PHYSICAL REVIEW E **72**, 025204(R) (2005)

Fractional kinetic model for chaotic transport in nonintegrable Hamiltonian systems

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(Received 14 April 2005; published 31 August 2005)

We propose a kinetic model of transport in nonintegrable Hamiltonian systems, based on a fractional kinetic equation with spatially dependent diffusion coefficient. The diffusion coefficient is estimated from the remainder of the optimal normal form for the given region of the phase space. After partitioning the phase space into building blocks, a separate equation can be constructed for each block. Solving the kinetic equations approximately and estimating the diffusion time scales, we convolve the solutions to get the description of the macroscopic behavior. We show that, in the limit of infinitely many blocks, one can expect an approximate scaling relation between the Lyapunov time and the diffusion (or escape) time, which is either an exponential or a power law. We check our results numerically on over a dozen Hamiltonians and find a good agreement.

DOI: 10.1103/PhysRevE.72.025204   PACS number(s): 05.45.−a, 05.60.Cd, 05.20.Dd

Statistical treatment of chaotic transport is one of the most difficult problems in nonintegrable Hamiltonian dynamics. Despite its importance for many practical problems in various fields, e.g., plasma physics [1,2] and dynamical astronomy [3], we still lack a general and consistent kinetic theory of transport. The main reason is the complicated nature of the phase space of the typical nonintegrable Hamiltonian system, since it usually contains a "topological zoo" of regular and chaotic structures mixed on an arbitrarily small scale. The most promising way for overcoming these difficulties is, in our opinion, the so-called fractional kinetics of the phase space [4]. Fractional kinetics has become a broad topic of research not only in Hamiltonian dynamics but also in very different areas such as solid-state physics [5] and physics of complex systems [6]. The basic advantage of the fractional kinetic equation (FKE) for describing chaotic transport is that its fractional nature allows one to include the self-similarity of phase space and time, which arises from the first principles, i.e., from the dynamical equations. Especially important is the phenomenon of the so-called stickiness [3] or dynamical trapping [7], which leads to long intervals of quasiregular motion.

The particular issue that has largely motivated this research is the phenomenon of approximate scaling of diffusion time scales with the Lyapunov exponents or perturbation strength. A number of papers have been published on this topic, e.g., [8]; we are also inspired by the building block method of [9].

The basic idea of our model is to consider a FKE in the action space with a nonhomogenous diffusion coefficient and to combine, i.e., convolve the results to obtain the expected macroscopic behavior. We use the following form of the FKE:

$$\frac{\partial^{\beta}P(I,t)}{\partial t^{\beta}} = \frac{\partial^{\alpha}[\mathcal{D}(I)P(I,t)]}{\partial |I|^{\alpha}} + \delta(I)t^{-\beta}/\Gamma(1-\beta), \tag{1}$$

where $0<\beta<1$ and $0<\alpha<2$. Its derivation from the Hamiltonian equations and discussion of assumptions involved can be found, e.g., in [4]. Although, strictly speaking, one should consider a vector of actions, we shall assume that diffusion along one action coordinate is independent of the others and consider I as a scalar; alternatively, one could interpret that as considering only one action variable, whereas the diffusion along the others is many orders of magnitude smaller. Both cases have been described in various systems [2,4].

We estimate the diffusion coefficient $\mathcal{D}$ as the remainder of the normal form for the dynamics in the vicinity of a stable domain, e.g., invariant torus. Splitting the Hamiltonian $H(I,\phi)$ into an action-only integrable part $H_0(I)=\omega I$ and the nonintegrable remainder $H_1(I,\phi)$, one can obtain the estimate for the remainder of the form $O(f(I))$, i.e., as a function of the action. Treating the influence of the nonintegrable remainder on the dynamics as the microscopic transport mechanism, we take $f(I)$ from the above estimate for the diffusion coefficient. Two optimal normal forms are known as Nekhoroshev and Birkhoff normal forms. Their remainders [10] give the diffusion coefficients $\mathcal{D}_N$ and $\mathcal{D}_B$;

$$\mathcal{D}_N = \mathcal{D}_0 \exp[-1/|I|^{\theta}], \tag{2a}$$

$$\mathcal{D}_B = \mathcal{D}_0 |I|^{\theta}, \tag{2b}$$

where $\mathcal{D}_0$ denotes the constant part, which is, in general, dependent on the properties of the Hamiltonian. For both cases, there is a constraint $\theta>2$. The two cases roughly correspond to local nonoverlapping or overlapping of the resonances.

The last step before solving the FKE is the estimation of the fractional exponents α and β. These are intimately related to the self-similarity of the structures involved, and can be determined from the exponents of the renormalization group of kinetics of the particular system. This has to be

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done numerically for all but the simplest systems [4]. In our computations, we have employed a "building block" approach similar to that of [9], partitioning the phase space into several regions, each described with its own FKE, with the diffusion coefficient (2a) or (2b). However, instead of considering only ballistic flights and Markovian diffusion, as in [9], we propose the adoption of a set of (α,β) pairs. The values of the exponents can then be determined by sampling the flights (longer than a certain threshold T_0), and then fitting the distribution of their lengths and durations as $\ell^{-(1+\alpha)}$ and $t^{-(1+\beta)}$, respectively.

It is hardly surprising that we were unable to find the exact solutions for the FKE (1), with the diffusion coefficients (2a) and (2b), in their most general form. However, the long-term behavior can be found by expanding the space derivative on the right-hand side of (1) according to the generalizations of the Leibniz's rule and chain rule for the fractional operator $d^\alpha/d|I|^\alpha$; see, e.g., [11] for mathematical details. For the case (2a), we obtain the solution, up to the normalization factor,

$$P(I,t) = E_\beta(-y_0^{4/\alpha} - y^{4/\alpha})\mathcal{I}_1\left(\frac{2e^{-y}}{\mathcal{D}_0^{3/2}}\sqrt{\frac{y_0}{t^\beta y}}\right), \tag{3}$$

where $\mathcal{I}$ denotes the modified Bessel function of the first kind, $y(I,t)=|I|/[(\theta-2)\sqrt{\mathcal{D}_0 I^\theta t^\beta}]$, and $y_0=y(I_0,t)$, with I_0 denoting the value of the action at $t=0$. The Mittag-Leffler function is denoted by E_β. For the Birkhoff case, one obtains

$$P(I,t) = \frac{y}{\sqrt{I}}E_\beta(-y_0^{4/\alpha} - y^{4/\alpha})\mathcal{I}_p(2y_0 y), \tag{4}$$

with $p=(\theta-1)/(\theta-2)$. We note that, for $I,t \gg 1$, both y and y_0 tend to zero. The asymptotic expansions of the Mittag-Leffler and the Bessel function can then be used to show that the solutions $P(I,t)$ fall off in the infinity sufficiently sharply to be valid probability distributions. They are the main exact result of our analysis. We shall use them here to apply the more advanced building block model and to obtain the approximate scaling relations between the diffusion and Lyapunov time scales.

Convolution over all the solutions ($\bigstar_{i=1}^N$) can be performed in the usual way, with some entrance probabilities (actually, statistical weights of each block) p_i,

$$P_{res}(I,t) = \bigstar_{i=1}^N p_i P_i(I,t), \tag{5}$$

which give the resulting probability distribution $P_{res}(I,t)$. We propose this way for examining the behavior of particular systems. In the limit of infinitely many blocks [20], however, one can derive a generic relation between the short-time and long-time diffusion scales.

We next proceed to estimate the typical diffusion time scales. These can be related to the "escape times" one often encounters in simulations, e.g., [8]. Strictly speaking, the escape time can only be defined in open systems, as the time to cross the Lyapunov curve (see [13] for a definition). Otherwise, escape time is usually a more or less qualitative term meant to describe, generally, the time needed to enter a large connected chaotic region ("stochastic see") or to experience a qualitative change of dynamical behavior. In what follows, we shall consider the escape time as the time scale needed to reach a fixed I; without loss of generality, we may assume $I=1$.

For fixed I, the solution (3) has a maximum about $2\sqrt{y_0/(t^\beta y)} \approx \mathcal{D}_0^{3/2}$. Solving this for time t, we obtain the estimate of the time to reach $I=1$,

$$T_{I=1} \approx \left(\frac{16(I/I_0)^{\theta-2}}{\mathcal{D}_0}\right)^{1/\beta}. \tag{6}$$

Similarly, (4) reaches its peak at $2yy_0 \approx 1$, which gives the following $T_{I=1}$:

$$T_{I=1} \approx \left(\frac{(II_0)^{1-\theta/2}}{(\theta-2)\mathcal{D}_0}\right)^{1/\beta}. \tag{7}$$

On the other hand, the short (microscopic) time scale of (1) is about $\mathcal{D}(I)/(\omega\epsilon^{\beta/\alpha})$, which may be interpreted as the average time between two "collisions;" in our case, this corresponds to a time needed to cross a single resonance, bearing in mind that resonance interactions and overlaps are the main physical mechanisms of transport. Moreover, this time scale is often considered to be a valid estimate of the Lyapunov time T_{Lyap} [1,3].

Let us now notice that the solutions (3) and (4), with their exit time scales (6) and (7), can be written in the form of Fox's H functions [6]. By convolving these functions, one gets, after a straightforward but tedious calculation, a Fox's function again, which may have two asymptotic behaviors. They scale with the short-time scale of (3) and (4) either as an exponential law or as a power law. The asymptotic behavior depends on the weights p_i and on the sum of transport exponents $2\beta_i/\alpha_i$ for each building block. Accepting this reasoning and inserting the above estimate for T_{Lyap} into (6) and (7), we obtain the approximate scalings for escape time T_{esc},

$$T_{esc} \propto \exp(T_{Lyap}^\kappa), \tag{8a}$$

$$T_{esc} \propto T_{Lyap}^\nu. \tag{8b}$$

Let us hold onto this result for a moment. The scaling of this type has been conjectured long ago (e.g., [14]), and it is implicitly suggested also by the classic work of Chirikov concerning the regimes of resonance nonoverlapping and overlapping [15] (the first one being known also as the Nekhoroshev regime). More recently, transition between the Nekhoroshev and Chirikov regime has been explored by Froeschle and others [16]. However, we show here that the scaling (8a) and (8b) arises from both basic regimes of chaotic dynamics, and that its type is determined also by the fractional exponents α and β of different building blocks. Physically, this means that the sticky (and thus non-Markovian) nature of self-similar structures in the phase space can "mimic" the effects of the resonance nonoverlapping. This is logical, since both phenomena effectively put a barrier into the transport channels. The scalings can be expected to be universal for a given system but are clearly nonuniversal for different systems, since they depend on the properties of the Hamiltonian. It should also be noted that, for N-dimensional ($N>2$) systems, one should take into ac-

TABLE I. Hamiltonians of the form $H_{Int}+\epsilon H_{Pert}$ explored in the simulations. For each Hamiltonian, we give the integrable part H_{Int}, the perturbation part H_{Pert}, the range of the values of ϵ in the simulations, the exponents of the scalings κ and ν, and the range of the values of ϵ for the transition regime. Variables (I_i,ϕ_i) denote the action-angle variables, whereas (x,y,z) are the physical space coordinates. HO2 and HO3 denote the harmonic oscillator in two and three dimensions, respectively. HH2 and HH3 refer to the integrable Henon-Heiles Hamiltonian [13] in two and three dimensions: $(\dot{x}^2+\dot{y}^2+x^2+y^2-2/3y^3)/2$ and $(\dot{x}^2+\dot{y}^2+\dot{z}^2+x^2+y^2+z^2-2/3z^3)/2$, respectively. Hamiltonian H_8 is the egg-crate system taken from [4], H_9 is the sixth-order Toda lattice, i.e., the integrable Henon-Heiles system perturbed with its sixth-order expansion [1], and H_{14} is taken from [16]. See the text for further comments.

H	H_{Int}	H_{Pert}	ϵ	κ	ν	ϵ_{trans}
H_1	HO2	ϵxy	1.00–4.00	0.65 ± 0.07	0.87 ± 0.05	1.50–1.60
H_2	HO2	$\epsilon x^2 y$	0.87–3.50	0.45 ± 0.05	1.98 ± 0.06	1.28–1.32
H_3	HO2	$-\epsilon x^2 y^2$	1.50–6.00	1.09 ± 0.03	1.70 ± 0.04	3.32–3.70
H_4	HH2	ϵxy	0.00–3.50	0.77 ± 0.08	0.53 ± 0.03	0.15–0.20
H_5	HH2	$\epsilon x^2 y$	1.00–4.00	0.15 ± 0.03	1.25 ± 0.06	1.12–1.16
H_6	HH2	$-\epsilon x^2 y$	1.00–4.00	0.71 ± 0.05	0.88 ± 0.04	1.55–1.66
H_7	HH2	$-\epsilon/\sqrt{x^2+y^2}$	0.00–3.50	0.33 ± 0.05	0.57 ± 0.03	1.60-1.70
H_8	$(\dot{x}^2+\dot{y}^2)/2+\cos x+\cos y$	$\epsilon \cos x \cos y$	0.00–2.00	0.22 ± 0.04	1.12 ± 0.08	0.34–0.37
H_9	HH2	sixth-order Toda lattice expansion	0.00–4.00	0.58 ± 0.03	1.44 ± 0.04	0.55–0.60
H_{10}	$I_1^2/2+2\pi I_2$	$\epsilon(\cos\phi_1+\cos(\phi_1-\phi_2))$	0.00–3.00	1.21 ± 0.04	1.82 ± 0.07	1.20–1.32
H_{11}	$I_1^2/2+2\pi I_2+\cos\phi_1$	$\epsilon(\cos(\phi_1-\phi_2)+\cos(\phi_1+\phi_2))$	0.00–3.00	0.45 ± 0.05	1.75 ± 0.07	0.85–0.90
H_{12}	HO3	$\epsilon x^2 yz$	0.00–2.00	0.22 ± 0.03	0.57 ± 0.03	0.33–0.45
H_{13}	HH3	ϵxz^2	0.80–4.00	0.41 ± 0.04	1.03 ± 0.08	1.20–1.31
H_{14}	$(I_1^2+I_2^2)/2+I_3$	$\epsilon/(\cos\phi_1+\cos\phi_2+\cos\phi_3+4)$	0.000–0.100	0.19 ± 0.03	1.00 ± 0.04	0.055–0.060

count the Arnold diffusion. However, this should be negligible as long as the number of the degrees of freedom is sufficiently low, especially if we take into account a recent result which proves its superexponentially slow nature for a certain class of systems [17].

We have performed thorough numerical tests of our results, by integrating ensembles of particles initially placed in a cell of the phase space of the given Hamiltonian. We have inspected the behavior of the perturbed (quasi-integrable) Hamiltonian systems, i.e., of the form $H=H_{Int}+\epsilon H_{Pert}$, since the constant part of the diffusion coefficient $\mathcal{D}_0$ can then easily be estimated as ϵ^2. We have observed the time evolution of the "distribution function," i.e., concentration of the particles in the phase space, the escape times, and the scaling exponents [by fitting to (8a) and (8b)]. We have also calculated the finite time Lyapunov exponent (FTLE, see [18] for a definition), as the numerical estimate for $1/T_{Lyap}$. The escape time was measured as the time of crossing the Lyapunov curves, for open systems, or as the time of the beginning of the first long interval of normal diffusion, for the closed systems [21]. Details on the simulations and on the approximate scalings of the form (8a) and (8b) found numerically are summed up in Table I.

Figure 1 gives the comparison between the analytically and numerically obtained distribution functions, for each of the cases (3) and (4). Overall agreement can be seen, although it is not perfect. Typical results for the $T_{esc}(T_{Lyap})$ relation are shown in Fig. 2. Agreement with the predicted approximate scalings is good. The regimes are rather clearly separated and the transient regime is short, although it does exist. This behavior could be described as a phase transition between two regimes of chaotic transport, an idea which is not new for dynamical systems.

We are unable to explain the abrupt transition from one scaling regime into another, which occurs in most of our simulations, and resembles a phase transition. This kind of behavior could be better described by a discrete model. An obvious choice is a multiply branched tree (as proposed in [19]) or a network, with the transition probabilities derived from our results for the distribution functions. This would actually be a formalization of the building block model, which already (implicitly) includes a network of blocks.

In conclusion, we have proposed a method for obtaining (and solving) the kinetic equations of chaotic diffusion. The

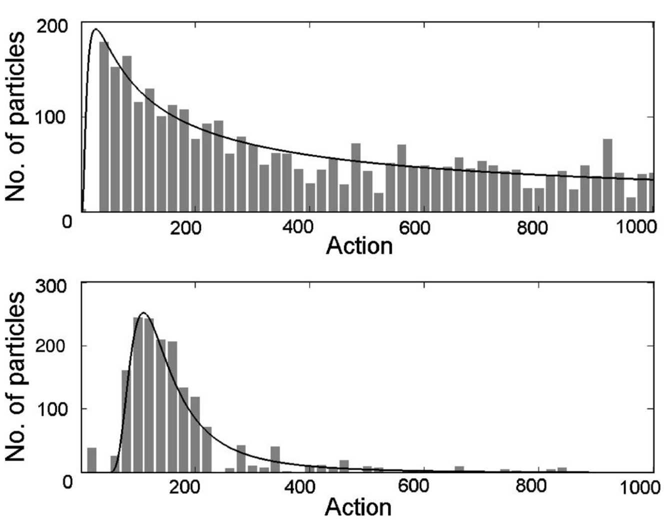

FIG. 1. Analytical (solid line) and numerical (histogram) distribution functions $P(I_1,t)$ for the Hamiltonian H_{14}. Action is in relative units. (a) Nonoverlapping resonances for $\epsilon=0.030$. (b) Overlapping resonances for $\epsilon=0.060$.

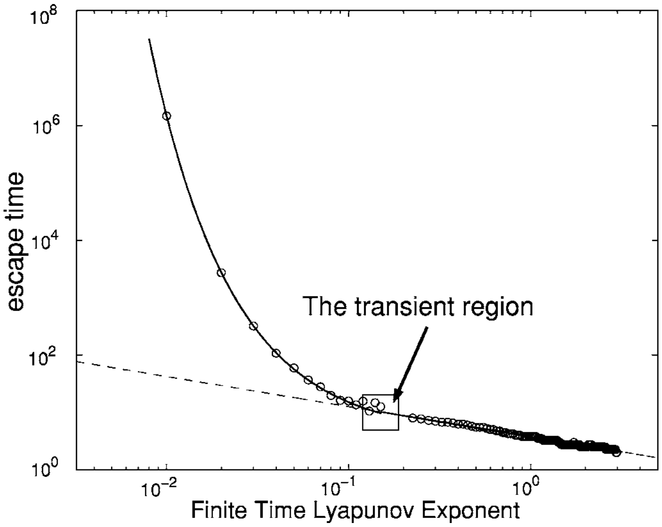

FIG. 2. An example of the scaling relations between finite time Lyapunov exponent and escape time. The solid lines denote the least-squares fit to the scaling relations (8). Scales are logarithmic on both axes, thus the power-law fit is a straight line. The dashed reference line for the power law is also shown, as well as the transient region. Time is in relative units from the simulation. The Hamiltonian is H_4.

method is based upon using the normal forms of dynamics as the basic blocks of kinetics. In general case, some parameters of the model, including the fractional exponents of FKE, have to be computed from the simulations, as the current state of Hamiltonian theory does not allow us to estimate them from the dynamical equations, as noted also in [4]. We have also demonstrated a generic approximate scaling of the macroscopic diffusion time, often regarded to in simulations as escape time, with the Lyapunov (microscopic) time scale. We especially underline that both the power law and the exponential form of scaling can arise from both possible forms of the diffusion coefficient, and that the scaling behavior arises from combining the two, i.e., as a kind of collective behavior.

I am grateful to researchers from the Group for Nonlinear Optics, Institute of Physics, Belgrade, for discussions and support during the preparation of this paper and for the processor time for the simulations. I am also indebted to Robert S. MacKay, Harry Varvoglis, and George M. Zaslavsky for helpful comments, and for some of the references. Work at the Institute of Physics is supported by the Ministry of Science and Environment Protection, under Project No. OI 1475.

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[20] This should be realistic for most systems, since each block, in a typical case, actually has a multifractal structure [12], which is analogous to consisting of many "sub-blocks," each one having different fractional exponents.
[21] The length of this interval has to be determined empirically. It should warrant that the particle has entered the large connected stochastic sea, so that the probability that the particle is trapped again is very low.