Exit Times and Chaotic Transport in Hamiltonian Systems

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A new statistical diagnostic tool for chaotic transport in Hamiltonian systems is proposed. The method, based on the concept of exit times, has an advantage over the calculation of diffusion coefficients in that it remains valid for nondiffusive transport processes. This method is tested on the Chirikov-Taylor standard map: One finds that it is more robust than the usual diffusion coefficient D and conveys the same information as D when the latter is meaningful, for all values of the nonlinearity parameter K.

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The major challenges raised by transport phenomena in nonlinear dynamical systems are related with the characterization, prediction, and control of these complex processes in space and time. Understanding them is important for many applications including heat and particle transport in fusion plasmas, astrophysics, fluid mixing, particle accelerators, and chemical reactions [1-3]. For instance, control of transport processes in tokamaks is a key issue in plasma confinement for controlled thermonuclear fusion [4]. These complex systems with a seemingly erratic behavior are generally governed by deterministic nonlinear equations, with solutions strongly sensitive to initial conditions and evolving along intricate trajectories. Transport is one aspect of the statistical nature of these nonlinear dynamical systems. In this Letter, we discuss a new approach and apply it to a well known area-preserving map, which mimics the Poincaré section of a 2 degrees of freedom Hamiltonian flow: The Chirikov-Taylor standard map.

When studying chaotic motion, there is a belief that transport and diffusive spreading for the density of some physical quantity are almost synonymous. This belief is so firm that, for instance, the prediction of a diffusion coefficient is a major goal in fusion research and the success of a transport model is assessed through its ability to predict this coefficient. The diffusion coefficient for a variable I is defined as the asymptotic spreading rate of its second moment

$$D=\lim_{t\to\infty}\frac{\langle (I_t-I_0)^2\rangle}{2t} \tag{1}$$

if the limit exists. This definition implies that it is possible for a chaotic orbit to wander in a (practically) unbounded domain (otherwise $D=0$); it cannot hold to properly describe stochastic behavior in bounded domains (which occurs for most physical problems). Beyond this definition, conventional wisdom expects that, on large time ($t=t'/\varepsilon^2$) and phase-space ($I=I'/\varepsilon$) scales, the rescaled motion $I'(t')=\varepsilon I_{[t/\varepsilon^2]}$ might approach a Brownian motion in the limit $\varepsilon\to 0$. While these questions are beyond the reach of present mathematical physics (see, e.g., [5]), conventional approaches go even further [1]: The quasilinear assumption estimates (1) by $\langle (I_\tau - I_0)^2\rangle/2\tau$, where τ is a typical "short" time scale (e.g., $\tau=1$ for the Chirikov-Taylor map). In other words, the correlation function of increments of I_t is approximated by a Dirac (or Kronecker) distribution. This assumption of the rapid decay (or even absence) of correlations is rather drastic. Rigorously speaking, diffusion coefficients are associated with Brownian motions and require a scale invariance usually not found in Hamiltonian systems. Indeed the phase space for Hamiltonians with 2 degrees of freedom is usually divided into stochastic and regular domains. Even in strong stochasticity regimes, chaotic domains contain small islands of stability which may constitute a finite measure fractal set in phase space [6]. The influence of these islands on stochastic trajectories has been discussed by various authors [7]; in particular, their stickiness was shown to induce specific long time correlations on chaotic orbits, which prevent a "naive" diffusional description of the process. In other words, the situation prevailing in chaotic transport is one for which the effective mean free path is at all times comparable in magnitude with a macroscopic length scale, whereas a diffusion model applies in the opposite case. Thus transport is generally governed by nondiffusive processes; this is well known in physics [8].

In this Letter, we develop a new statistical diagnostic describing chaotic transport in deterministic systems, based on the exit time concept and valid for nondiffusive transport processes as well. Characteristic times have already been used by several authors [7,9-11] to describe chaotic motion in relation with local structures in phase space: They do not probe the large scale properties of the system. Here, instead, we discuss an average exit time, which is defined more generally than diffusion coefficient D and conveys essentially the same information as D when the latter is meaningful.

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Given a domain Ω of phase space and a point $x_0 \in \Omega$, we define the exit time $\tau(x_0,\Omega)$ as the time [1] needed by the orbit of x_0 to leave Ω (and $\tau=\infty$ if x_t remains in Ω for all times $t>0$). Then, given a probability density f_0 of initial conditions (particles) on Ω, the ensemble average exit time from Ω for f_0 is

$$\langle \tau(\Omega)\rangle_{f_0} = \int_\Omega \tau(x_0,\Omega) f_0(x_0)dx_0 . \tag{2}$$

The choice of f_0 (e.g., uniform on a subset of Ω) is important. If it gives a positive weight to an invariant subset of Ω, then $\langle\tau(\Omega)\rangle_{f_0}$ is infinite. A natural choice for f_0, from a dynamical viewpoint, is associated with ergodic measures, but these are seldom known *a priori:* One usually finds them by following trajectories. Moreover, when stable islands are large or numerous, it may be difficult to choose appropriate initial conditions outside these islands. Therefore we introduce a second definition of the exit time by averaging τ along trajectories. Given an initial point x_0 at $t_0=0$, we choose a first domain Ω_0 containing x_0 and find the exit time $t_1=\tau(x_0,\Omega_0)$; then we associate to the new position x_{t_1} (outside Ω_0) a new domain Ω_1 (e.g., by shifting Ω_0, or by another symmetry) and determine the exit time $\tau(x_{t_1},\Omega_1)$; we iterate this procedure and denote by $\langle T\rangle(x_0)$ the orbit average of the successive exit times, if it exists:

$$\langle T\rangle(x_0) = \lim_{n\to\infty} \frac{1}{n}\sum_{k=0}^{n-1} \tau(x_{t_k},\Omega_k) . \tag{3}$$

As an orbit may wander through phase space, $\langle T\rangle$ describes "global" aspects of transport (like D) while $\langle\tau\rangle$ describes more "local" aspects [as a "local" coefficient $D(x)$ does].

With reasonable choices of domains Ω, $\langle\tau\rangle$ and $\langle T\rangle$ can be finite in two cases where D is meaningless: (i) When the orbit belongs to an accelerator mode, $\langle (I_t - I_0)^2\rangle/t$ diverges like t; (ii) when the chaotic domain is bounded, $\langle (I_t-I_0)^2\rangle/t$ decays like t^{-1}. However, one should note that $\langle T\rangle(x_0)$ is undefined $[\tau(x_0,\Omega)=\infty]$ if x_0 belongs to an invariant island contained in Ω_0. An alternative definition of the diffusion coefficient has been proposed to discard this influence of islands [10]: $D_{\text{har}} = \alpha|\Delta I|^2\langle\tau^{-1}\rangle$, with the harmonic average exit time $\langle\tau^{-1}\rangle = \int_\Omega [1/\tau(x_0,\Omega)] f_0(x_0)dx_0$ from a domain of size ΔI (α is a numerical constant).

Finally, one should refer to the theory of stochastic processes [12]. For one-dimensional Brownian motion with space-dependent diffusion constant $D(x)$ and drift $V(x)$, the expected exit time $\sigma(x_0)=\langle\tau(x_0,\Omega)\rangle$ from a slab $\Omega=[-L/2,L/2]$ with initial condition $x_0\in\Omega$ obeys the differential equation $(V\sigma)'+(D\sigma')'=-1$ with $\sigma(-L/2)=\sigma(L/2)=0$. In particular, for $V=0$ and constant diffusion coefficient D,

$$\langle\tau(x_0,\Omega)\rangle_D = (L^2-4x_0^2)/8D \tag{4}$$

so that, for initial data distributed according to a uniform distribution f_0 on $[-r/2,r/2]$:

$$\langle\tau\rangle_{f_0} = (L^2 - r^2/3)/8D . \tag{5}$$

We will use this latter expression to compare with (2) and (3) at scales on which we try to model the dynamics by a stochastic process.

For illustration, consider the standard map

$$I_{n+1} = I_n + K\sin\theta_n , \tag{6a}$$

$$\theta_{n+1} = \theta_n + I_{n+1} , \tag{6b}$$

which describes a model of a kicked rotator; parameter K controls the strength of the kicks. For $K\gg 1$, model (6) is strongly chaotic and trajectories look close to Brownian motions [1,11]. Large scale transport occurs for $K > K_c = 0.9716\ldots$ and a diffusion coefficient D_{num} can be estimated numerically. Unexpectedly, the rescaled coefficient D_{num}/K^2 was found to oscillate strongly and regularly [13].

We compute the average exit time along an orbit $\langle T\rangle(x_0)$ for the standard map by fixing the domain Ω_0 as a band of width ΔI and shifting it by a quantity $\pm\Delta I/2$ so that $x_{t_1}\in\Omega_1$, and repeating the procedure. To ensure that the particle needs a few time steps to exit the current Ω (which gives smoother statistics), we choose a width $\Delta I > K$, because K is the largest step allowed in one iteration of (6). Moreover, this width should rather be a multiple of 2π because of the periodicity of phase space with respect to I, but this condition is obsolete if K is very large as the system seems then practically ergodic. Thus we take $\Delta I = 2\pi K m$, where $m\ge \max(1/K,1)$ and can be varied continuously. Then we compute the average exit time as a function of the coupling parameter K for a fixed value of m.

To propose theoretical estimates for $\langle T\rangle$, we assume that the orbit average behaves as an ensemble average like (5) with a Brownian diffusion coefficient. Though one has not established rigorously whether the orbits generated by (6) diffuse in action according to a Markov process on large space and time scales, a Fourier representation of $\langle (I_t-I_0)^2\rangle/2t$ yields [1,13] the following asymptotic expansion D_{asy} of the diffusion coefficient for $K\to\infty$:

$$D_{\text{asy}} = D_{\text{QL}}\left[1 + c\left(\frac{8}{\pi K}\right)^{1/2} + c^2\frac{4}{\pi K} + o(K^{-1})\right] , \tag{7}$$

where $D_{\text{QL}} = K^2/4 = \langle (I_1-I_0)^2\rangle/2$ is the "quasilinear" coefficient, and $c=\cos(K-\pi/4)$. The agreement between $D_{\text{asy}}/D_{\text{QL}}$ and $D_{\text{num}}/D_{\text{QL}}$ is reasonable for values of K for which there are no accelerator islets.

In Fig. 1 we plot the average exit time $\langle T\rangle$ vs K computed for $m=4$. It is nicely fitted by $C(m)D_{\text{QL}}/D_{\text{asy}}$; the constant $C(m)\approx 2\pi^2 m^2$ for $m\to\infty$ in agreement with (5). Figure 1 shows that $\langle T\rangle$ exhibits the same oscillations as $D_{\text{QL}}/D_{\text{asy}}$ and $D_{\text{QL}}/D_{\text{num}}$. But, whereas $D_{\text{num}}/D_{\text{QL}}$ also displays peaks due to the divergence of (1) in the presence of stable accelerator modes [1,13], $\langle T\rangle$ does not vanish and behaves smoothly for such values of K:

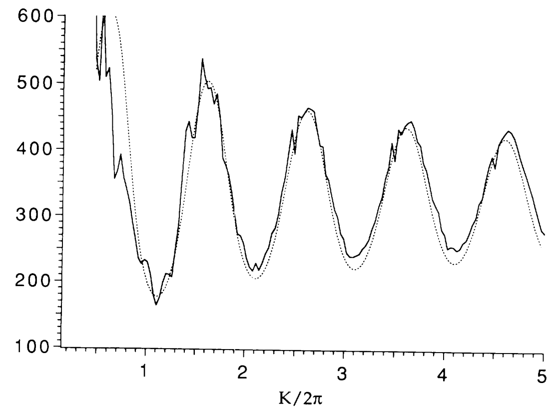

FIG. 1. Average exit time $\langle T \rangle$ vs coupling parameter K for standard map. Solid line: numerical results for one particle, 10^7 iterations, $\Delta I = 2\pi K m$, $m = 4$. Dashed line: plot of $2\pi^2 m^2 D_{\mathrm{QL}}/D_{\mathrm{asy}}$ to order $1/K$.

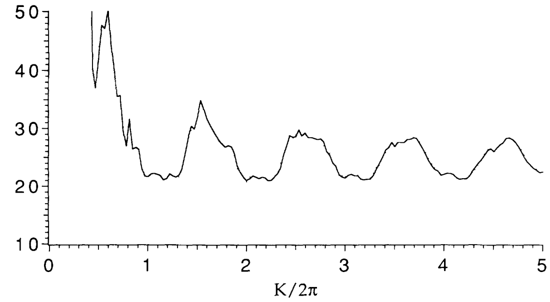

FIG. 2. Solid line: first exit time averaged over a uniform initial distribution ($|I_0| \leq K$). Dots: averaged exit time from second band (10^5 particles, bands $\Delta I = 2\pi K$).

This shows the robustness of the averaged exit time to these modes with our choice of Ω and that these oscillations are not mere artifacts. The transition time defined by Chirikov in his seminal work [11] and a first study of the harmonic average exit time [10] did not reveal such oscillations because they took $\Delta I = 2\pi$: These oscillations can only be observed if one takes the dominant behavior $\langle T \rangle \sim \Delta I^2/K^2$ into account and if the numerical estimation of $\langle T \rangle$ involves enough statistics (i.e., particles spend enough time steps in the domains).

We now discuss how the statistics of exit time depend on initial distributions of particles. To test the equivalence between the expected value (2) of the exit time for an ensemble and the expected value (3) along an orbit, one must check that the influence of the initial distribution is not significant. Indeed, if we start with a uniform distribution of initial data (I_0, θ_0) in a band of width ΔI, the actions after the first exit from Ω will be distributed (nonuniformly) over two sidebands, each one with a width K. The shift by $\pm \Delta I/2$ "glues" these two bands and yields a new "initial" distribution of particles, for which we repeat the procedure. One hopes that, on iterating this process, the distribution will converge towards a limit corresponding to averaging along an orbit. This intuition is supported by Fig. 2, which displays the ensemble averaged exit time from the first domain Ω_0 ($|I| \leq \Delta I/2$) and from the second domain Ω_1; for these domains we chose $\Delta I = 2\pi K$, and our initial data were distributed at random in a band ($|I_0| \leq K$) of width $2K$ (which is the width of the asymptotic support). This computation shows an important similitude between the first and second exit times, and the oscillations of the average second exit time are smoother than those of the average first exit time.

For the standard map, the Brownian limit corresponds to $K \to \infty$ and $m \to \infty$, so that each particle step after every iteration is negligible compared to the size of Ω. We checked numerically that, in this limit, the averaged exit time coincides with the Brownian estimate.

Moreover, Fig. 3 shows the phase-averaged (for phases θ_0 chosen at random according to a uniform distribution) exit time as a function of I_0 for points (I_0, θ_0) from a band $0 \leq I \leq \Delta I$ for $K = 100$, $m = 4$. Except for an overall shift, this average exit time agrees quite well with parabola (4), using (7) for the diffusion coefficient. Yannacopoulos and Rowlands [14] also checked that the probability that the particle remains in a slab as a function of time approaches that of a diffusion process for the standard map with $K = 20$, $\Delta I = 200$.

Our last figure (Fig. 4) shows that, near the large scale stochasticity threshold K_c, $\langle T \rangle$ scales according to a power law $\langle T \rangle \sim (K - K_c)^{-\alpha}$ with $\alpha \approx 3$ in agreement with previous observations [7,11]. Note that our data for $K - K_c \leq 0.02$ involve too few exits to be statistically sharp.

These results show that the averaged exit time defined by (3) enables us to retrieve the (large scale) transport properties of the standard map not only for large values of K, but also for intermediate ones and near the strong stochasticity threshold. In particular, $\langle T \rangle$ is useful when

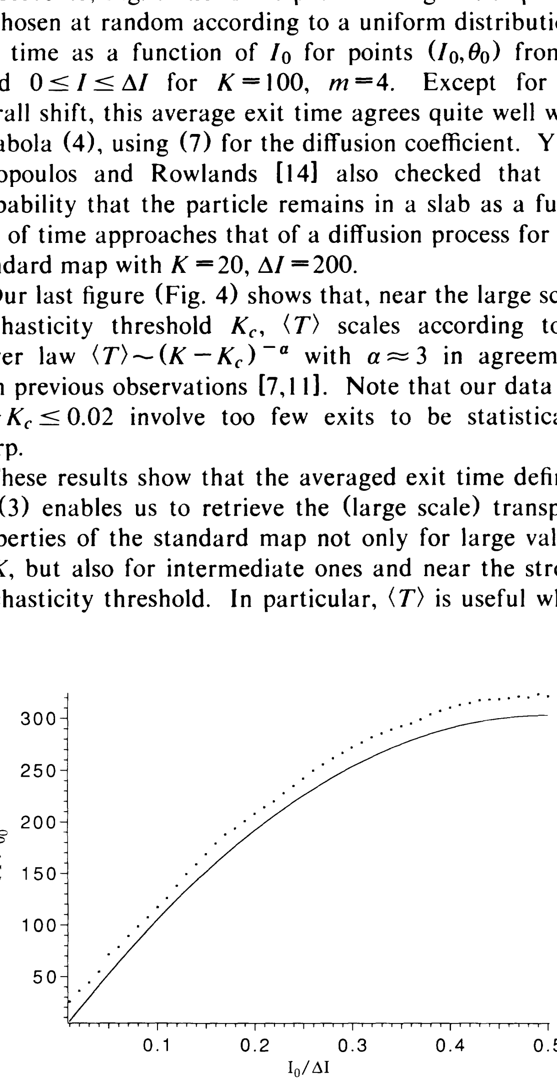

FIG. 3. Squares: phase-averaged exit time $\langle T \rangle_{\theta_0}$ vs I_0 for $K = 100$, $\Delta I = 2\pi K m$, $m = 4$ (10^5 particles per point). Solid line: parabola (4) with D given by (7).

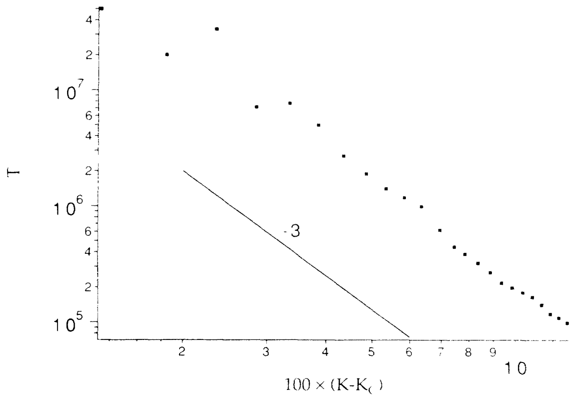

FIG. 4. Average exit time $\langle T \rangle$ vs $K - K_c$ near large scale stochasticity threshold for the standard map, in log-log scale (one particle, $\Delta I = 4\pi$, 10^8 iterations per point).

the chaotic domain encloses large islands.

To summarize, we have shown numerically, using the standard map, that transport in Hamiltonian chaos can be characterized by means of the averaged exit time. Provided one chooses domains Ω with insight, this new diagnostic tool remains valid in situations where diffusion coefficients are ill defined, in particular when phase space contains invariant closed curves acting as complete barriers to transport, and cantori and chains of islets acting as partial barriers; and when D is relevant, the average exit time conveys essentially the same information. Near stochastic threshold, the averaged exit time is still meaningful, and easily computed in a system of sufficiently large extension. Finally, when chaotic motion is bounded, this new statistical tool enables one to probe "limited transport" which is also investigated from a promising more geometrical viewpoint [9].

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