Fractals and dynamical chaos in a two-dimensional Lorentz gas with sinks

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We consider a two-dimensional periodic reactive Lorentz gas, in which a moving point particle undergoes elastic collisions on fixed hard disks and annihilates on absorbing disks, called sinks. We present clear evidence of the existence of a fractal repeller in this open system. Moreover, we establish a relation between the reaction rate, describing the macroscopic evolution of the system, and two characteristic quantities of the microscopic chaos: the average Lyapunov exponent and the Hausdorff codimension of the fractal repeller.

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I. INTRODUCTION

Many recent works have been devoted to an understanding of macroscopic irreversible processes, such as diffusion or reaction, studied from a microscopic point of view, using deterministic chaotic models [1–7]. An efficient way to establish relations between the characteristic quantities of microscopic chaos and the macroscopic transport coefficients is the escape-rate formalism [3–7]. In this formalism, a dynamical quantity called the Helfand moment $G^{(\alpha)}$ is associated with each transport property [8]. For large enough systems and long enough times, this Helfand moment has a diffusive evolution determined by the transport coefficient α considered. This diffusionlike process can be characterized by the escape rate of trajectories out of a phase-space region defined by bounds on the Helfand moment $-\chi/2 \leq G_t^{(\alpha)} \leq \chi/2$, χ being real and positive [4]. Almost all trajectories escape after a finite time. The trajectories that remain trapped forever in the prescribed bounds form an unstable fractal set in the phase space. This set is called the fractal repeller. In the case of diffusion, the Helfand moment is simply the position $\mathbf{r}$: the particle itself escapes out of a region defined in the configuration space.

The fractal repeller is characterized by its chaotic and fractal properties, which can be studied in the large-deviation formalism, in particular, in terms of the topological pressure $P(\beta)$ [9]. This function depends on a real parameter β. Varying its value allows us to scan the dynamical structure of the system. Moreover, the average Lyapunov exponent and, for a system with escape, the escape rate and the dimension of the fractal repeller, can be calculated from the topological pressure $P(\beta)$. This formalism has already been applied to diffusion in the one-dimensional lattice Lorentz gas [10–14].

Escape processes have been considered for different systems such as one-dimensional mappings [15,16], chaotic-scattering systems [7,17,18], and systems with a color dynamics [19], as well as in spatially extended systems with absorbing boundaries on the external borders of the system [3,6,7]. Until now, little work has been devoted to the escape of particles or trajectories from inside the system. In this direction, Kaufmann *et al.* studied processes of transient chaotic diffusion in one-dimensional mappings and in chains with lateral escape besides an escape from the ends of the chain [20,21]. For those systems, Kaufmann generalized the escape-rate formula of Ref. [3] (see Ref. [21]).

The purpose of the present paper is to study a two-dimensional (2D) periodic reactive Lorentz gas with the possible escape of particles from inside the system due to the presence of absorbing disks, modeling reactive centers where the moving point particle is annihilated. In a previous paper [22], we considered a 2D periodic reactive Lorentz gas, where the reaction is a reversible isomerization of the point particle between states A and B, also known as a color dynamics. In the present paper, our aim is to study a similar model but with a reaction of annihilation, instead of an isomerization. As in Ref. [22], the point particle undergoes elastic collisions on hard disks fixed in the plane. Some of the disks—called sinks or absorbers—have absorbing boundaries: the point particle is absorbed upon collision on one of those absorbing disks. All the other disks are inert for the reaction, so that the reaction scheme is the following if we call X the moving particle:

$$X + \text{inert disk} \leftrightarrow X + \text{inert disk}, \tag{1}$$

$$X + \text{sink} \rightarrow \emptyset + \text{sink}. \tag{2}$$

In the periodic case, the inert disks and the sinks form regular arrays. This system is an open Lorentz gas in the sense that the point particle escapes when colliding on a sink. Therefore, most particles will disappear from the system except for a set of zero probability forming a fractal repeller composed of the trajectories which move forever between the sinks. The decay in the number of particles due to the annihilation is characterized by an escape rate which is equivalent to the reaction rate in such models.

In the present paper, one of our aims is to establish a relationship between the reaction rate, on the one hand, and the characteristic quantities of the fractal and chaotic properties of the repeller, on the other hand, which are its Hausdorff dimension and the average Lyapunov exponent.

The paper is organized as follows. The model is introduced in Sec. II. The escape process and the fractal repeller are studied in Sec. III. A nonequilibrium measure defined on the fractal repeller is defined in Sec. IV, which allows us to calculate the average Lyapunov exponent in Sec. V. The pressure function defined in the case of the Lorentz gas is

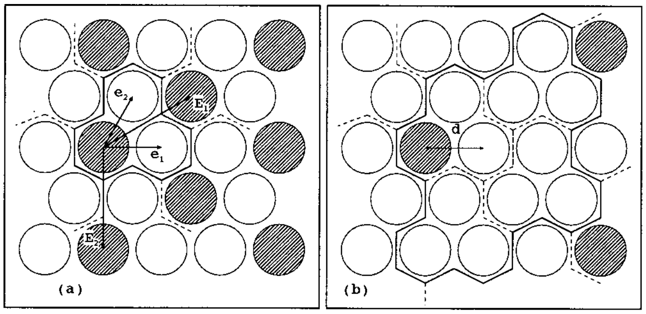

FIG. 1. (a) Elementary cell of the superlattice of the sinks, in the case $n=1$; (b) in the case $n=2$.

presented in Sec. VI, with the derivation of relations between the escape rate, the dimensions of the fractal repeller, and the average Lyapunov exponent. Finally, the dependence of the escape rate and of the codimension of the fractal repeller on the density of sinks is presented in Sec. VII. The conclusions are drawn in Sec. VIII.

II. DESCRIPTION OF THE MODEL

In a two-dimensional periodic Lorentz gas, a point particle undergoes elastic collisions on hard disks fixed in the plane and forming a regular triangular lattice. Let us denote the distance between the centers of the disks as d, and their radius, being equal to unity in the numerical calculations, as a. We shall work in the finite horizon regime $2a<d<4a/\sqrt{3}$, for which the diffusion coefficient is known to be finite [23,24]. In our model, some of the disks are sinks which absorb the moving particle upon collision. These sinks form a regular triangular superlattice over the disk lattice. The fundamental vectors of the disk lattice are $\mathbf{e}_1=d(1,0)$ and $\mathbf{e}_2=d(\frac{1}{2},\sqrt{3}/2)$. Those of the sink superlattice are $\mathbf{E}_1=nd(\frac{3}{2},\sqrt{3}/2)$ and $\mathbf{E}_2=nd(0,-\sqrt{3})$, where n is an integer parameter controlling the density of sinks in the system: in the directions of $\mathbf{E}_1$ and $\mathbf{E}_2$, one disk over n is a sink. Configurations with $n=1$ and $n=2$ are depicted in Fig. 1. For $n=1$, the fundamental cell of the superlattice contains three disks, among which one is a sink which can be chosen as shown in Fig. 1(a). The shape of this fundamental cell is used as the building block for the fundamental cell for larger n, as shown in Fig. 1(b) for the case $n=2$. Therefore, for larger n, the fundamental cell of the superlattice is made of $n\times n$ of these blocks of three disks. Accordingly, one disk over $N=3n^2$ is a sink, so that the density of all the disks ρ_d and the density of the sinks ρ_s are:

$$\rho_d=\frac{2}{\sqrt{3}d^2} \tag{3}$$

and

$$\rho_s=\frac{\rho_d}{N}=\frac{2}{3\sqrt{3}(nd)^2}, \tag{4}$$

respectively. The phase-space coordinates of the particle are its position and its velocity (x,y,v_x,v_y). The collisions with the disks being elastic, the energy of the particle is conserved and the magnitude of the velocity is a constant of motion $\|\mathbf{v}\|=v$. In the numerical calculations, we shall take it equal to unity, $\|\mathbf{v}\|=1$. The energy shell defines a three-dimensional phase space where the coordinates of the particle are (x,y,ψ), ψ being the angle between the velocity and the x axis. Using the periodicity of this system, we can study its dynamics in an elementary cell of the sinks superlattice, containing $N=3n^2$ disks. We shall use the Birkhoff coordinates $\mathbf{x}=(j,\theta,\varpi)$, with $1<j<N=3n^2$, $0\leqslant\theta<2\pi$, and $-1\leqslant\varpi\leqslant1$. The integer j defines the disk of the elementary cell on which the collision takes place, θ is an angle giving the position of the impact on this disk, and $\varpi=\sin\phi$ is the sine of the angle ϕ between the velocity after collision and the normal at the impact. At an elastic collision, the velocity of the point particle changes instantaneously according to the collision rule

$$\mathbf{v}_i^{(+)}=\mathbf{v}_i^{(-)}-2(\mathbf{n}_i\cdot\mathbf{v}_i^{(-)})\mathbf{v}_i^{(-)}, \tag{5}$$

where $\mathbf{v}_i^{(+)}$ is the velocity after the ith collision, $\mathbf{v}_i^{(-)}$ is the velocity before the ith collision, and $\mathbf{n}_i$ is the normal at the impact point. We notice that, in Birkhoff coordinates, the dynamics reduces to a mapping which is known to be area preserving [7].

III. ESCAPE AND FRACTAL REPELLER

Our model is an open Lorentz gas: the point particle escapes when it is absorbed by a sink. Another type of open Lorentz gas, without reaction but with absorbing boundaries of large spatial extension, was studied in Ref. [6]. The methods developed in Ref. [6] extend to the present model, as we explain below.

For a typical initial condition $\Gamma_0=(x_0,y_0,\psi_0)$, the particle will collide on a sink and escape after a finite time: this time is called the escape time $\mathcal{T}_n(\Gamma_0)$, where n refers to the configuration of the sinks. Although this time is finite for most trajectories, there exist trajectories that never collide on a sink and remain trapped forever in the Lorentz gas. These trajectories can be periodic or nonperiodic. Because of the defocusing character of the collisions on the disks, these trajectories are unstable and form a fractal set of zero Lebesgue measure in phase space: this set is therefore called the fractal repeller $\mathcal{F}_n$. This fractal repeller is typical of the chaotic-scattering processes [6,7,16–18].

An evidence of the fractal character of this repeller is given by the escape time as a function of the initial condition, as shown in Fig. 2. This function is finite for almost all initial conditions, since the particle collides on a sink after a finite time. However, this time is infinite for trajectories trapped in the fractal repeller. They correspond to initial conditions on the stable manifold of a trapped trajectory. The singularities of the escape-time function are thus on a fractal set formed by the stable manifolds of the fractal repeller, $W_s(\mathcal{F}_n)$.

Figure 2 shows this escape time as a function of the initial

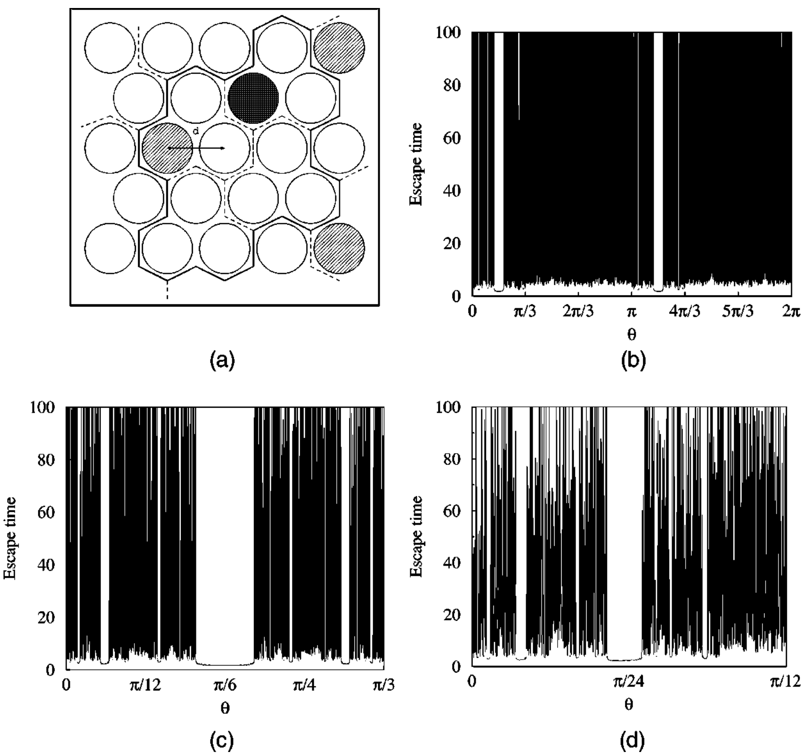

FIG. 2. Escape time function in the case when $n=2$ and $d=2.15$. (a) the initial positions are taken at a varying angle θ_0 around the black disk, the dashed ones being the sinks; the initial velocity is always taken along the normal of the disk so that $\varpi_0=0.0$ in Birkhoff coordinates. (b) $\theta_0 \in [0,2\pi]$. (c) $\theta_0 \in [0,\pi/3]$. (d) $\theta_0 \in [0,\pi/12]$. The scaling behavior appears in (c) and (d).

position at an angle θ_0 around a next-nearest-neighbor disk of the sink, shown in black in Fig. 2(a), in the case where $n=2$, and $d=2.15$. The velocity is normal to the disk. As can be seen in Fig. 2(b), the singularities seem to occupy most of the initial conditions, although they are of zero Lebesgue measure. This is due to the fact that the Hausdorff dimension of the fractal set is close to 1 (see below). The two largest windows of the escape time are centered at $\theta_0=\pi/6$ and $7\pi/6$. They correspond to the trajectories directly colliding on the two nearest sinks. The self-similar character of the fractal set appears in Figs. 2(c) and 2(d).

The escape dynamics of this system can be further described by a quantity called the escape rate [6]. Let us take N_0 initial conditions, forming a set $\{\Gamma_0^{(j)}\}$, chosen according to an initial measure ν_0 so that

$$d\nu_0(\Gamma)=\lim_{N_0\to\infty}\frac{1}{N_0}\sum_{j=1}^{N_0}\delta(\Gamma-\Gamma_0^{(j)})d\Gamma, \qquad (6)$$

where $\Gamma=(x,y,\psi)$. After a time t, only a number N_t of particles will remain in the system. This number will decrease monotonically with t. The set of particles remaining in the Lorentz gas at time t is given by those having an escape time $\mathcal{T}_n(\Gamma_0)$ larger than t:

$$\Upsilon_n(t)=\{\Gamma_0 : t<\mathcal{T}_n(\Gamma_0)\}. \qquad (7)$$

The decay of the number of particles is then described by

$$\lim_{N_0\to\infty}\frac{N_t}{N_0}=\nu_0[\Upsilon_n(t)]=\int_{\Upsilon_n(t)}d\nu_0(\Gamma_0). \qquad (8)$$

This decay is expected to be exponential since the trapped trajectories are exponentially unstable and the system is spatially periodic. The escape rate is thus defined as

$$\gamma=\lim_{t\to+\infty}-\frac{1}{t}\ln\nu_0[\Upsilon_n(t)]. \qquad (9)$$

The escape rate is a characteristic quantity of the system, independent of the initial measure ν_0 chosen, as long as this latter is smooth enough. The escape rate is easily accessible by numerical computations, as shown in Fig. 3. The logarithm of the fraction of particles remaining in the system after a time T, N_T/N_0, is plotted as a function of T. The slope gives the escape rate. In this example, $n=2$ and $d=2.25$, and we obtain $\gamma=0.0378$.

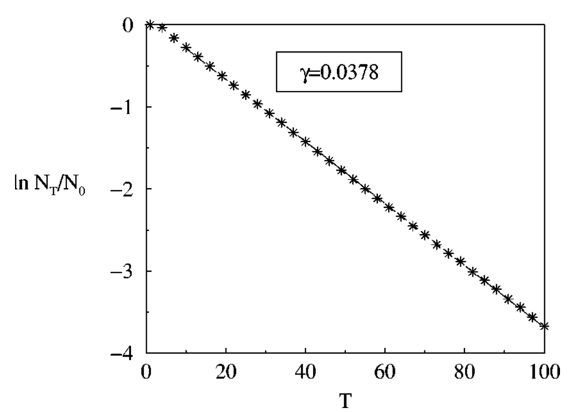

FIG. 3. Logarithm of the fraction of particles remaining in the Lorentz gas at time T, N_T/N_0, as a function of time T, in the case when $n=2$ and $d=2.25$. The slope gives the escape rate: here $\gamma=0.0378$.

IV. NONEQUILIBRIUM PROBABILITY MEASURE

For a system with escape, the ergodic hypothesis is not appropriate since most trajectories escape after a finite time: a time average does not provide interesting information. On the contrary, we are expecting that the important information is contained in the trajectories forever trapped inside the system. The invariant measure we are interested in thus has the fractal repeller $\mathcal{F}_n$ as support. This invariant measure can be constructed by considering statistical averages over all the trajectories which have not yet escaped during a time-reversal symmetric interval $[-T/2,+T/2]$ and, thereafter, taking the limit $T\to\infty$. Indeed, the trajectories which do not escape during $[0,+T/2]$ have initial conditions on the stable manifolds of the repeller, $W_s(\mathcal{F}_n)$, in the limit $T\to\infty$. On the other hand, the initial conditions of the trajectories which do not escape during $[-T/2,0]$ approach the unstable manifolds $W_u(\mathcal{F}_n)$ in the same limit. In the limit $T\to\infty$, imposing no escape over the whole interval $[-T/2,+T/2]$ selects trajectories which approach closer and closer the repeller given by the intersection:

$$W_s(\mathcal{F}_n)\cap W_u(\mathcal{F}_n)=\mathcal{F}_n . \tag{10}$$

Statistical averages over these selected trajectories define an invariant measure having the fractal repeller for support [5,7].

In systems with a time-reversal symmetric collision dynamics such as the present one, statistical averages calculated over the aforementioned invariant measure are equivalent to statistical averages over a conditionally invariant measure defined by selecting the trajectories which do not escape during $[0,+T/2]$ only and taking the limit $T\to\infty$ (for further information, see Refs. [5–7,25]). This conditionally invariant measure was shown in Ref. [6] to be given by

$$d\mu_{\rm ne}(\Gamma)=\lim_{T\to+\infty}\frac{1}{T}\int_0^T dt\frac{1}{\nu_0[\Upsilon_n(T)]}I_{\Upsilon_n(T)}(\Phi^{-t}\Gamma)\,d\nu_0(\Phi^{-t}\Gamma), \tag{11}$$

where $I_{\mathcal{E}}(\Gamma)$ is the indicator function of the set $\mathcal{E}$ in phase space and ν_0 is the initial measure [Eq. (6)]. The ensemble average is here taken over the trajectories which are still in the system at time T. In the limit of low densities of sinks, we note that the system tends to the closed Lorentz gas, whereupon the invariant and the conditionally invariant measures reduce to the microcanonical equilibrium invariant measure. In this limit, the escape process stops and the fractal repeller fills the whole phase space. Using measure (11), we shall now define the average Lyapunov exponent, the topological pressure and the fractal dimensions of the repeller for the open system.

V. AVERAGE LYAPUNOV EXPONENT

According to the conditionally invariant probability measure [Eq. (11)], the positive Lyapunov exponent is defined as the average of the logarithm of the stretching factors Λ_T at time T over the N_T particles still in the system at this time [6],

$$\lambda=\lim_{T\to\infty}\lim_{N_0\to\infty}\frac{1}{T}\frac{1}{N_T}\sum_{j=1}^{N_T}\ln\Lambda_T(\Gamma_0^{(j)}). \tag{12}$$

In the case of the Lorentz gas, the stretching factor can be obtained as follows [6].

Consider a front of particles issued from the same initial position but with different velocity angles. This front is characterized by a radius of curvature $R(\Gamma_t)$, Γ_t being a reference trajectory considered at time t. For Γ_t, the ith collision is supposed to occur at the time t_i. Between two collisions, this radius of curvature increases linearly with the time as

$$R(\Gamma_t)=v(t-t_{i-1})+R_{i-1}^{(+)}, \tag{13}$$

where v is the particle velocity, t_{i-1} is the time of the previous collision, and $R_{i-1}^{(+)}$ is the radius of curvature after the previous collision. Therefore, the radius of curvature before the ith collision is given by $R_i^{(-)}=R(\Gamma_{t_i})$. At an impact, the radius of curvature is modified according to the geometry of the collision: the relation between the curvature before and after the ith collision is given by

$$\frac{1}{R_i^{(+)}}=\frac{1}{R_i^{(-)}}+\frac{2}{a\cos\phi_i}, \tag{14}$$

where ϕ_i is the angle between the vectors $\mathbf{v}_i^{(+)}$, and $\mathbf{n}_i$ introduced in Eq. (5).

Using Eqs. (13) and (14), we can calculate the stretching factor [6,7], and we obtain

$$\Lambda_T(\Gamma_0)=\exp\int_{T_0}^{T}\frac{v}{R(\Gamma_t)}dt =\frac{t_1}{T_0}\left\{\prod_{i=2}^{n}\left[1+\frac{v(t_i-t_{i-1})}{R_{i-1}^{(+)}}\right]\right\}\left[1+\frac{v(T-t_n)}{R_n^{(+)}}\right] \tag{15}$$

for a segment of trajectory with n collisions such that $0<T_0<t_1$ and $t_n<T$. The time integral in Eq. (15) should start from a strictly positive time $T_0>0$ since here we assume that the radius of curvature is set equal to zero at the initial condition, $R_0^{(+)}=0$. We note that several choices are here possible, which all lead to the same value for the average Lyapunov exponent [Eq. (12)].

Numerically, the positive Lyapunov exponent is obtained by plotting the average of the logarithm of the stretching factor as a function of time according to Eq. (12), the slope giving the Lyapunov exponent. An example is depicted in Fig. 4, in the case when $n=2$ and $d=2.25$: here $\lambda=1.9$. An important observation is that the Lyapunov exponent varies very slightly with the density of sinks: the dependence is smaller than the numerical error. A similar robustness was observed for the open Lorentz gas with external absorbing boundaries [6].

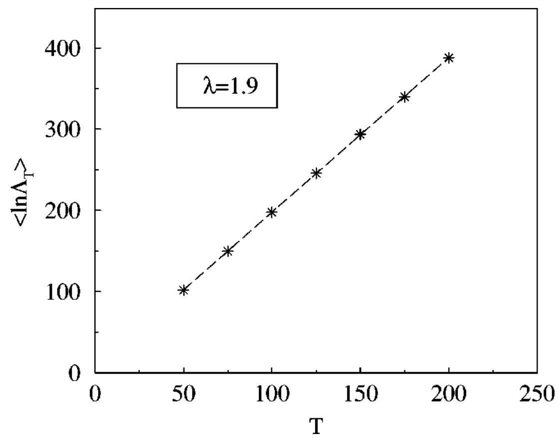

FIG. 4. Average of the logarithm of the stretching factors, as a function of time T, in the case when $n=2$ and $d=2.25$. The slope gives the average Lyapunov exponent $\lambda=1.9$.

VI. LARGE-DEVIATION FORMALISM

A. Topological pressure

The dynamics on the fractal repeller can be characterized in an efficient way thanks to the large-deviation formalism and, in particular, in terms of the topological pressure. This function depends on a real parameter β: by varying its value, we are able to scan the dynamical structure of the system [9]. In the case of a Lorentz gas, the topological pressure can be defined as follows [6]:

$$P(\beta)=\lim_{T\to+\infty}\lim_{N_0\to\infty}\frac{1}{T}\ln\frac{1}{N_0}\sum_{j=1}^{N_T}[\Lambda(\Gamma_0^{(j)})]^{1-\beta}. \quad (16)$$

Using the definition of the escape rate [Eqs. (8) and (9)], Eq. (16) can be rewritten as

$$P(\beta)=-\gamma+\lim_{T\to+\infty}\lim_{N_0\to\infty}\frac{1}{T}\ln\frac{1}{N_T}\sum_{j=1}^{N_T}[\Lambda(\Gamma_0^{(j)})]^{1-\beta}. \quad (17)$$

As can be seen from Eq. (16), for $\beta<1$, the dominant contribution to $P(\beta)$ is due to the most unstable trajectories corresponding to the largest values of Λ. Conversely, for $\beta>1$, the less unstable trajectories dominate. For $\beta=1$, Eq. (17) reduces to [9]

$$P(1)=-\gamma. \quad (18)$$

Moreover, the derivative of $P(\beta)$ with respect to β taken at $\beta=1$ gives us the Lyapunov exponent [9]

$$\lambda=-P'(1). \quad (19)$$

The topological pressure has been computed numerically, using Eq. (16), in the case when $n=2$ and $d=2.25$, as shown in Fig. 5. The value of the escape rate obtained from Eq. (18), $\gamma=0.0378$, is equal to the simulation result shown in Fig. 3. In Fig. 5, corresponding to a periodic Lorentz gas with a finite horizon, we observe that the pressure function is regular, so that no dynamical phase transition occurs in this case.

B. Generalized fractal dimensions

Important tools to characterize the fractal properties of the repeller are its generalized fractal dimensions. When a probability measure is associated with a fractal, as is the case here, it forms most often a multifractal with nontrivial generalized fractal dimensions D_q. The embedding dimension of the repeller is here equal to three, since we are working in a three-dimensional phase space. Therefore, the fractal dimensions of the repeller belong to the interval $0\leq D_q<3$. We are not going to calculate immediately the dimensions D_q of the fractal repeller of the flow itself. Instead, we consider a line $\mathcal{L}$ across the stable manifolds of the fractal repeller $\mathcal{F}_n$. The intersection of this line with the stable manifolds of the fractal repeller is another fractal f_n, which is characterized by so-called *partial* fractal dimensions belonging to the interval $0\leq d_q<1$.

For given q, the dimension D_q is related to the partial dimension d_q by

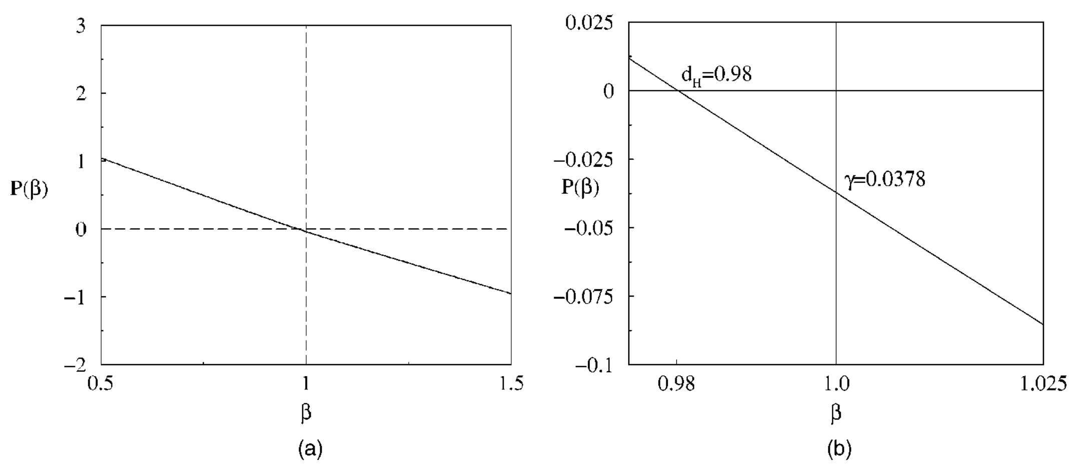

FIG. 5. (a) Topological pressure $P(\beta)$ in the case when $n=2$ and $d=2.25$. (b) Zoom of the region around $\beta=1$; the zero of $P(\beta)$ gives the value of the Hausdorff dimension $d_H=0.98$, and the value of $P(\beta=1)$ gives the escape rate $\gamma=0.0378$.

$$D_q = 2d_q + 1, \tag{20}$$

because the system is time reversal symmetric, so that the partial dimension in the stable direction is equal to the one in the unstable direction. Furthermore, the direction of the flow contributes a partial dimension equal to unity.

If we suppose a covering of the fractal f_n by intervals of equal length l, the generalized dimensions are defined as [26]

$$d_q = \lim_{l\to 0} \frac{1}{q-1} \frac{1}{\ln l} \ln \sum_{j=1}^{N_l} p_j^q, \tag{21}$$

where N_l is the number of intervals. For $q=0$, we find the usual definition of the Hausdorff dimension

$$d_H = d_0 = \lim_{l\to 0} -\frac{\ln N_l}{\ln l}. \tag{22}$$

For $q=1$, we obtain the so-called information dimension

$$d_I = d_1 = \lim_{q\to 1} d_q = \lim_{l\to 0} \frac{1}{\ln l} \sum_{j=1}^{N_l} p_j \ln p_j. \tag{23}$$

For a uniform probability measure, $p_j = p = 1/N$ for all the intervals, and the information dimension d_{I} is equal to the Hausdorff dimension d_H. In general, we expect the probability measure to be nonuniform and, therefore, the repeller to be multifractal, in which case $d_{\mathrm{I}} \neq d_H$.

A more general definition of d_q implies a covering of the fractal by intervals of various lengths l_j, $l_j < l$ [26]. The dimension d_q is obtained by imposing the quantity

$$\lim_{N\to\infty} \sum_{j=1}^{N} \frac{p_j^q}{l_j^{(q-1)d}} \tag{24}$$

to be of the order of unity. This is only the case for a critical value $d = d_q$ which defines the generalized dimension d_q.

In order to evaluate d_q in the case of our fractal repeller, let us consider the escape-time function along the line $\mathcal{L}$. The set of initial conditions for which the escape time is larger than T is composed of many small intervals forming a covering of the fractal f_n. If we consider a reference initial condition $\Gamma_0^{(j)}$ in a given interval j, the length l_j of this interval is inversely proportional to the stretching factor up to time T [6,15,16,29,30],

$$l_j \sim \frac{1}{\Lambda_T(\Gamma_0^{(j)})}, \tag{25}$$

and the probability of this interval is given by

$$p_j \sim \frac{\exp(\gamma T)}{\Lambda_T(\Gamma_0^{(j)})}. \tag{26}$$

Considering this covering, definition (24) of the generalized dimension d_q can be rewritten in terms of the topological pressure given by Eq. (17), as shown in Refs. [6,15,16,30]:

$$q\,\gamma = -P[q + (1-q)d_q]. \tag{27}$$

For $q=0$, the Hausdorff dimension d_H is thus found to be given by

$$0 = P(d_H). \tag{28}$$

Numerically, in the case when $n=2$ and $d=2.25$, the zero of the topological pressure gives us $d_H = 0.98$, as can be seen in Fig. 5(b).

By differentiating Eq. (27) with respect to q and taking $q=1$, the escape rate is obtained as

$$\gamma = -P'(1)(1-d_I) = \lambda(1-d_I). \tag{29}$$

We introduce the fractal codimensions as [6]

$$c_H = 1 - d_H, \tag{30}$$

$$c_I = 1 - d_I. \tag{31}$$

Equation (29) can thus also be written as

$$\gamma = \lambda c_I, \tag{32}$$

which expresses the escape rate—or reaction rate—in terms of the positive Lyapunov exponent and the information codimension.

C. Hausdorff codimension by the algorithm of Maryland

A numerical algorithm developed by the group of Maryland allows us to calculate the Hausdorff codimension of the fractal repeller [6,31]. The basic idea of this algorithm is to consider an ensemble of pairs of initial conditions, separated by ε, along the line $\mathcal{L}$ defined in Sec. VI B. A pair is said to be uncertain if there is a singularity of the escape-time function between both initial conditions. On the other hand, when the pair is certain, the initial conditions belong to an interval of continuity of the escape-time function. The fraction of uncertain pairs is known to depends on ε as

$$f(\varepsilon) \sim \varepsilon^{c_H}. \tag{33}$$

In the case of the Lorentz gas, a pair will be certain if the two trajectories undergo their successive collisions on the same disks. If we associate with each trajectory a symbolic sequence $\omega_0\omega_1\cdots\omega_n$, ω_i labelling the disk on which the ith collision takes place, the sequences are identical for a certain pair. The details of the algorithm used here are described in Ref. [6].

In Fig. 6, we have plotted the logarithm of the fraction of uncertain pairs as a function of the logarithm of the small ε separating the two initial conditions of a pair. The linear curve confirms the power-law behavior [Eq. (33)] and the slope gives us a value of the Hausdorff codimension equal to $c_H = 0.02$. This is in perfect agreement with the value of the Hausdorff dimension $d_H = 0.98$ obtained as the zero of the topological pressure in Fig. 5(b).

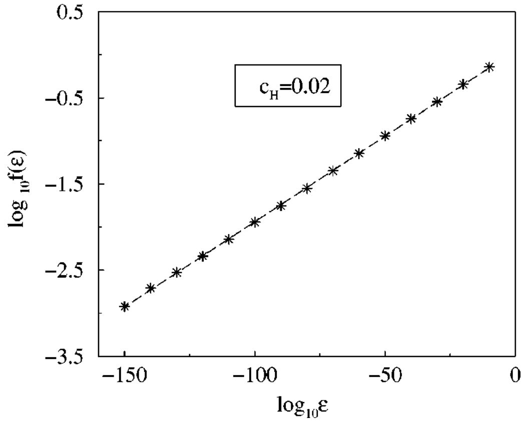

FIG. 6. Maryland algorithm: the logarithm of the fraction of uncertain pairs as a function of the logarithm of the difference ε between the two initial conditions of the same pair, in the case when $n=2$ and $d=2.25$, corresponding to Fig. 5. The slope gives the Hausdorff codimension $c_H=0.02$.

D. Escape rate in terms of the Hausdorff codimension and the average Lyapunov exponent

Thanks to the Maryland algorithm, we have numerically access to the Hausdorff codimension. It would therefore be interesting to rewrite the reaction rate [Eq. (32)] in terms of the Hausdorff codimension c_H instead of the information codimension c_I. For this purpose, we expand the pressure around $\beta=1$ to the second order in β and use expressions (18) and (19), as shown in Ref. [6]:

$$P(\beta)=-\gamma-\lambda(\beta-1)+\tfrac{1}{2}P''(1)(\beta-1)^2+o[(\beta-1)^2]. \tag{34}$$

This expansion is justified as long as the pressure function is regular around $\beta=1$, as observed in Fig. 5. The Hausdorff dimension being defined by Eq. (28) and the Hausdorff and information codimensions by Eqs. (30) and (32), we obtain

$$c_H=\frac{\gamma}{\lambda}-P''(1)\frac{\gamma^2}{2\lambda^3}+o(\gamma^2)=c_I-\frac{P''(1)}{2\lambda}c_I^2+o(c_I^2). \tag{35}$$

From this relation, we can deduce that the difference between c_H and c_I will become smaller and smaller when c_I itself decreases, which means when the information dimension of the fractal repeller d_I increases. The dimension of the fractal repeller increases when the escape rate decreases, that means for a low density ρ_s of sinks, i.e., of reacting centers. We can thus expect that the reaction rate [Eq. (32)] is given by

$$\gamma\simeq\lambda c_H \quad \text{in the limit} \quad \rho_s\rightarrow 0, \tag{36}$$

i.e., in the limit where the geometric parameter n of our model defined in Sec. II is large enough. Relation (36) is well verified numerically, as can be seen in Fig. 7 for different values of the interdisk distance d, in the case $n=2$. In Fig. 7(b), we depict the ratio $c_H/(\gamma/\lambda)$ of the Hausdorff codimension obtained by the Maryland algorithm to the information codimension given by $c_I=\gamma/\lambda$. We observe that this ratio is very close to the unit value, already for the configuration $n=2$ with only $N=12$ disks for one sink in the fundamental cell of the superlattice. This result confirms expectation (36).

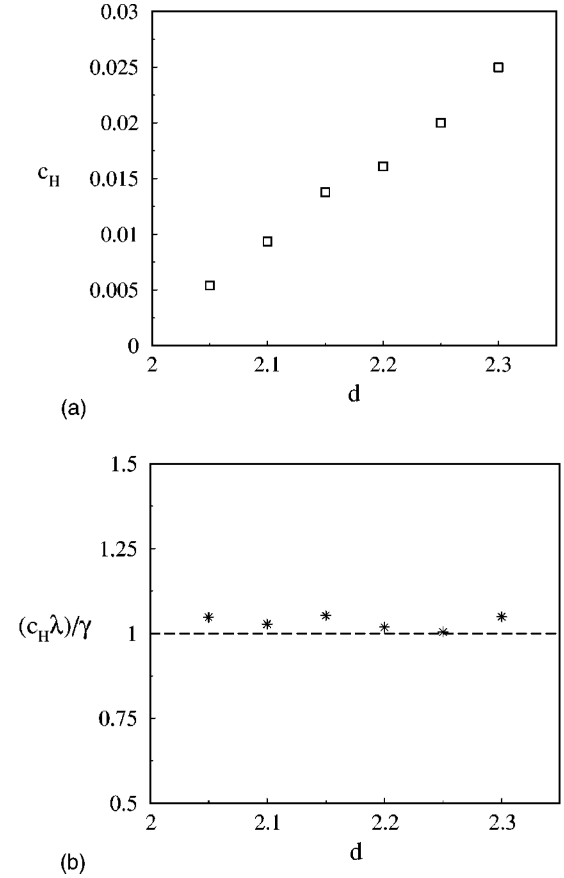

FIG. 7. (a) Hausdorff codimension as a function of the interdisk distance d, in the case $n=2$. (b) The ratio $c_H/(\gamma/\lambda)$ as a function of d, in the case $n=2$.

The remarkable feature of relation (36) is that it connects directly two quantities characterizing the microscopic chaotic dynamics of the Lorentz gas, namely, the average Lyapunov exponent λ and the Hausdorff codimension c_H of the fractal repeller, together with a third quantity describing the global macroscopic behavior of this open system, namely, the escape rate γ which is identical to the reaction rate.

VII. DEPENDENCE OF THE ESCAPE RATE AND HAUSDORFF CODIMENSION ON THE DENSITY OF SINKS

If the sinks are dilute in the periodic Lorentz gas, the density ρ of the moving particle may be assumed to evolve according to the diffusion equation

$$\partial_t\rho\simeq D\nabla^2\rho \tag{37}$$

on spatial scales larger than the interdisk distance d but smaller than the mean distance between the sinks. For the periodic Lorentz gas with a finite horizon, the diffusion coefficient D is positive and finite [23,24], and its values are known numerically [7,27].

For low enough sink densities, the annihilation reaction is thus controlled by the diffusion of the moving particle among the disks of the Lorentz gas. In the limit $\rho_s \to 0$, we can therefore obtain an estimation of the reaction rate by a method first proposed by Smoluchowski [32]. Because of the annihilation reaction at each sink, the moving particle escapes at a rate γ, which causes the solutions of Eq. (37) to decay exponentially $\rho \sim \exp(-\gamma t)$. The escape rate γ can thus be estimated by the eigenvalue problem

$$\left(\nabla^2 + \frac{\gamma}{D}\right)\rho = 0. \tag{38}$$

Because of the absorption of the moving particle at the sink, the density ρ should be assumed to vanish on the border of the sink, where we impose a Dirichlet boundary condition

$$\rho(r=a,t)=0. \tag{39}$$

Strictly speaking, Eqs. (38) and (39) are not valid in the small scale $r \simeq a$, but we must impose an absorbing boundary condition at the sink, and Eq. (39) is a convenient way to satisfy this condition within Smoluchowski's theory [32].

Furthermore, the triangular symmetry of the superlattice implies that Neumann boundary conditions should be considered on the border of hexagonal cells centered on each sink of the superlattice,

$$\partial_n \rho(r,t)|_{\rm hex} = 0, \tag{40}$$

where ∂_n denotes a derivative perpendicular to the border. Indeed, the escape rate should correspond to the leading eigenfunction of Eq. (38), which is expected to be extremum on the borderlines between the sinks. These borderlines form hexagons centered on each sink.

The solution of the eigenvalue problem [Eqs. (38)–(40)] can be obtained in polar coordinates by expanding the eigenfunction in a basis formed by the Bessel functions of integer order, $J_m(qr)$ and $Y_m(qr)$, multiplied by the trigonometric functions $\cos(m\theta)$ and $\sin(m\theta)$, with $\gamma = Dq^2$. The coefficients of this expansion should be determined by imposing boundary conditions (39) and (40) on the eigenfunction. Moreover, the escape rate should be given by the leading eigenvalue. In this way, we obtain the following asymptotic dependence for the escape rate on $N=3n^2$,

$$\gamma \simeq C \frac{D}{d^2 N \ln N} \quad \text{for} \quad N \to \infty, \tag{41}$$

where D is the diffusion coefficient, d is the interdisk distance, one disk over N is a sink, and C is a dimensionless constant. We note that the logarithmic correction $\ln N$ in the escape rate [Eq. (41)] has its origin in the two-dimensional character of the Lorentz gas.

In Eq. (41), the dimensionless constant C can be approximated by imposing boundary condition (40) on a circle of radius $r = nd/2$, instead of a hexagon. In this approximation, the leading eigenfunction of Eq. (38) is simply given by a linear superposition of the zeroth-order Bessel functions, $J_0(qr)$ and $Y_0(qr)$ with $\gamma = Dq^2$, and the boundary conditions are satisfied if

$$Y_0(qa) J_1\left(\frac{qnd}{2}\right) \simeq J_0(qa) Y_1\left(\frac{qnd}{2}\right). \tag{42}$$

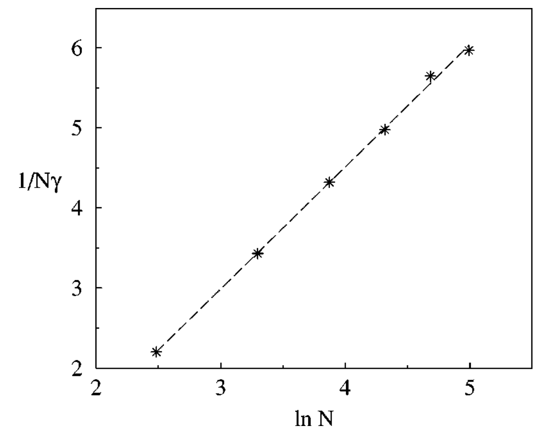

FIG. 8. Dependence of the escape rate γ on the sinks density: one disk over N is a sink, N taking the values 12,27,48,75,108, and 147 (with $d=2.25$). The dependence $\gamma \sim 1/N \ln N$, predicted by Smoluchowski's theory, is verified here.

Using the known expansions of the Bessel functions near $q=0$ [28], we obtain as asymptotic expression [Eq. (41)] with an approximate value $C \simeq 16$ for the approximation of the hexagon by a circle. We remark that the constant C turns out to be determined only by the Neumann boundary condition [Eq. (40)] and not by the small scale where the absorbing boundary condition [Eq. (39)] is taken.

When the Neumann boundary condition [Eq. (40)] is imposed on a hexagon, a numerical approximation can be computed for the same constant C, as performed in a previous work devoted to another type of two-dimensional reactive Lorentz gas [22]. In Ref. [22], the continuous diffusion process of Eq. (38) was approximated by a random walk model, and the numerical approximation $C \simeq 15.5$ was obtained in the limit $N \to \infty$ for boundary conditions corresponding to Eqs. (39) and (40) with a hexagon. We should thus expect that the exact dimensionless constant is close to the value $C \simeq 15.5$ in Eq. (41).

In order to verify the theoretical prediction [Eq. (41)] here, we have computed the escape rate γ by simulation of the deterministic and reactive Lorentz gas for $N=27,48,75,108$, and 147, with $d=2.25$. We have then plotted $1/N\gamma$ as a function of $\ln N$, as can be seen in Fig. 8. The linear behavior of this curve confirms the dependence $\gamma \sim 1/N \ln N$. Moreover, the value of the slope, here 1.526, allows us to check the value of the constant C. Since the diffusion coefficient for the Lorentz gas in the case $d=2.25$ is equal to $D=0.205 \pm 0.003$ [6], our simulation gives the value $C=16.15 \pm 0.40$, which is in reasonable agreement with the value expected from Smoluchowski's theory. We attribute the deviation to the relative smallness of

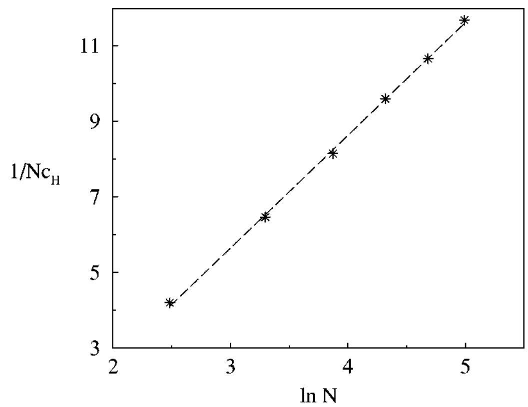

FIG. 9. Dependence of the Hausdorff codimension c_H on the sinks density: one disk over N is a sink N, taking the values 12,27,48,75,108, and 147 (with $d=2.25$). Considering the relation $\gamma \simeq \lambda c_H$, we expect a dependence of c_H on N of the form $c_H \sim 1/N \ln N$, that is indeed observed here.

the configurations for which the present simulation has been carried out. The agreement should improve if the simulation was pushed to still larger sizes N.

According to relation (36), we can expect the same dependence on N for the Hausdorff codimension c_H, with a constant $C' = C/\lambda$. We have computed c_H using the Maryland algorithm, for $N=27,48,75,108$, and 147, and $d=2.25$. Figure 9 depicts $1/Nc_H$ as a function of $\ln N$. Again we observe a linear behavior, the slope being equal to 2.985. C' is then equal to 8.5, which is in good agreement with the value $C/\lambda = \frac{16.15}{1.9} = 8.5$ expected from the direct numerical simulation of the escape rate.

Combining Eqs. (36) and (41) and expressing the result in terms of densities (3) and (4), we obtain a theoretical estimation for the Hausdorff codimension of the fractal repeller in a periodic Lorentz gas with a superlattice of sinks

$$c_H \simeq \frac{\sqrt{3}C}{2} \frac{D(\rho_d)}{\lambda(\rho_d)} \frac{\rho_s}{\ln(\rho_d/\rho_s)} \quad \text{for} \quad \rho_s \to 0. \tag{43}$$

This Hausdorff codimension is given in terms of the diffusion coefficient D, the positive Lyapunov exponent λ, the density of disks ρ_d, the density of sinks ρ_s, and a dimensionless constant C determined only by the geometry of the superlattice of sinks. We note that, in the limit $\rho_s \to 0$, both the diffusion coefficient D and the Lyapunov exponent λ tend to their value for the periodic Lorentz gas without sink. In this limit, both quantities D and λ depend only on the density of disks ρ_d and on the geometry of the lattice of disks, provided that the horizon is finite in order for $D(\rho_d)$ to take a finite value. Formula (43) confirms that the fractal repeller fills the whole phase space as the density of sinks decreases because the Hausdorff codimension vanishes in this limit.

VIII. CONCLUSIONS

In this paper, we have studied an annihilation process induced by the dynamical chaos of the two-dimensional Lorentz gas, for periodic configurations of disks and sinks. We have shown the existence of a fractal repeller formed by the trajectories of particles that never escape out of the system. We have defined a nonequilibrium measure on the fractal repeller, which allows us to characterize its chaotic and fractal properties. In this way, we have obtained the different characteristic quantities of the repeller, which are the escape rate, the positive Lyapunov exponent, and the fractal dimensions. From the expression of the topological pressure, relation (36) between the escape rate γ, the positive Lyapunov exponent λ, and the Hausdorff codimension c_H of the fractal repeller has been obtained in the limit of low densities of sinks. This relation has been numerically verified. In the present model, the importance of relation (36) holds in the fact that the escape rate gives the reaction rate, which can thus be expressed in terms of the underlying microscopic chaos. On these grounds, we have studied the dependence of the escape rate γ and of the Hausdorff codimension c_H on the density of sinks.

In the periodic system with one sink over N disks, we have observed that the escape rate decreases with a dependence of the form $\gamma \simeq C(D/d^2 N \ln N)$, as predicted by the diffusion theory of two-dimensional systems. We have numerically verified that the Hausdorff codimension c_H has a similar dependence on N, which is in good agreement with Eq. (36). This result led us to derive expression (43) for the Hausdorff codimension as a function of the densities of disks or sinks. The two-dimensional character of the Lorentz gas, together with the periodicity of the system, is at the origin of a logarithmic correction on the densities.

In conclusion, this work reveals that fractals are of special importance in chaotic models of reactions by annihilation in spatially extended systems, and that the properties of such reactive processes can be quantitatively studied by the escape-rate formalism. In particular, the reaction rate can be expressed in terms of the Lyapunov exponent and the Hausdorff dimension of fractal sets dynamically generated by the reaction.

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