Deterministic diffusion in flower-shaped billiards

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We propose a flower-shaped billiard in order to study the irregular parameter dependence of chaotic normal diffusion. Our model is an open system consisting of periodically distributed obstacles in the shape of a flower, and it is strongly chaotic for almost all parameter values. We compute the parameter dependent diffusion coefficient of this model from computer simulations and analyze its functional form using different schemes, all generalizing the simple random walk approximation of Machta and Zwanzig. The improved methods we use are based either on heuristic higher-order corrections to the simple random walk model, on lattice gas simulation methods, or they start from a suitable Green-Kubo formula for diffusion. We show that dynamical correlations, or memory effects, are of crucial importance in reproducing the precise parameter dependence of the diffusion coefficent.

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I. INTRODUCTION

One of the central themes in the theory of nonequilibrium statistical mechanics is to assess the importance of deterministic chaos for understanding transport processes such as diffusion [1,2]. Simple model systems appear to be most suited for studying the detailed relation between microscopic chaos and macroscopic transport. Along this line of research, the parameter dependent diffusion coefficients of strongly chaotic dynamical systems have been investigated for one- and two-dimensional mappings [3–7], periodic Lorentz gases [8], and billiards in an external field [9]. That diffusion coefficients can be fractal functions of control parameters was first observed in a simple one-dimensional mapping generalizing a random walk on the line [5,6]. The origin of this fractality may be attributed to the topological instability of orbits under parameter variation, which affects the parameter dependence of the diffusion coefficient in a nontrivial way. Based on the analysis of such simple systems, it was conjectured that fractal diffusion coefficients are rather generic for low-dimensional fully chaotic dynamical systems exhibiting some spatial periodicity [5,6]. Indeed, recently it was found that in case of billiards in an external field the diffusion coefficient again exhibits a highly irregular structure [9].

The standard periodic Lorentz gas is one of the typical models for studying deterministic normal diffusion (see, e.g., Refs. [1,2] and further references therein). That it is strongly chaotic and exhibits normal diffusion was proven by Bunimovich and co-workers [10–12]. Machta and Zwanzig have calculated the diffusion coefficient of this model from computer simulations at some parameter values, and they have matched their results to a simple analytical random walk approximation [13]. That the diffusion coefficient in the standard periodic Lorentz gas is indeed a nontrivial function of the parameter was first reported in Ref. [8]. Here the analysis by Machta and Zwanzig was refined by suggesting two methods for systematically correcting their random walk approximation. However, whether the numerically detected irregularities in the diffusion coefficient were of a fractal nature remains an open question. More recently, a third approximation scheme was proposed by deriving a Green-Kubo formula that exactly generalizes the Machta-Zwanzig approximation [14]. Applying all these methods led to the conclusion that including long-term correlations, or memory effects, was indispensable for reproducing the precise functional form of the parameter dependent diffusion coefficient for the standard periodic Lorentz gas.

One of the essential problems in the analysis of diffusion in the standard periodic Lorentz gas is that the parameter range of normal diffusion is very limited. In this small region, the irregular behavior of the parameter dependent diffusion coefficient shows up on very fine scales and appears to be rather smooth within the range of precision available from computer simulations [8,15]. Consequently, the question about the existence of a fractal diffusion coefficient is very difficult to answer for this model. As the main reason for this behavior, it might be suspected that the topological instability of the standard periodic Lorentz gas under parameter variation is not strong enough to generate more pronounced irregularities in this region. The main purpose of this paper is therefore to propose a billiard without an external field, which is very similar to the standard periodic Lorentz gas, but which has a geometry, and an associated range of control parameters exhibiting normal diffusion, with stronger topological instabilities. This way, we intend to learn more about the emergence of possible fractal structures for diffusion coefficients in billiards. As we will show, our model indeed generates a considerably stronger irregular parameter dependence of the diffusion coefficient than in the standard Lorentz gas. By applying the set of approximation methods mentioned above we argue that long-range dynamical correlations, or memory effects of orbits, are again at the origin of this irregularity, as in the case of simple one- and two-dimensional maps.

Our paper is composed of seven sections. In Sec. II, we introduce the flower-shaped billiard. Numerical results depicting the nontrivial parameter dependence of the diffusion coefficient are shown in Sec. III. In Secs. IV, V, and VI, we briefly review the different approaches to understanding the parameter dependence of diffusion coefficients in deterministic dynamical systems, i.e., the Machta-Zwanzig approximation, Klages-Dellago correction methods, as well as the approach based on a suitable Green-Kubo formula for diffusion, and we apply them to the flower-shaped billiard. Summary and conclusions are contained in Sec. VII.

II. THE FLOWER-SHAPED BILLIARD

The two-dimensional class of billiards we consider here consists of a point particle of mass m moving in a plane such that its Hamiltonian is

$$H=\frac{1}{2m}p_x^2+\frac{1}{2m}p_y^2, \tag{1}$$

where x and y denote the Cartesian coordinates of the position in the plane, while p_x and p_y are the corresponding momenta. The point particle undergoes elastic collisions with obstacles that are fixed in the plane. All the obstacles have the same shape, and their centers are situated on a triangular lattice according to

$$\mathbf{q}_c=m_c\boldsymbol{\ell}_1+n_c\boldsymbol{\ell}_2, \tag{2}$$

as defined in terms of the fundamental translation vectors of the triangular lattice,

$$\boldsymbol{\ell}_1=(0,1) \tag{3}$$

and

$$\boldsymbol{\ell}_2=\left(\frac{\sqrt{3}}{2},\frac{1}{2}\right), \tag{4}$$

where m_c and n_c are integers.

If all the pairs of integers are selected, we fill the whole triangular lattice with hard wall obstacles, and the billiard is invariant under the group of spatial translations generated by the vectors Eq. (2). Accordingly, the whole lattice can be mapped onto a so-called Wigner-Seitz cell with periodic boundary conditions. The elementary Wigner-Seitz cell of the triangular lattice is a hexagon of area

$$A_{WS}=|\boldsymbol{\ell}_1\times\boldsymbol{\ell}_2|=\frac{\sqrt{3}}{2}. \tag{5}$$

In this paper, we propose an open billiard consisting of flower-shaped obstacles instead of disks, which belongs to

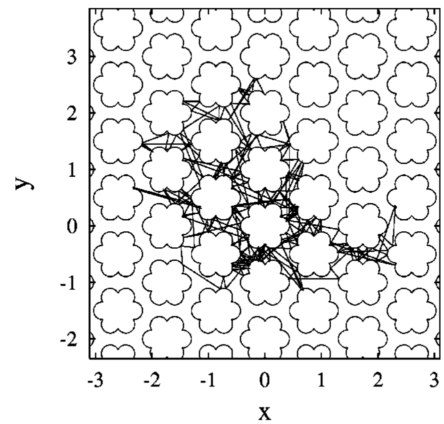

FIG. 1. The modified Lorentz gas as composed of a point particle moving freely in the spaces between the flower-shaped obstacles, which scatters elastically with the obstacles. In our case, mass $m=1$ and velocity $v=1$. The quantities plotted here and in the following figures are dimensionless.

the general class of periodic Lorentz gases whose normal diffusion has been proven by Bunimovich and co-workers [10–12]. The mixing property and the extension of such billiards to higher-dimensional gases have been studied by Chernov [16]. As shown in Fig. 1, the space between the obstacles forms the two-dimensional domain of the billiard, where the point particle moves freely and collides with the obstacles obeying the law of elastic reflection.

A single scatterer of our billiard is defined as follows. First, we consider the inner hexagon whose vertices are on the middle points of the sides of the hexagon of the elementary Wigner-Seitz cell, as depicted by the dotted lines in Fig. 2. Next, we join six arcs that have the same radii and touch the inner hexagon. Then we obtain the flower-shaped obstacle shown in Fig. 2. Note that the radius r of one arc that consists in a petal of the flower-shaped obstacle can be changed from $1/(4\sqrt{3})$ to infinity. According to this construction, the position space forms a two-dimensional torus. The motion of the point particle in the infinite lattice is unbounded so that transport by diffusion is *a priori* possible. Indeed, we will show that the diffusion of point particles in

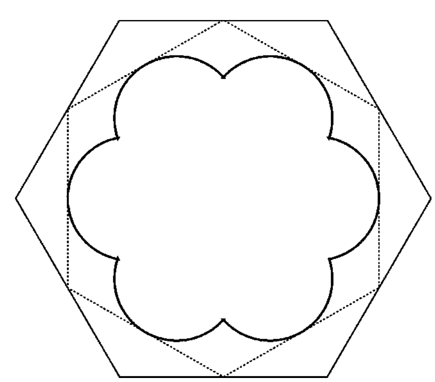

FIG. 2. Definition of a flower-shaped obstacle. The bigger hexagon (bold lines) is the elementary Wigner-Seitz cell. The arc always touches the smaller hexagon (dotted lines), which prohibits any infinite horizon.

the billiard of the flower-shaped obstacles is normal. When the dynamics is reduced to the Wigner-Seitz cell, the position of the particle inside this cell must be supplemented by a lattice vector of the type of Eq. (2) in order to determine the actual position of the particle in the infinite lattice. This lattice vector changes in discrete steps at each crossing of the border of the elementary Wigner-Seitz cell.

A billiard whose obstacles are disks, or, in higher dimensions, spheres, is called a periodic Lorentz gas, and this model serves as a typical example for studying deterministic diffusion [10–13,16,17]. The diffusion coefficient of this standard periodic Lorentz gas has been studied in various ways both analytically and numerically, where recent work focused particularly onto its density dependence (see Refs. [8,14] and further references therein). However, the density of this model cannot be varied much because of the condition of a finite horizon, which prohibits collision-free ballistic motion and thus guarantees the existence of normal diffusion [10–12,16]. Consequently, the diffusion coefficient exists in a very limited range of parameters only, and whether the diffusion coefficient of the standard periodic Lorentz gas is a fractal function of the density of scatterers appears to be an open question.

Let us introduce the Liouville equilibrium invariant measure given by

$$d\mu_e = I(x,y)\,\delta(H-E)\,dx\,dy\,dp_x\,dp_y\,, \tag{6}$$

where $I(x,y)$ is the indicator function of the billiard domain, and E is the energy of the point particle. Averages over this invariant measure are denoted by $\langle\cdot\rangle$. This measure is normalizable for the reduced dynamics in an elementary Wigner-Seitz cell, where the area of the billiard domain takes a finite value. In this finite case, the Liouville invariant measure is a probability measure, which defines the microcanonical ensemble of equilibrium statistical mechanics. The flower-shaped billiard belongs to the class of dispersing billiards whose hyperbolicity has been proven by Sinai [18]. Consequently, it is known that the motion of the point particle in the elementary Wigner-Seitz cell of our billiard is hyperbolic, in the sense that all orbits are unstable and of saddle type with nonvanishing Lyapunov exponents, and time averages are equal to averages over the Liouville equilibrium invariant measure.

III. CURVATURE DEPENDENCE OF THE DIFFUSION COEFFICIENT

Since the system of flower-shaped obstacles is fully chaotic, and by working in the regime of finite horizon, we may expect that diffusion is normal in the sense that the position is asymptotically a Gaussian random variable with a variance growing linearly in time. Consequently, the diffusion coefficient exists and is finite [10–12,16]. Indeed, we checked numerically that the variance is proportional to time after sufficiently long time evolution.

The diffusion coefficient D is given by the Einstein formula

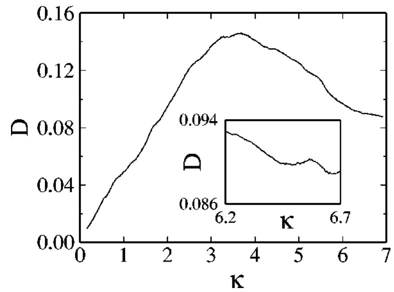

FIG. 3. Diffusion coefficient D (solid line) versus the curvature κ of the petal of the flower-shaped obstacles. The diffusion coefficient inceases approximately linearly for small enough κ until it reaches a global maximum. Inset: enlargement of the curve of the diffusion coefficient for larger κ showing the irregularity of this curve on fine scales.

$$D = \lim_{t\to\infty}\frac{1}{4t}\langle\{\mathbf{q}(t)-\mathbf{q}(0)\}^2\rangle, \tag{7}$$

and according to this formula the diffusion coefficient was calculated from computer simulations in the flower-shaped billiard, where the curvature κ of the petals is varied from 0 to its maximum, $4\sqrt{3}$. The results are depicted in Fig. 3. In this figure, we observe a nontrivial structure depending on the curvature κ of the arc defining the petal of the flower-shaped obstacles.

The gross features of the curvature dependence for the diffusion coefficient can qualitatively be explained as follows: When the curvature of the petal of the flower-shaped obstacle is zero, the inner hexagon shown by the dotted lines in Fig. 2 connects to the six hexagons surrounding it. In this case, the point particle remains forever localized in compact domains bounded by the three neighboring hexagons. For this specific value of the control parameter, the motion of the point particle is completely predictable because the compact domain is an equilateral triangle, and the system is integrable.

When the curvature becomes positive, the point particle can run away from the compact domain, and diffusion occurs. As already explained, at all positive curvatures of the petal, even if they are very small, the motion of the point particle is fully chaotic and the horizon is finite, hence diffusion is expected to be normal. The diffusion coefficient starts to increase from zero according to the linear increase of the curvature of the petal, and related to the fact that the space between petals also increases.

When the radius of the petal is equal to $R_L = \sqrt{3}/4 \simeq 0.433$, which is the distance between the center of the hexagon and the tangent point to the hexagon, the obstacle becomes a disk of radius R_L, that is, for this parameter value our billiard is precisely the same as the conventional periodic Lorentz gas. This point corresponds to the curvature $\kappa \simeq 2.309$ in Fig. 2.

When the radius r of the curvature of the petal decreases below R_L, the point particle is much more likely to be trapped in the space between two obstacles. This appears to be due to the formation of wedges between any two petals of a flower-shaped obstacle.

The inset of Fig. 3 depicts an enlargement of the curve showing the fine structure on smaller scales with respect to curvature. We remark that the apparently continuous fluctuations therein are within the numerical errors, that is, we confirmed the convergence of our results within a precision of order 10^{-4} by taking an average over 10^{10} initial conditions. Unfortunately, with our computational power it is impossible to check whether this oscillatory behavior persists on even finer scales.

IV. MACHTA-ZWANZIG APPROXIMATION FOR DIFFUSION COEFFICIENTS

In Ref. [13], Machta and Zwanzig have obtained a simple analytical approximation for the diffusion coefficient of the periodic Lorentz gas, which yields asymptotically correct results in the limit of small gaps between disks. In this case, the particle is somewhat trapped for a long time in the triangular regions between three adjacent scatterers. Hence, the particle is supposed to loose the memory of its past itinerary due to the multiple scattering in the trap region, and the transition probabilities to the neighboring triangular cells are assumed to be equivalent. As was shown in Ref. [13], the average rate τ^{-1} of such transitions can be calculated from the fraction of phase space available for leaving the trap divided by the total phase space volume of the trap, leading to

$$\tau = \pi A/(3W), \tag{8}$$

where A is the area of the trap and W is the width of the gap between the disks.

The flower-shaped billiard has similar types of traps as the periodic Lorentz gas. Accordingly, the Machta-Zwanzig approximation can be applied to the flower-shaped billiard as well, and Eq. (8) holds again for the average trapping time. Hence, we only need to calculate the areas of the trap and the gap between the petals from simple geometrical considerations, yielding

$$A = \frac{3\sqrt{3}}{4} - 3h[\sqrt{3}h + \sqrt{r^2 - h^2}] \tag{9}$$

and

$$W = \tfrac{1}{2} - [\sqrt{3}h + \sqrt{r^2 - h^2}], \tag{10}$$

where

$$h = \frac{1}{2}\left(\frac{\sqrt{3}}{4} - r\right). \tag{11}$$

In the above, r denotes the radius of the curvature of the petal.

The distance l between the centers of the flower-shaped obstacles is $1/\sqrt{3}$. Assuming that the gap size W is very narrow leads to the Machta-Zwanzig random walk approximation for the diffusion coefficient

$$D_{MZ} = \frac{l^2}{4\tau}, \tag{12}$$

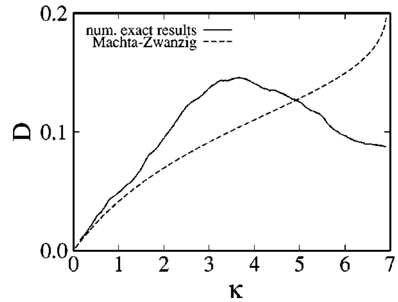

FIG. 4. Diffusion coefficient D (solid line) versus the curvature κ of the petal of the flower-shaped obstacle. The solid curve corresponds to the numerically exact results, while the dotted curve yields the Machta-Zwanzig random walk approximation Eq. (12).

with τ being given by Eq. (8) and supplemented by Eqs. (9)–(11) for the flower-shaped case. As is shown in Fig. 4, the Machta-Zwanzig approximation works very well in the vicinity of zero curvature of the petal only.

V. KLAGES-DELLAGO CORRECTIONS OF THE MACHTA-ZWANZIG APPROXIMATION

In Ref. [8], Klages and Dellago have generalized the Machta-Zwanzig approximation for the standard periodic Lorentz gas by taking memory effects of orbits into account. Their generalization is based on the observation that, except in the asymptotic limit of narrow gap sizes, the diffusive dynamics is not a simple Markov process, in the sense that there exist nonvanishing dynamical correlations. By mapping the orbit of a particle onto a suitable symbolic dynamics they numerically calculated the probabilities to obtain certain symbol sequences of finite length. Increasing the length of these symbol sequences yielded systematic corrections of the Machta-Zwanzig approximation. In Ref. [8], two schemes directly emerging from this approach were discussed, one suggesting simple heuristic corrections to the simple random walk model of diffusion Eq. (7), and another one employing lattice gas computer simulations defined by these probabilities. In this section, we apply these two methods to the flower-shaped billiard in order to systematically correct the Machta-Zwanzig approximation. A third scheme starting from a Green-Kubo formula for diffusion will be discussed in Sec. VI.

The Machta-Zwanzig approximation assumes that a particle jumps from one trap to a neighboring trap situated on the hexagonal lattice of traps. However, there exist nonvanishing probabilities that a particle can jump to next nearest neighbors, or even farther, without collisions. Accordingly, we should correct the Machta-Zwanzig approximation for the flower-shaped billiard by using the probabilities p_{cf1} and p_{cf2} of those collisionless flights which lead from one cell directly to its second nearest neighbors, or to its third nearest neighbors, respectively. The distances l_1 and l_2 between the center of a trap to the respective second and third neighbors are

$$l_1 = \sqrt{3}l, \quad l_2 = \sqrt{7}l. \tag{13}$$

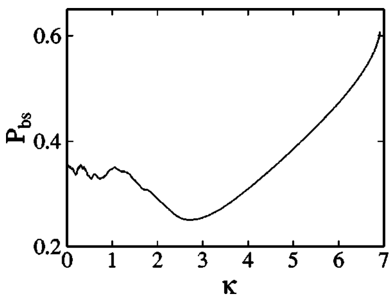

FIG. 5. Backscattering probability $p(z)$ (solid line) versus the curvature κ of the petal of the flower-shaped obstacle. In the case of a Markovian process it is equal to 1/3.

The diffusion coefficient D_{cf} with corrections due to these collisionless flights then reads

$$D_{cf}=(1-p_{cf1}-p_{cf2})D_{MZ}+p_{cf1}\frac{l_1^2}{4\tau}+p_{cf2}\frac{l_2^2}{4\tau}$$

$$=(1+2p_{cf1}+6p_{cf2})D_{MZ}. \qquad (14)$$

Next we take memory effects of orbits due to backscattering into account. For this purpose, orbits are coded by labeling the entrance through which a particle enters a trap as *z*, the exit to the left of this entrance as *l*, and that to the right as *r*. Thus, an orbit can be mapped onto a sequence of symbols z,l, and r. For example, $p(z)$ is the backscattering probability p_{bs}, which is the probability of the moving particle to leave the trap through the same gate where it entered. The Machta-Zwanzig approximation assumes that $p(z)=p(l)=p(r)=1/3$. However, in general, $p(z)$ is not close to 1/3 as shown in Fig. 5, because the actual orbits do not loose their memory during their itineraries.

A more profound explanation for the complicated functional form of $p(z)$ may be provided in terms of the theory of chaotic scattering: Chaotic scattering systems with multiple exit modes typically have fractal phase space boundaries separating the sets of initial conditions (basins) going to the various exits. However, open systems such as a three-disk scatterer of the periodic Lorentz gas possess the even stronger property of being *Wada*, that is, any initial condition which is satisfied on the boundary of one exit basin is also simultaneously satisfied on the boundaries of all the other exit basins [19]. Changing the curvature κ sensitively affects the highly irregular structure of these basin boundaries. Consequently, Fig. 5 may be understood as reflecting the topological instabilities of Wada basins under parameter variation, and as we will now show this is reflected in the parameter dependence of the diffusion coefficient.

Modifying the Machta-Zwanzig random walk by including the backscattering probability $p(z)$ we obtain the diffusion coefficient

$$D_{BS}=\frac{[1-p(z)]l_2^2}{4(2\tau)}=[1-p(z)]\frac{3}{2}D_{MZ}. \qquad (15)$$

Combining the effects of collisionless flights and backscattering yields as a first-order approximation

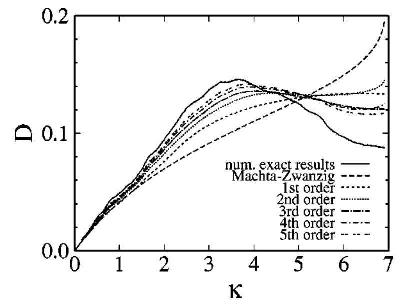

FIG. 6. Diffusion coefficients of higher-order approximations due to including higher-order backscattering probabilities. The solid curve corresponds to numerically exact results, while the other curves represent approximate solutions.

$$D_1=\tfrac{3}{2}[1-p(z)](1+2p_{cf1}+6p_{cf2})D_{MZ}. \qquad (16)$$

Higher-order approximations of the diffusion coefficient, as related to longer symbol sequences and respective probabilities such as $p(lrz\cdots)$, can be derived in the same way [8]. For the flower-shaped billiard, respective results are shown in Fig. 6.

The above correction methods assume that all orbits follow higher-order Markov processes, where correlations are present in the form of initial transient times before the variance becomes linear in time. This dynamics appears to be more suitably represented in the form of lattice gas simulations on a honeycomb lattice, where the sites of the lattice represent the traps. Indeed, for the periodic Lorentz gas, such lattice gas simulations were performed in Ref. [8] confirming the fast convergence to the numerically exact results. Compared to that scheme, the convergence of the intuitive correction method described above is, first slower, and, second, not everywhere converging to the numerically exact results, which is due to the fact that this approach was purely of a heuristic nature.

We also performed lattice gas simulation in case of the flower-shaped billiard according to the following prescription: Particles hop from site to site with frequency τ^{-1}, which is identical to the hopping frequency used in the Machta-Zwanzig approximation. The hopping probabilities are given by the backscattering probability $p(z)$ and by those corresponding to respective longer symbol sequences. The diffusion coefficient is then obtained from the Einstein formula Eq. (7) in the limit when the variance is becoming proportional to time. The correlations in the actual orbits are thus systematically and exactly filtered out according to the length of the symbol sequences.

In Fig. 7, the results of such higher-order approximations according to lattice gas simulations are shown. One can see that the convergence to the numerically exact results is not only much better than in Fig. 6, but even exact. Strong memory effects are clearly visible especially after the diffusion coefficient curve takes its maximum. In the previous heuristic modifications to the simple random walk model, the dynamics was only modeled for a limited number of time steps as a Markov process. Figure 6 suggests that correlations as contained in the symbol sequences are more suitably represented by higher-order iterations in the form of lattice

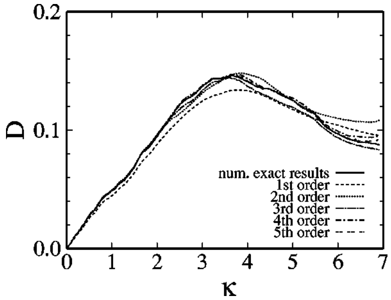

FIG. 7. Diffusion coefficient as obtained from lattice gas simulations based on higher-order backscattering probabilities. The solid curve corresponds to numerically exact results, while the other curves yield higher-order approximations.

gas simulations. However, a disadvantage is that the lattice gas scheme requires a second round of computations, which is put on top of the previous simulations, by again looking at the time evolution of an initial ensemble of points.

VI. THE GREEN-KUBO FORMULA APPROACH

The main drawbacks of the two methods described above were, first, that the heuristic corrections of the Einstein formula were not converging exactly to the numerically exact results, and, second, that the lattice gas simulations were merely a numerical scheme without being represented in the form of analytical approximations. These deficiencies were essentially resolved in Ref. [14] by the derivation of a Green-Kubo formula which employs the symbolic dynamics on the hexagonal lattice of traps introduced in Sec. V. The result reads

$$D=\frac{1}{4\tau}C_0+\frac{1}{2\tau}\sum_{n=1}^{\infty}C_n, \tag{17}$$

with

$$C_n:=\langle \mathbf{j}(\mathbf{x}_0)\cdot\mathbf{j}(\mathbf{x}_n)\rangle \tag{18}$$

being the velocity autocorrelation function related to jumps $\mathbf{j}(\mathbf{x}_n)$ on the hexagonal lattice at time step n. These jumps are suitably defined in terms of the lattice vectors Eqs. (3),(4). That is, any symbol sequence of an orbit on the hexagonal lattice of traps defines a respective chain of lattice vectors. The averages indicated by the brackets in Eq. (18) are calculated by weighting the respective scalar products of lattice vectors with the corresponding conditional probablities $p(\alpha\beta\gamma\cdots),\alpha,\beta,\gamma\in\{l,r,z\}$. In Eq. (17), τ is the mean time of free flight between symbol changes, and it is given by Eq. (8). Equation (17) is thus the honeycomb lattice analog to the Green-Kubo formula derived by Gaspard for the Poincaré-Birkhoff map of the periodic Lorentz gas [1,20].

It is easy to see that the first term in Eq. (17) yields the Machta-Zwanzig approximation Eq. (12). Higher-order corrections can then be calculated by defining the hierarchy of approximations,

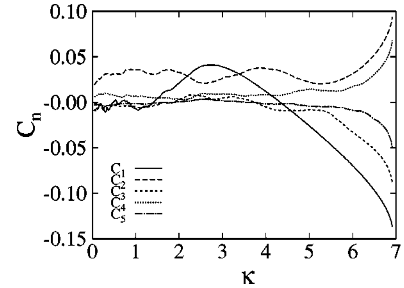

FIG. 8. Parameter dependence of the time-dependent correlation function C_n, see Eq. (18), as defined with respect to the symbolic dynamics on the hexagonal lattice of traps. At any parameter, C_n decays exponentially related to the fact that the Green-Kubo formula Eq. (17) is a convergent series. The speed of the convergence depends on the curvature. Obviously, in the large curvature region the correlation function decays more slowly than for small curvature.

$$D_n=\frac{l^2}{4\tau}+\frac{1}{2\tau}\sum_{\alpha\beta\gamma\cdots}p(\alpha\beta\gamma\cdots)\ell\cdot\ell(\alpha\beta\gamma\cdots), \tag{19}$$

with $n>0$ being the number of symbols and $D_0(w)$ given by Eq. (12), where, again, $\ell(\alpha\beta\gamma\cdots)$ are suitable lattice vectors.

The impact of dynamical correlations on the diffusion coefficient can now be understood by analyzing the single contributions in terms of the correlation function C_n as contained in the Green-Kubo formula Eq. (17). In fully chaotic systems such as the periodic Lorentz gas and the flower-shaped billiard, the velocity correlation function decays exponentially, which is in agreement with the results depicted in Fig. 8. By comparing this figure to Fig. 9 one can learn how the irregularities of the correlation function determine the parameter dependent diffusion coefficient: Let us start with the first-order approximation of Eq. (19), which reads $D_1=D_0+D_0[1-3p(z)]$. The functional form of $p(z)$ in Fig. 5 thus qualitatively explains the position of the global maximum of the diffusion coefficient, because at this value of the curvature the probability of backscattering is minimal. Adding up the three-jump contributions coming from C_2, furthermore, yields the most important quantitative contributions in this region of the curvature. In the region of large

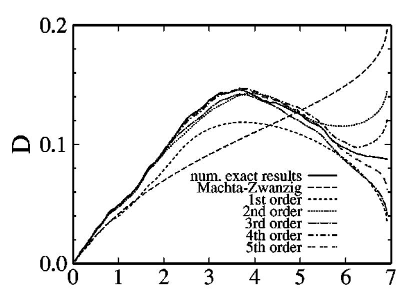

FIG. 9. Diffusion coefficients as obtained from the Green-Kubo formula Eq. (19). The solid curve corresponds to the asymptotic, numerically exact results, while the other curves yield the respective hierarchy of approximations.

curvature the diffusion coefficient decays monotonically according to the effect of two-hop correlations covered by C_1. However, note the large fluctuations of the correlation function C_n as well as of the diffusion coefficient approximations D_n in this regime, both indicating the dominant effect of long-range higher-order correlations. Studying the detailed convergence of the approximations depicted in Fig. 9 shows that correlations due to orbits with longer symbol sequences yield irregularities in the parameter dependence of the diffusion coefficients on finer and finer scales.

VII. SUMMARY AND CONCLUSION

In this paper, we have introduced a variant of the periodic Lorentz gas by assigning a flower-shaped geometry to the scatterers. Although both systems are rather similar in the sense that they are both fully chaotic and exhibit normal diffusion in a certain parameter range, we have found that the diffusion coefficient in the flower-shaped geometry is considerably more irregular under parameter variation than that obtained from circular disks as scatterers. We have analyzed these irregularities by three different methods, which all start from correcting the Machta-Zwanzig random walk approximation for the diffusion coefficient. All these improved approximation schemes use a symbolic dynamics, which maps the orbits of moving particles to symbol sequences according to traps situated on a hexagonal lattice. We have discussed the convergence of these different approximation schemes, and we have shown how they enable a detailed understanding of the precise shape of the parameter dependent diffusion coefficient in the flower-shaped billiard in terms of long-range dynamical correlations.

The Green-Kubo formula introduced in Ref. [14] appears to be most suitable for understanding the irregular behavior of the parameter dependent diffusion coefficient, because it conveniently transforms the diffusive dynamics into a sum over the velocity correlation function, whose specific parameter dependence can in turn be analyzed step by step. In particular, this approach yields an exact convergence to the parameter dependent diffusion coefficient as obtained from simulations.

Interestingly, when the correlation function decays in time, the frequency of oscillations as a function of the control parameter increases. The relation between this decay in time and the increase of the frequency of these oscillations determines the strength of the irregularities on fine scales of the resulting parameter dependent diffusion coefficient. The question of the existence of fractal diffusion coefficients in billiards such as periodic Lorentz gases with circular or flower-shaped scatterers might thus be answered by using Green-Kubo formulas if the respective correlation functions could be evaluated more precisely for large enough times. Indeed, in Ref. [9] the highly irregular diffusion coefficient of an open billiard in an external field has already been investigated along these lines by relating the Poincaré-Birkhoff version of the Green-Kubo formula to fractal Weierstrass functions. The joint efforts compiled in Refs. [8,9,14] may therefore be considered as first steps towards answering the conjecture of Refs. [5,6], which suggested a possible universality of fractal diffusion coefficients in low-dimensional fully chaotic dynamical systems exhibiting some spatial periodicity, for the case of chaotic Hamiltonian dynamical systems such as particle billiards.

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