Dynamical crossover in deterministic diffusion

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(Received 18 October 1996)

We study diffusion in a one-dimensional periodic array of scatterers modeled by a simple map. The chaotic scattering process of the map can be changed by a control parameter and exhibits a dynamics analogous to a crisis in chaotic scattering. We show that the associated strong backscattering induces a crossover between different asymptotic laws for the parameter-dependent diffusion coefficient. These laws are obtained from exact diffusion coefficient results and are supported by simple random walk models. We conjecture that the main physical feature of this crossover is present in many other dynamical systems exhibiting nonequilibrium transport. [S1063-651X(97)50502-2]

PACS number(s): 05.45.+b, 05.60.+w

One of the basic mechanisms in the theory of chaotic dynamical systems are crisis events, where the asymptotic dynamics of the system change dramatically with respect to the variation of a control parameter [1–3]. Recently, it was found that related events occur in simple chaotic scattering systems when the scattering rules are varied. This phenomenon has been called a crisis in chaotic scattering [4]. On the other hand, considerable literature has developed in which the origin of transport in nonequilibrium statistical mechanics has been connected to the characteristics of chaotic scattering processes [5]. One problem studied was deterministic diffusion in simple one-dimensional maps [6–9], where parameter-dependent diffusion coefficients have been computed by taking the complete equations of motion of the dynamical systems into account [10,11]. Related one-dimensional maps have been proposed in Ref. [4] as simple models that exhibit a crisis in chaotic scattering. Thus, the question arises whether features of a crisis in chaotic scattering have an impact on deterministic diffusion. We study a periodic continuation of the map of Ref. [4] on the real line so that it exhibits diffusive behavior. We find that the diffusion coefficient has a global structure with a crossover from linear to quadratic dependence on the slope. These algebraic laws have already been noticed by previous authors for similar maps, either obtained from simple approximations, or based upon calculations for special values of the slope [6,7,12]. We show that their suggestive arguments are quantitatively supported by the accurate parameter-dependent diffusion coefficient of the map and qualitatively by two simple random walk models. More detailed studies of the diffusion coefficient, and of the microscopic scattering process in this model, reveal that the specific shape of the crossover region depends on whether the map exhibits the dynamics of a crisis in chaotic scattering or not. However, generically this crossover is due to backscattering, and it should be encountered in many dynamical systems with nonequilibrium transport.

In the following, we consider discrete one-dimensional piecewise linear chaotic maps with uniform slope, $x_{n+1}=M_h(x_n)$, where h is a control parameter, and x_n is the position of a point particle at discrete time n. $M_h(x)$ is continued periodically beyond the interval $[0,1)$ onto the real line by a lift of degree one, $M_h(x+1)=M_h(x)+1$. We assume that $M_h(x)$ is antisymmetric with respect to $x=0$, $M_h(x)=-M_h(-x)$, i.e., that there is no drift imposed on a point particle [13]. As an example, we consider the sawtooth map sketched in Fig. 1. It was chosen as a periodic continuation of the map studied in Ref. [4], which exhibits a crisis in chaotic scattering. The control parameter is here the height h of the map, which is related to the absolute value of the slope a by $h=(a-3)/4$. The diffusive properties of similar maps have been studied in Refs. [6,7,9]. For this sawtooth map the parameter-dependent diffusion coefficient has been computed by solving the Frobenius-Perron equation of the dynamical system [2],

$$\rho_{n+1}(x)=\int dy \quad \rho_n(y) \quad \delta(x-M_h(y)), \tag{1}$$

where $\rho_n(x)$ is the probability density for points on the real line, and $M_h(y)$ is the map under consideration. There exists

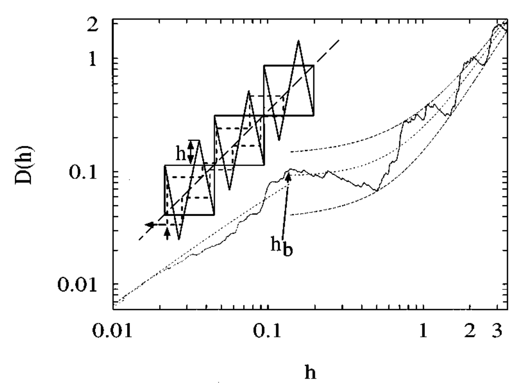

FIG. 1. Double logarithmic plot of the diffusion coefficient $D(h)$ with respect to the height h for the sawtooth map shown in the figure. The graph is based on 38 889 single data points. Two random walk solutions (dotted lines) and two curves, which approximately give the boundaries of the oscillations of $D(h)$ for values of h above the backscattering point h_b (dashed lines), are included.

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a dense set of parameter values h for which one can construct Markov partitions for the map, and for each of these parameter values Eq. (1) can be written as a matrix equation [10,11],

$$\boldsymbol{\rho}_{n+1}=(1/|a|)\ T\ \boldsymbol{\rho}_n . \tag{2}$$

$\boldsymbol{\rho}_n$ represents a column vector of the probability densities in each part of the Markov partition at time n, and T is a topological transition matrix, which can be obtained from the Markov partition. However, instead of solving the eigenvalue problem of T [10], here solutions for the probability density vector $\boldsymbol{\rho}_n$ have been obtained by iterating Eq. (2),

$$\boldsymbol{\rho}_{n+1}=(1/|a|^n)T^n\boldsymbol{\rho}_0 . \tag{3}$$

Starting with any probability density vector $\boldsymbol{\rho}_0$ this iteration method enables us to compute the exact time-dependent probability density ρ_n at any time step n and all other dynamical quantities based on probability density averages for maps of the type of $M_h(x)$ [11,14,15]. In particular, it provides an efficient way to calculate diffusion coefficients by employing an Einstein formula [6,8,9,12],

$$D(h)=\lim_{n\to\infty}\frac{1}{2n}\int dx\ \rho_n(x)x^2, \tag{4}$$

where the integral is the second moment of the time-dependent probability density [16].

Figure 1 shows a log-log plot of the diffusion coefficient as a function of h up to $h=3.5$. Included are four curves that describe the coarse-grained behavior of the exact results. There exist several methods to compute the diffusion coefficient for maps of this type for integer values of the height analytically [6,7,9–11]. By applying the eigenvalue method of Ref. [10] we get

$$D(h)=\frac{2h^3+3h^2+h}{12h+9}\to\frac{h^2}{6}\ \ (h\to\infty),\quad h\in N. \tag{5}$$

The two dashed curves give approximate limits for the oscillations of the exact diffusion coefficient in the range $h>h_b$. They are obtained by fitting the diffusion coefficient with the functional form of Eq. (5) at $h=(2k+1)/2$ and $h=(4k+3)/4$, $k\ \in N_0$, for the upper and lower curve, respectively. The two *dotted* curves show two simple random walk approximations, where it is assumed that the probability density of a scatterer is uniform. For large heights the distance a point particle travels at one time step by moving from one unit interval to another is taken into account exactly [2], and we get

$$D_{rw1}(h)=\int_0^{1/2}dx[M_h(x)-x]^2\to\frac{h^2}{6}\quad(h\to\infty), \tag{6}$$

which gives the dotted line plotted for $h>h_b$. For small heights the absolute value of the distance is approximated to either zero or one, depending on whether the particle remains on a unit interval or leaves it [6,8,12]. This leads to

$$D_{rw2}(h)=\frac{2h}{4h+3}\to\frac{2}{3}\ h\quad(h\to 0). \tag{7}$$

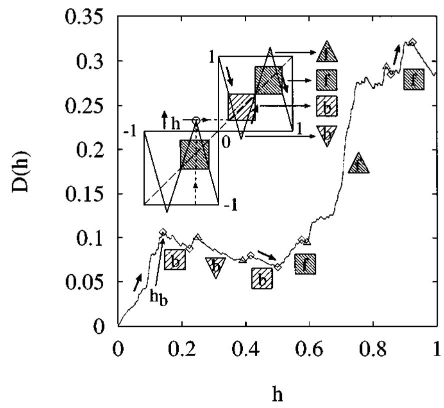

FIG. 2. Chaotic scattering in the sawtooth map and its connection to the behavior of the diffusion coefficient $D(h)$. Certain microscopic scattering mechanisms of the map are identified by shaded squares and triangles. The same symbols are shown along the $D(h)$ curve, where they indicate the impact of the respective scattering regions on the diffusion coefficient. The graph consists of 10 268 single data points.

These approximations indicate three different regions of coarse-grained behavior for the exact diffusion coefficient: The first one is a simple initial region, where the diffusion coefficient behaves linearly for small heights. For $h\geqslant h_b$ it decreases slightly on increasing the height. Finally, for $h\geqslant 0.5$ it starts to grow quadratically in the height, but with strong oscillations on a fine scale. The transition between the two different types of asymptotic coarse-grained behavior, which occurs in the crossover region of $h_b\leqslant h\leqslant 0.5$, can be understood by referring to the action of certain microscopic scattering mechanisms. They are introduced in Fig. 2, where certain regions of the map have been distinguished by shaded squares and triangles: The triangles refer to parts where points of one unit interval get mapped from that interval into another unit interval. Additionally, if points enter a square they preferably move into the triangular escape region above or below the respective square after some iterations. These squares are identical to the squares of an analogous scattering model, where they provide the basic mechanism for a crisis in chaotic scattering [4]. The abbreviations f (‘‘forward’’) and b (‘‘ backward’’) in these scattering regions refer to the dynamics of the critical point of the map, which is indicated by a small circle. Its first iteration is shown by the dashed line with the arrows. At its second iteration, and by increasing the height h continuously up from zero, the orbit of the critical point, denoted as the *critical orbit* in the following, travels along the graph of the map in the next right box from the upper left to the lower right, as indicated by bold black arrows. This way, the critical orbit explores all the different scattering regions of the map as h is increased from zero. If the orbit hits a region labeled by a b it is in a position to get *backscattered* into the box to the left. *Vice versa*, if the orbit enters an f region it is in a preferable position to move further *forward* to the next box to the right. The critical point indicated in Fig. 2 is part of a forward scattering region. Note that there is a dense set of points around the critical point that exhibits the same dynamics, at least for the first few iterations. An event dynamically analogous to the one that occurs at a crisis in chaotic scattering now occurs at the *point of strong backscattering*, defined by the parameter value of the height h_b for which the critical orbit of the forward scattering region hits the boundary of a backward scattering region in the next right box after one iteration for the first time. This case is illustrated in Fig. 2 and, for the map shown, is determined by $h_b=(\sqrt{17}-3)/8\simeq 0.1404$. We emphasize that this process is *topologically* not identical to a crisis, or a crisis in chaotic scattering, since it is not generated by the merging of two formerly isolated invariant sets in the phase space. Nevertheless, we argue that *dynamically* this process provides the same characteristics as a crisis in chaotic scattering, especially the onset of strong backscattering [4,11]. The squares and the triangles along the diffusion coefficient curve now refer to parameter regions where the critical orbit gets mapped into the respective scattering regions. The different symbols on the curve denote boundary points where the critical orbit enters, or leaves, these regions. The diffusion coefficient clearly decreases globally if the critical orbit enters a backscattering region, and it increases globally if it exhibits forward scattering. Hence, the different microscopic scattering mechanisms defined above are connected to regions in the macroscopic diffusion coefficient which exhibit different parameter-dependent behavior. We remark that the parameter region of backscattering corresponding to the broad crossover region in Fig. 1 is precisely identical to the respective parameter region in the model of Ref. [4] where enhancement of chaotic scattering, triggered by a crisis, occurs. Moreover, the backscattering point h_b indicates the first strong local maximum of the curve, as shown in Fig. 2. Magnifications reveal that the fine structure of the curve changes dramatically from quite regular below h_b to much more irregular just above, and that the curve is fractal [10]. These features can be understood in detail by refining the procedure explained above and reflect a drastic change in the microscopic dynamics of the model, which at the backscattering point h_b develops from rather simple to more complex motion [11,14].

Thus, the onset of strong backscattering affects the diffusion coefficient of the sawtooth map not only on a fine scale, but also on a coarse-grained scale. This phenomenon may be understood as a *backscattering-induced dynamical crossover in deterministic diffusion*. The extension and specific shape of the crossover region are due to the sawtooth map exhibiting the dynamics of a crisis in chaotic scattering. On the other hand, an onset of strong backscattering must eventually occur in any map of the type of $M_h(x)$ at a certain parameter value, independently of its special functional form. This can be checked by identifying the forward and backward scattering regions of a map and applying the definition of the backscattering point given above. As an example, the piecewise linear, discontinuous, nonsawtooth map studied in Ref. [10] has been analyzed. We find that the respective backscattering point of the map again corresponds to the first strong local maximum of the diffusion coefficient curve, and that again this point is related to a change between two different laws for the asymptotic diffusion coefficient. Since this map does not mimic the dynamics of a crisis in chaotic scattering, it lacks a broad crossover region right above its backscattering point. However, again the diffusion coefficient grows linearly for small values of the height, only the slope being different from that of the sawtooth map, and in the limit of large heights, the diffusion coefficient increases quadratically with a factor of 1/6, as in the case of the sawtooth map. Analogous results for asymptotic diffusion coefficients have been reported in Refs. [6,7] for many other maps of the type of $M_h(x)$, although in this previous work diffusion coefficients could be computed exactly only for special values of the height, and the asymptotic regimes could not be verified rigorously with respect to the full parameter-dependent diffusion coefficient. These results indicate that a backscattering-induced dynamical crossover should be typical for diffusive maps of the type of $M_h(x)$. In the limit of small heights, the asymptotic diffusion coefficient must always decrease linearly, as can be understood by a simple geometrical argument [6,12]. In the limit of large heights, we expect that it always increases quadratically with a factor of 1/6. Similar results may be obtained for certain classes of two-dimensional maps [2,17].

We conjecture that the main physical feature of this crossover, i.e., a connection between the onset of strong microscopic backscattering and a change in the behavior of macroscopic parameter-dependent transport coefficients, is quite common as well in more realistic Hamiltonian systems: For example, in Ref. [18] diffusion in two-dimensional periodic Coulombic potentials has been studied, and an energy threshold has been proved to exist above which the diffusion coefficient increases with a power law in the particle energy, whereas below this threshold no diffusion coefficient exists. In Ref. [4] it has been found that related models exhibit a crisis in chaotic scattering. The existence of this energy threshold might thus be linked to the dynamics of a crisis in chaotic scattering as in case of the dynamical crossover discussed above. Furthermore, for a crisis in chaotic scattering the significance of orbiting collisions has been pointed out, indicating the onset of strong backscattering [4]. However, orbiting collisions have already been studied in the framework of the kinetic theory of gases for Lennard-Jones fluids at low densities, and at low temperatures a qualitative connection between the onset of these collisions and a small change in the temperature-dependent behavior of transport coefficients has been noted [19]. Thus, physically one may connect the occurrence of certain microscopic chaotic scattering processes, or in special cases even crisis events, to a specific behavior of transport coefficients. These events may be linked to macroscopic dynamical crossover phenomena or, in certain cases, possibly even to dynamical phase transitions [20,21].

In summary, (a) the sawtooth map under consideration here was chosen as a diffusive version of a one-dimensional dynamical system exhibiting a crisis in chaotic scattering. A crossover in the parameter-dependent diffusion coefficient of this map has been found, linked to the dynamical mechanism of this crisis event. This suggests that the dynamics of a crisis in chaotic scattering can trigger a dramatic effect in nonequilibrium transport. (b) The dynamical crossover found here affects the diffusion coefficient of the model not only on a fine scale, but also on a coarse-grained scale, and induces a transition between two different algebraic laws for the asymptotic diffusion coefficient. (c) The crossover is understood physically by relating the onset of strong microscopic backscattering to a change in the behavior of the macroscopic parameter-dependent transport coefficient. This main physical feature is conjectured to be quite common in dynamical systems exhibiting non-equilibrium transport.

Helpful discussions with Chr. Beck, A. Latz, E. Ott, E. Schöll, T. Tél, and J. Yorke are gratefully acknowledged. R.K. is indebted to C. Grebogi for his continuing interest and support of this work, and he wants to thank S. Hess, the NaFöG Commission Berlin, the IPST, and the DFG for financial and other support. J.R.D. wishes to acknowledge support from the National Science Foundation under Grant No. PHY-93-21312 and No. PHY-96-00428.

[1] C. Grebogi, E. Ott, and J.A. Yorke, Phys. Rev. Lett. **48**, 1507 (1982); Physica D **7**, 181 (1983); C. Grebogi *et al.*, Phys. Rev. A **36**, 5365 (1987).

[2] E. Ott, *Chaos in Dynamical Systems* (Cambridge University Press, Cambridge, 1993).

[3] K.T. Alligood, T. Sauer, and J.A. Yorke, *Chaos: An Introduction to Dynamical Systems* (Springer, Berlin, 1997).

[4] Y.-Ch. Lai *et al.*, Phys. Rev. Lett. **71**, 2212 (1993); Phys. Rev. E **49**, 3761 (1994).

[5] See P. Gaspard and J.R. Dorfman, Phys. Rev. E **52**, 3525 (1995), and references therein.

[6] H. Fujisaka and S. Grossmann, Z. Phys. B **48**, 261 (1982); Phys. Rev. A **26**, 1179 (1982).

[7] Ch.-Ch. Chen, Phys. Rev. E **51**, 2815 (1995).

[8] M. Schell, S. Fraser, and R. Kapral, Phys. Rev. A **26**, 504 (1982).

[9] S. Grossmann and S. Thomae, Phys. Lett. **97A**, 263 (1983); T. Geisel and S. Thomae, Phys. Rev. Lett. **52**, 1936 (1984); R. Artuso, Phys. Lett. A **160**, 528 (1991); Physica D **76**, 1 (1994); R. Artuso, G. Casati, and R. Lombardi, Phys. Rev. Lett. **71**, 62 (1993); H.-Ch. Tseng, Phys. Lett. A **195**, 74 (1994).

[10] R. Klages and J.R. Dorfman, Phys. Rev. Lett. **74**, 387 (1995).

[11] R. Klages, *Deterministic Diffusion in One-Dimensional Chaotic Dynamical Systems* (Wissenschaft & Technik Verlag, Berlin, 1996).

[12] H.G. Schuster, *Deterministic Chaos*, 2nd ed. (VCH Verlagsgesellschaft mbH, Weinheim, 1989).

[13] The case with drift will be discussed elsewhere [J. Groeneveld, R. Klages, and J.R. Dorfman (unpublished)].

[14] R. Klages and J.R. Dorfman (unpublished).

[15] Applying the iteration method to large sets of parameter values of the height, time-dependent Gaussian probability densities with strong periodic fine structures have been obtained for the sawtooth map and for the piecewise linear map of Ref. [10]. Moreover, the kurtosis, time-dependent diffusion coefficients, and velocity autocorrelation functions have been computed. All these quantities show the characteristics of a simple statistical diffusion process on a coarse-grained scale; i.e., they increase linearly, or decrease exponentially, respectively, but with certain oscillations on a fine scale [11,14].

[16] The iteration method leads to values for $D(h)$, which are precise up to an order of 10^{-7} after maximally 15 iteration steps. Therefore, no error bars appear for the results presented in Figs. 1 and 2. Another approach to compute diffusion coefficients for maps of the type of $M_h(x)$ is based on a Green-Kubo formula and relates the parameter-dependent diffusion coefficient to a class of fractal functions which is defined by certain functional equations [11,14]. An even more efficient method has been developed by J. Groeneveld (unpublished).

[17] see I. Dana, N.W. Murray, and I.C. Percival, Phys. Rev. Lett. **62**, 233 (1989); J.D. Meiss, Rev. Mod. Phys. **64**, 795 (1992), and further references therein.

[18] A. Knauf, Commun. Math. Phys. **110**, 89 (1987); B. Nobbe, J. Stat. Phys. **78**, 1591 (1995); Diploma thesis, Technische Universität Berlin, 1995 (unpublished).

[19] R. Klages, S. Hess, and W. Loose, Verh. Dtsch. Phys. Ges. **26**, 1002 (1991); R. Klages, Diploma Thesis, Technische Universität Berlin, 1992 (unpublished).

[20] S.K. Nayak, R. Ramaswamy, and C. Chakravarty, Phys. Rev. E **51**, 3376 (1995); V. Mehra and R. Ramaswamy, *ibid.* **53**, 3420 (1996); Ch. Dellago and H.A. Posch, Physica A **230**, 364 (1996).

[21] Recent results indicate that an analogous dynamical crossover occurs in the diffusion coefficient of the two-dimensional periodic Lorentz gas with respect to the density of scatterers as a control parameter. Cf. Ch. Dellago, H. Posch, and R. Klages (unpublished).