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Transient chaos: the origin of transport in driven systems

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Abstract. – In open Hamiltonian systems transport is governed by chaotic saddles which are low-dimensional if a single-particle description can be used. We show that in systems where the motion of the particle is biased towards one direction, the chaotic set is never space filling. Its escape rate splits into two parts: *a*) a term proportional to the square of the bias; *b*) a term also present in the non-driven case which vanishes in the large system limit. These general results are equivalent to previous ones on thermostatted systems if the systems have identical entropy production.

The stochastic properties of chaotic dynamical systems make the description of transport processes in a deterministic single-particle picture possible. The relation between microscopic chaotic dynamics and macroscopic transport properties has been studied in closed thermostatted driven systems [1]-[3], as well as in open Hamiltonian non-driven systems [4]-[8]. Here we present a Hamiltonian approach to open systems driven in a given direction.

In infinite Hamiltonian systems subjected to external forces the kinetic energy of the particle would grow without bound. To avoid this growth, a Gaussian thermostat has been used in ref. [1]-[3] introducing dissipation into the systems. In such cases the particle dynamics exhibits chaos on a chaotic attractor. We take a different point of view avoiding the use of a thermostat. Open Hamiltonian systems of finite size L are considered where the dynamics is biased and transiently chaotic due to an underlying chaotic saddle [9]. The bias gives rise to a drift velocity v which can exhibit two different types of scaling in the limit of large system size: i) $v \sim 1/L$ or ii) $v = \text{const}$. The first type of behavior is found in single-particle motions among fixed scatterers under the influence of an external field F in the x direction. An example for this billiard-like picture is the driven Lorentz gas. The field has to be sufficiently weak so that the kinetic energy E_{kin} does notchange significantly when the particle crosses the system: $FL \ll E_{\mathrm{kin}}$ ([1]). Thus, the drift velocity v, which is proportional to F, is bounded from above by E_{kin}/L. The second type of behavior is characteristic for certain collective models of transport [10] where the drift velocity does not depend on the system size for large but fixed values of L (the largest allowed system size must, however, be on the order of $1/v$, *i.e.* $L_{\max} = C/v$). In both cases particles undergo a chaotic Hamiltonian dynamics in the interval $0 \le x \le L$, and under passing the borders at $x = 0$ or $x = L$ they escape in free motion. In the Poincaré surface-of-section, this can be modelled by a spatially extended area-preserving map with bias and absorbing boundaries.

Our approach is in spirit close to that of Gaspard and Nicolis who described diffusion in unbiased systems [4], [5]. Here we show that biased systems behave in a qualitatively different manner: the escape rate κ has a new contribution proportional to the square of the bias, and this can be the dominating term in the limit of large system size. We also find a remarkable relation between open Hamiltonian and thermostatted systems, since the present approach is equivalent to the description of transport by thermostatted systems if the systems produce the same amount of (irreversible) entropy.

For our general purpose the particular form of the dynamics is not important. We solely use the openness of the system and the Hamiltonian character of the dynamics, which imply chaotic scattering behavior of particles [11]. Thus, only exceptional trajectories are trapped in $0 < x < L$ forever, the majority escapes. According to the theory of transient chaos [9], for a broad class of systems, called hyperbolic, the escaping process is exponential. For any smooth initial distribution of particles, the number of survivors $N(t)$ decays after a sufficiently long time t as $N(t) \sim N_0 \exp[-\kappa t]$, where the escape rate κ is a basic characteristic of the chaotic saddle. This holds, for example, for any perturbed (or slightly opened) Lorentz gas [12]. Since we are interested in cases with macroscopic chaotic lifetimes, the escape rate has to be small.

We derive a relation between the (microscopic) escape rate, on the one hand, and the (macroscopic) drift and diffusion coefficients, on the other. To that end we demand the microscopic dynamics to be consistent with a (macroscopic) Fokker-Planck equation. Besides the drift v one has to take into account the random feature of deterministic chaos characterized by a constant diffusion coefficient D:

$$\frac{\partial P(x,t)}{\partial t} = -v \frac{\partial P(x,t)}{\partial x} + \frac{D}{2} \frac{\partial^2 P(x,t)}{\partial x^2}. \qquad (1)$$

Equation (1) has been shown to be valid for both the field-free Lorentz gas [13], and the limit of weak fields [3] provided that the scattering process is hyperbolic. Based on this, we take for granted that the macroscopic behavior of driven systems of the type considered here is governed by eq. (1). The open ends of the system are modelled by imposing $P(0,t) = P(L,t) = 0$. The solution of eq. (1) is then given by $P(x,t) = \sum_{n=1}^{\infty} c_n \exp[-\gamma_n t] \exp[\alpha x] \sin\left(\frac{n\pi}{L} x\right)$, where $\gamma_n = v^2/(2D) + n^2\pi^2 D/(2L^2)$, $\alpha = v/D$, and the coefficients c_n follow from the initial condition. The long-time behavior is dominated by the slowest decay mode $n = 1$ with decay rate γ_1. Consistency requires the identification of the microscopic and macroscopic rates so that

$$\kappa = \frac{1}{2} \frac{v^2}{D} + \frac{1}{2} \frac{D\pi^2}{L^2}. \qquad (2)$$

This is a key relation connecting the escape with transport quantities. The relation holds for

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([1]) This condition can indeed be fulfilled in macroscopic conductors. At room temperature an electron has a kinetic energy of about 30 meV, and a conductor has typically a specific resistivity of 1.5–10 $\times 10^{-8}$ Ohm m. In a wire with a length of 1 m and a cross-section of 1 mm^2, a current of 0.05–0.3 A is created by a potential difference 5 mV, so that $\Delta E_{\mathrm{kin}} = 5\,\mathrm{mV} \ll E_{\mathrm{kin}} = 30\,\mathrm{mV}$.

any open dynamical system that is compatible with the Fokker-Planck equation (1) in the macroscopic limit. In the special case of unbiased systems ($v = 0$) we recover the result of Gaspard and Nicolis [4]. The new observation is that in driven systems the escape rate has an additional term (the first one on the r.h.s. of eq. (2)) proportional to the square of the drift. In the billiard case it scales as $E_{\rm kin}^2/L^2$, and for large kinetic energy it can dominate eq. (2). Similarly, if the drift is constant, the first term dominates provided $Lv \gg D$ ([2]). In any case, in the drift-dominated limit one finds $\kappa = v^2/(2D)$. This corresponds to the physically interesting limit of taking large systems with a weak current running through them.

From the point of view of macroscopic transport our problem is one-dimensional. We do not need to specify the microscopic dynamics in detail, but it has to be Hamiltonian. This requires at least two degrees of freedom and a flow in a three-dimensional energy shell. The chaotic motion is related to an underlying chaotic saddle, and it can faithfully be represented by a two-dimensional Poincaré map. Asymptotically, transport is governed by trajectories that stay inside the scattering system for a long time. The corresponding particles concentrate more and more along the unstable manifold of the chaotic saddle. In the Poincaré plane, the general relation $d_1 = 2 - \kappa/\lambda$ connects the information dimension d_1 of this manifold with the escape rate κ and the average Lyapunov exponent λ of the chaotic saddle [14]. From eq. (2) we obtain d_1 in leading order in v and $1/L$:

$$d_1 = 2 - \frac{1}{2}\frac{v^2}{D\lambda_{\infty,0}} - \frac{1}{2}\frac{D\pi^2}{L^2\lambda_{\infty,0}}, \tag{3}$$

where $\lambda_{\infty,0}$ is the Lyapunov exponent in the infinite unbiased system. The dimension d_1 of the unstable manifold can thus be expressed via macroscopic parameters, and $\lambda_{\infty,0}$ as the only microparameter. The deviation from the value 2 contains a term proportional to v^2, and a term due to diffusion. The first two terms of eq. (3) yield d_1 in the drift-dominated limit. They are exactly of the form of d_1 of the chaotic attractor present in biased thermostatted systems as predicted by Vance [2] and Chernov *et al.* [3]. The first and the last terms are equivalent to the formula of Gaspard and Nicolis valid in unbiased systems [4]. Our result thus provides a connection between these cases. An explanation of this correspondence can be given in terms of identical entropy production [15].

We now illustrate the general result of eq. (2) by means of an analytically tractable model, which is an extension of Gaspard's multi-baker map [5] to driven systems. It consists of a chain of N identical boxes of linear size a coupled to each other along the x-axis (fig. 1 *a*)). Each box has the same internal dynamics, which is defined in fig. 1 *b*) and carried out at integer multiples of a discrete time unit τ. The area ratio of the two middle horizontal strips in fig. 1 *b*) is p/q, such that $s_2 = (1-l-r)p$ and $s_1 = (1-l-r)q$, where $q = 1-p$. These strips remain inside the square under the mapping. The parameters p and q specify the internal dynamics inside the boxes, while l and r characterize the coupling between neighboring boxes. The full chain has free ends that allow particles to escape. The dynamics is area preserving, and the motion of a particle in the chain is described by chaotic scattering. In order to study the time evolution of phase space densities, let us consider a partitioning of the chain by the vertical strips defined by the one-step dynamics. There are four strips in each box. In box k, the symbols $4k$, $4k+1$, $4k+2$, and $4k+3$ mark the strips (fig. 1 *c*)). The partition is generating [16], *i.e.* it defines a unique symbolic dynamics, which for the chain of length N consists of $4N$ symbols.

The chaotic properties of a system with a generating partition can be described by a transfer matrix T [17]. The elements $t_{i,j}$ of T represent the probability to go from strip i to strip j. In

([2]) The right-hand side of eq. (2) coincides with the exact slowest decay rate of certain lattice-gas models of finite size (G. M. Schütz, private communication).

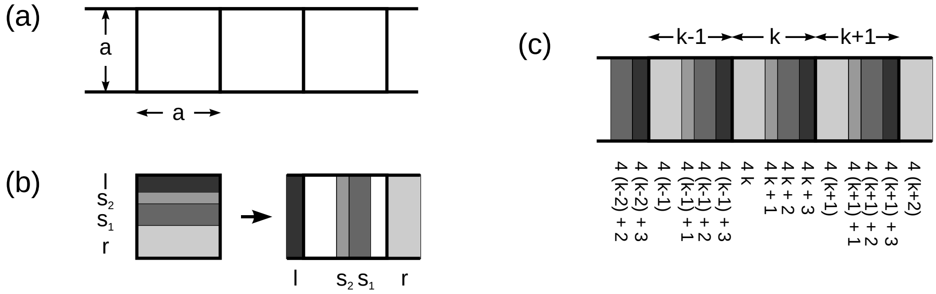

Fig. 1. – The biased multi-baker map. *a*) Geometry. In an open multi-baker map, there are N squares of size $a \times a$, each of which contains a baker map that allows for escape to and entering from the neighboring squares. *b*) Action of the map on a single cell. Four horizontal strips are squeezed and stretched such that the map is area-preserving and the resulting vertical strips exactly fit into the boxes. The two strips of width $s_1 a$ and $s_2 a$ in the middle stay inside the same square; the strips of width ra and la leave the square to the right and the left, respectively. Strips from the neighboring boxes are mapped to the corresponding free spaces. *c*) $4N$ vertical strips inside the chain form a generating partition defining a symbolic dynamics which describes the dynamics on the chaotic saddle responsible for transport.

our case the non-zero matrix elements occur only for stripes i, j in the same or neighbouring cells. They can be expressed by the parameters l, s_1, s_2, and r. The escape rate κ from the chaotic saddle of the chain is directly related to the largest eigenvalue ξ of T [9]: $\kappa\tau = -\ln \xi$. With the condition $P(0,t) = P(N+1,t) = 0$, we find

$$\kappa\tau = -\ln\left[s + 2\sqrt{lr}\cos\left(\pi/(N+1)\right)\right], \tag{4}$$

where $s = 1 - l - r$. For large N, κ tends to a constant with a correction $\sim N^{-2}$.

To discuss other characteristics of chaotic scattering, we use the so-called free-energy function $\beta F(\beta)$, which is the Legendre transform of the spectrum of local Lyapunov exponents [11], [17]. From this function one can extract quantities characterizing the chaotic dynamics. A straightforward generalization of the transfer matrix concept to arbitrary parameters β [17] leads to the statement that there is a matrix $T(\beta)$ whose largest eigenvalue is $\chi(\beta) = \exp[-\beta F(\beta)]$. This matrix has the same structure as T but the elements are now of the form $t^{\beta}_{i,j}$. Using the same argument as above, we find

$$\beta F(\beta) = -\ln\left[s^{\beta}(p^{\beta} + q^{\beta}) + 2(lr)^{\beta/2}\cos\frac{\pi}{N+1}\right]. \tag{5}$$

This expression interpolates between the single-cell result ($N = 1$) and the large-system result obtained in the limit $N \to \infty$.

Finally, we discuss the connection between the microscopic and the macroscopic description of transport. The transfer matrix description via $T(\beta = 1)$ is equivalent to a Markov chain description [18] of a random walk, because it only depends on the jump probabilities, and not on the intra-cell dynamics. There is a limit of random walk processes that leads to the Fokker-Planck equation (1). This limit requires $D \equiv \frac{a^2}{\tau}(r + l) \gg \frac{a^2}{\tau}(r - l) \equiv a\,v$, where a is the cell size and τ the unit time; the jump probabilities are

$$l = \frac{1}{2}\left(D\frac{\tau}{a^2} - v\frac{\tau}{a}\right), \quad r = \frac{1}{2}\left(D\frac{\tau}{a^2} + v\frac{\tau}{a}\right), \tag{6}$$

i.e. the sum of these probabilities is much larger than their difference. This is the condition for having a result compatible with eq. (1). This condition contains both macroscopic parameters

D and v of the Fokker-Planck equation. For large system size and small drift velocity one indeed recovers eq. (2) by inserting eq. (6) into eq. (4) with $L \equiv aN$ as the total length of the chain.

Note that the escape rate is the only characteristic of chaos that can be expressed by parameters independent of the intra-cell dynamics. In all other cases the micro parameters, like p or the time or space units, remain involved (cf. eqs. (5), (6)).

To conclude, we have shown that the escape from biased dynamical systems with large but finite extent is closely related to two macroscopic phenomena: drift and diffusion. This Hamiltonian approach to discuss transport is equivalent to the thermostatted one [1]-[3] if the production of thermodynamic entropy is the same. Moreover, the approach can be extended to deal with other transport coefficients such as viscosity or heat conductivity: the close connection between the respective transport coefficients has been pointed out in a recent generalization of the unbiased escape rate formalism [6]. Equation (2) remains valid in the general case, too, where v and D denote the bias and the diffusion coefficient of the generalized transport process, respectively.

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