(s) = L[Q(t)]$ means the Laplace transform,

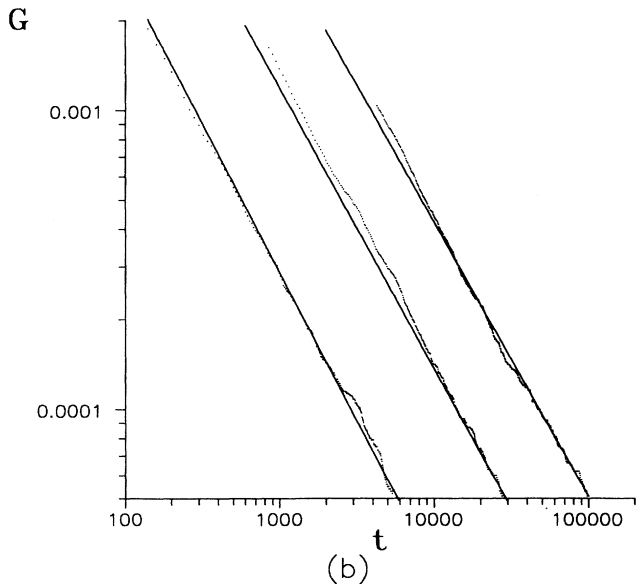
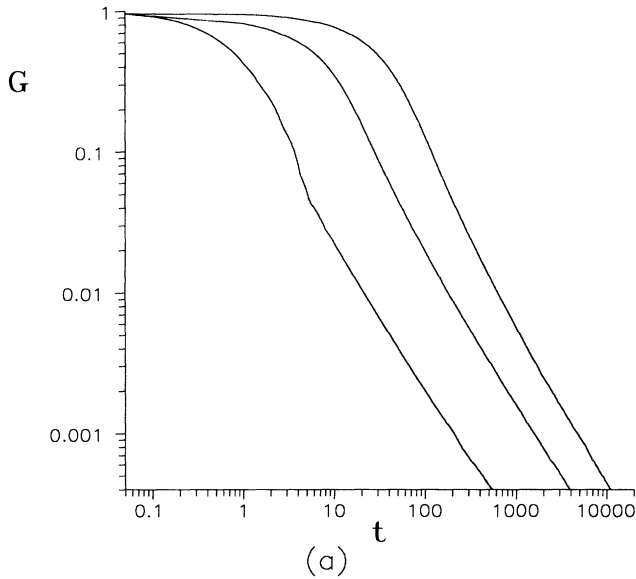


FIG. 1. (a) Numerical results of G for $D = 2, 3, 4$. We have fixed a (the side of the D -dimensional square well) as the unit of length and $a/\sqrt{2(E + V_0)}$ as the unit of time. The log-log plot shows G vs t for radius $R = 0.23$ of the central scatterer. (b) The long time tail together with the best fit to G vs t that is consistent with the exponent $\delta = 1$ for $D = 2, 3, 4$.

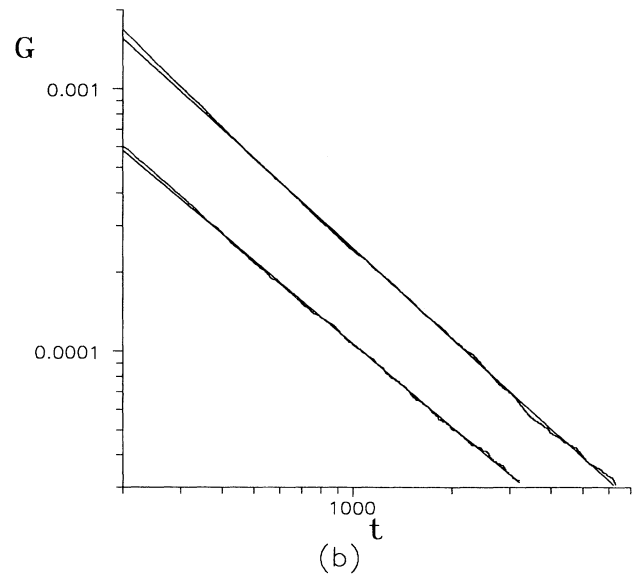
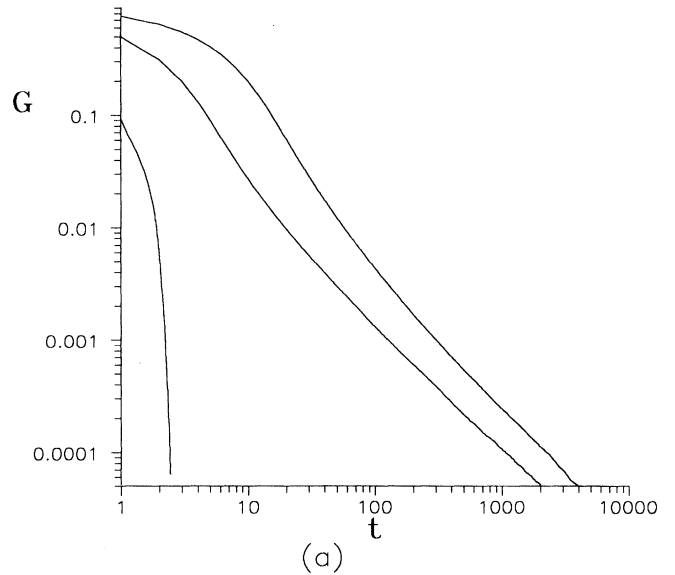


FIG. 2. (a) Numerical results of G for $D = 2, 3, 4$. The units are the same as in Fig. 1. The log-log plot shows G vs t for radius $R = 0.4$ of the central scatterer. (b) The long time tail together with the best fit to G vs t that is consistent with the exponent $\delta = 1$ for $D = 3, 4$.

$$Q(t) = 1 - \frac{N(t)}{N_0}, \quad (4.2)$$

and $N(t)/N_0$ is the fraction of particles present in the well at time t (the decay law). Taking into account the equation

$$dg/dt = -g(0)f(t), \quad (4.3)$$

so that

$$\hat{f}(s) = 1 - s\hat{g}(s)/g(0), \quad (4.4)$$

we finally find

$$\hat{Q}(s) = \frac{\omega_D \hat{g}(s)/s}{1 + (1 - \omega_D)[\hat{g}(s)s/g(0) - 1]}. \quad (4.5)$$

The preceding equation is a straightforward extension of the one that we have obtained in I for the two-dimensional problem, being in that case $\omega_{D=2} = w$. To know $Q(t)$, we must be able to inversely transform (4.5). Computing the leading term of (4.5) and employing (4.2) we obtain

$$N(t) \sim \omega_D \int_{t'=t}^{t'=\infty} g(t') dt'. \quad (4.6)$$

We must center our attention on the function $g(t)dt$ for our D -dimensional problem to study the long time behavior (4.6) of the decay law.

We will extend the definition of corridors to higher dimensions. For that we must appeal to the periodic Lorentz gas in the D -dimensional case for which statistical properties in the hyperbolic domain (finite horizon) have been studied in detail in a recent reference [9] and a numerical study of some universal properties was performed in [6]. We will say that a D -dimensional periodic Lorentz gas has an infinite horizon if the length of the free motion is unbounded. The first trivial extension is to define the corridors in D dimensions by the directions of the velocity \vec{v} that satisfy $v_i/v_j = z_1/z_2 \forall(i, j)$, where z_1 and z_2 are coprime integers. These are not the only directions that lead in D dimensions to unbounded free motion. For example, for $D = 3$ the direction $v_1 = 0$, with v_2 and v_3 arbitrary (compatible with the condition that the modulus of the velocity $|\vec{v}|$ is 1), is also a corridor in the meaning of free unbounded motion. The main characteristic to note is that as the dimension increases it is possible to find more directions that define unbounded motion for any value of the radius of the scatterer $R \leq 0.5$, which means that there is no critical value R_c that destroys the corridors, as there was in two dimensions. However, R_c influences the number of open corridors, since there are some corridors that disappear when $R > R_c$.

All the trajectories that contribute to the long time tail of the decay lie almost entirely in some corridor. In terms of the Sinai well we say that these initial conditions are asymptotic to the parabolic periodic orbits that exist in D dimensions, leaving the bounded region with probability ω_D after one collision with the D -dimensional

scatterer.

At this point it is necessary to emphasize that apart from the corridors whose asymptotic initial conditions contribute to the algebraic long time tail of the decay with an exponent $\delta = 1$ (we call them principal corridors), there are other corridors in which initial conditions asymptotic to them lead to an algebraic tail of the decay ($1/t^\mu$) with the exponent $\mu > 1$. A proof of the existence of these other corridors is given in Fig. 3. It shows for $D = 4$ and $R = 0.4$, there are two curves G as a function of t . In one (dashed line) all the corridors have been populated and the exponent for the long time tail is $\delta = 1$; in the other (solid line) we do not consider initial conditions to be asymptotic to the principal corridors, resulting in an exponent for the long time tail different from 1.

Since the global behavior of the decay law for long times is $(1/t)$ independent of the dimension D , we call these other corridors hidden corridors because there is no evidence of them in the long time tail of the decay law. On the other hand, the intermediate behavior of the decay law, which it is related to asymptotic conditions to the hidden corridors, results in a superposition of algebraic decays with exponents greater than and different from one, this behavior being more and more complicated as the dimension increases.

We devote the remainder of this section to derive the explicit dependence on t of the distribution $g(t)dt$ for initial conditions that are asymptotic to the principal corridors using the D -dimensional periodic Lorentz gas model. Without loss of generality we will compute $g(t)dt$ for the initial conditions that lie in the principal corridor ($D = 3$) defined by the directions of the velocity $v_1/v_2 = \pm 1$ and v_3 arbitrary that satisfy the condition $|\vec{v}| = 1$,

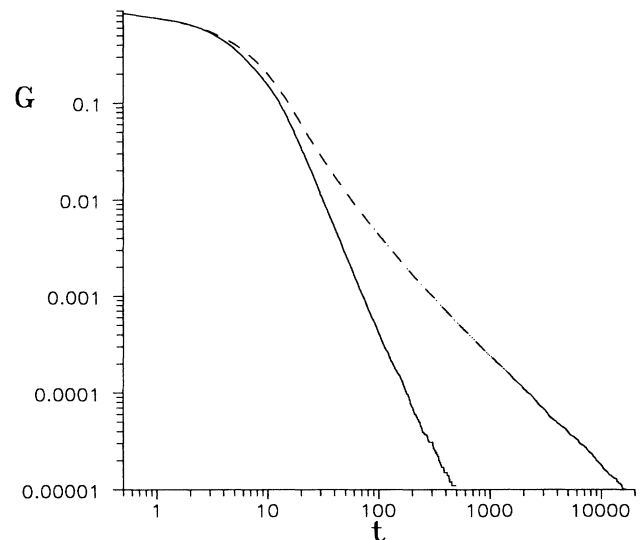


FIG. 3. Numerical results of G for $D = 4$. The units are the same as in Fig. 1. The log-log plot shows G vs t for radius $R = 0.4$ of the central scatterer. The dashed curve corresponds to initial conditions in all phase space. The solid curve results from not having populated any principal corridors. The algebraic long time tail is originated by the hidden corridors. The best fit is consistent with an exponent $\delta = 2$.

corresponding this case to $R < R_c$. In Fig. 4 we show a schematic representation of the mentioned corridor of width l in which we have cut with the plane $z = \text{const}$ the spherical scatterers at their centers in order to simplify the figure. We remark that as $|\vec{v}| = 1$ the distributions in times are equivalent to distributions in lengths.

Let $n(t^*)$ be the fraction of initial conditions for which the first collision with some scatterer occurs in times $t > t^*$. As we are interested in the large t behavior, the angle α is proportional to $n(t^*)$

$$n(t^*) \sim \alpha \sim \frac{l}{t^*} \quad (4.7)$$

and

$$-dn/dt^* \sim \frac{l}{t^{*2}} \sim g(t^*) \quad (4.8)$$

where $g(t^*)dt^*$ is the fraction of initial conditions for which the first collision with the scatterer occurs between t^* and $t^* + dt^*$. To be more precise we must consider the integration over the solid angle, but this gives 2π , so we can conclude that inside a principal corridor

$$g(t) \sim \frac{\text{const}}{t^2}. \quad (4.9)$$

Use of the expression (4.9) in (4.6) leads to the mentioned behavior of the long time tail of the decay

$$N(t) \sim \frac{\omega_D}{t}. \quad (4.10)$$

We stress that the derivation (4.10) is also valid for the other principal corridors. In the case of the hidden corridors, vestiges of some principal corridors when $R > R_c$, the integration over the solid angle leads to an additional

$1/t$ dependence, so in that case

$$g(t) \sim \frac{\text{const}'}{t^3}. \quad (4.11)$$

The preceding arguments can be extended to higher dimensions. For the principal corridors the dependence on t is exactly the same ($\sim 1/t$). For the hidden corridors, as the dimension D increases, the integration over the solid angle gives rise to contributions of the type $1/t^\mu$ with the $2 \leq \mu \leq D$.

C. The decay law in terms of the Laplace transform

We begin computing the decay law $N(t)$ as the inverse Laplace transform of a function $q(\lambda)$,

$$N(t) = \int_0^\infty q(\lambda) e^{-\lambda t} d\lambda, \quad (4.12)$$

where $q(\lambda)$ can be seen as the fraction of initial conditions that decay at time t and which decay rate varies between λ and $\lambda + d\lambda$. In the context of (4.12), the whole decay law can be thought of as the result of infinitely many decay processes of exponential type, each one characterized by a decay rate λ ; this interpretation is independent of the dimension D . Our purpose is to relate the function $q(\lambda)$ to $\hat{g}(s)$, the Laplace transform of the function $g(t)$, which, as we have shown in the preceding subsection, determines univocally the decay law. Employing (4.2) and (4.12)

$$Q(t) = 1 - \int_0^\infty q(\lambda) e^{-\lambda t} d\lambda \quad (4.13)$$

and making the Laplace transform of (4.13)

$$\int_0^\infty \frac{q(\lambda)}{\lambda + s} d\lambda = \frac{1}{s} - \hat{Q}(s). \quad (4.14)$$

The left-hand side of (4.14) is the Stieltjes transform of the function $q(\lambda)$ and arises naturally from the iteration of the Laplace transform. Inversely transforming (4.14) we can determine univocally $q(\lambda)$ from $\hat{Q}(s)$. Here we do not give the exact expression for the inversion of (4.14). For further details see [10]. We would like to emphasize that this point of view enables us to determine the fraction of initial conditions that decay at time t with a decay rate between λ and $\lambda + d\lambda$ when the function $\hat{g}(s)$ is known.

V. SUMMARY AND CONCLUSIONS

In the present work we have studied the decay of the Sinai well in D dimensions, this system being an extension to higher dimensions of the previous one studied in detail in I. The main difference between the ($D > 2$)-dimensional system and the analog in two dimensions is that being both completely chaotic, the first one has an invariant parabolic trapped set for all the values of the radii R of the scatterer, whereas in the second one the invariant trapped set can be fully hyperbolic or have a

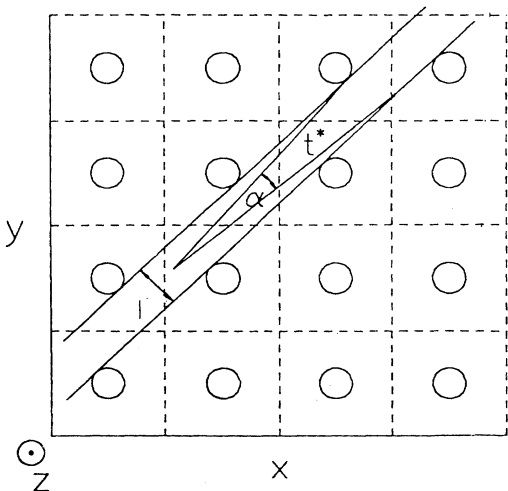


FIG. 4. Periodic configuration of scatterers in $D = 3$ dimensions for a constant value of the coordinate z . The coordinate z has been chosen in order to cut the spherical scatterers at their centers. The principal corridor defined by $v_1/v_2 = 1$ and v_3 arbitrary, which satisfied the condition $|\vec{v}| = 1$, is shown. The width of the corridor is l and the angle α ($\sim l/t^*$) is proportional to the number of initial conditions that collide with some scatterer in a time $t > t^*$.

parabolic trapped subset if $R < \frac{\sqrt{2}}{4}$. In terms of the decay law this means that for the present system the decay law is always of algebraic type for long times (related to initial conditions asymptotic to the parabolic periodic orbits in $D > 2$ dimensions). We have related the decay law in D dimensions to internal distributions that characterize the dynamics and concluded that the exponent δ for the algebraic long time tail is $\delta = 1$ irrespective of the dimension. This behavior is in agreement with the results encountered in Ref. [11]. In that work the authors investigate in D dimensions a system like a Sinai billiard [3] and allow the decay providing a small window in one of the walls of the container. They conclude that for the regular case (without a scatterer in the center) the decay law is algebraic ($\sim 1/t$), independent of D . As the trapped set of the regular system coincides with the parabolic periodic orbits of the Sinai well, the result is consistent with our conclusion. We also studied the intermediate behavior of the decay law and concluded that it is related to the so-called hidden corridors, which asymptotic initial conditions contribute to the decay law with a temporal dependence of the type $(1/t^\mu)$, with $2 \leq \mu \leq D$.

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APPENDIX

In this appendix we derive the explicit expression for ω_D , the transition probability from the bounded to the free region after one collision with the scatterer. It can be evaluated using ergodic theory as the ratio between all orientations of momentum in the free region and all possible orientations of momentum.

The space of momenta is a D -dimensional unit sphere (the modulus of \vec{p} is 1). Let $d\Psi_{\text{lim}}(D)$ be the solid angle subtended by Ψ_{lim} , where Ψ_{lim} is given in expression (2.2) and $\Omega(D)$ is the total solid angle in D dimensions. As we have established in (2.3),

$$\omega_D = \frac{d\Psi_{\text{lim}}(D)}{\Omega(D)}, \quad (\text{A1})$$

so for computing ω_D we must have the explicit expressions for $\Omega(D)$ and $d\Psi_{\text{lim}}(D)$.

Introducing the polar coordinates in D dimensions ($D \geq 3$)

$$(r, \phi, \theta_1, \dots, \theta_{D-2}) \quad (\text{A2})$$

with $r = 1$, $0 < \phi < 2\pi$, and $0 < \theta_i < \pi$, $i = 1, \dots, D-2$, we can derive the expression

$$\Omega(D) = 2\pi \prod_{i=1}^{D-2} \int_0^\pi \sin^i \theta_i d\theta_i. \quad (\text{A3})$$

Employing the well-known formula [12]

$$\int_0^\pi \sin^i \theta_i d\theta_i = \sqrt{\pi} \frac{\Gamma(i+1/2)}{\Gamma(i+2/2)} \quad (\text{A4})$$

and putting it back in (A3), we obtain

$$\Omega(D) = \frac{\pi^{D-2}}{\Gamma(D/2)}. \quad (\text{A5})$$

In order to compute $d\Psi_{\text{lim}}(D)$ we must perform the integration in the variables θ_i with $i = 1, \dots, D-3$ between $0 < \theta_i < \pi$ and $0 < \theta_{D-2} < \Psi_{\text{lim}}$,

$$d\Psi_{\text{lim}}(D) = 2\pi \prod_{i=1}^{D-3} \int_0^\pi \sin^i \theta_i d\theta_i \times \int_0^{\Psi_{\text{lim}}} \sin^{D-2} \theta_{D-2} d\theta_{D-2}. \quad (\text{A6})$$

After a straightforward calculation we obtain

$$d\Psi_{\text{lim}}(D) = \frac{2 (\sqrt{\pi})^{D-1} \Psi_{\text{lim}}^{D-1}}{(D-1) \Gamma(D-1/2)} \quad (\text{A7})$$

and from (2.3), (A5), and (A7)

$$\omega_D = \frac{2 \Gamma(D/2) \Psi_{\text{lim}}^{D-1}}{\sqrt{\pi} (D-1) \Gamma(D-1/2)} \quad (\text{A8})$$

results.

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