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Resonances and Diffusion in Periodic Hamiltonian Maps

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Chaotic diffusion in periodic Hamiltonian maps is studied by the introduction of a sequence of Markov models of transport based on the partition of phase space into resonances. The transition probabilities are given by turnstile overlap areas. The master equation has a Bloch band spectrum. A general exact expression for the diffusion coefficient D is derived. The behavior of D is examined for the sawtooth map. We find a critical scaling law for D, extending a result of Cary and Meiss. The critical scaling emerges as a *collective* effect of many resonances, in contrast with the standard map.

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Evidence for the existence of a diffusion coefficient D in Hamiltonian maps has been provided by extensive numerical and analytical calculations.[1-4] The analytical studies give explicit formulas for the diffusion coefficient in the form of infinite sums that, for most parameter regimes, converge rapidly to give useful and accurate estimates of D. However, the methods employed in these studies do not have a transparent connection to the details of the dynamics.

An important step in rectifying this situation was the introduction of Markov models for systems of two degrees of freedom to simulate the actual dynamics near the critical breakup of Kolmogorov-Arnol'd-Moser tori.[5-7] These models are based on a partition of phase space into regions (called states) which are separated from each other by "partial barriers" formed from cantori. Unfortunately these models are not easily generalized to the case of large fluxes, or to systems where all fluxes are of the same order of magnitude. In these cases it is unclear how to choose a *countable* subset of cantori for a partition of the phase space.

Resonances[8,9] give a natural partition of phase space. A resonance may be defined[8] as a region of phase space bounded by two "partial separatrices" formed from orbits homoclinic to a hyperbolic periodic orbit. Recall that an orbit is homoclinic to a given periodic orbit if it converges to the given orbit both forwards and backwards in time. The total flux exchanged per iteration by the resonance with the rest of phase space is determined by the turnstiles associated with the two partial separatrices. The partial fluxes exchanged by any two resonances are determined from the areas of overlap of their turnstiles, as illustrated in Fig. 1.

In this Letter we introduce a Markov model of transport based on resonance dynamics in Hamiltonian maps on the cylinder of the form

$$p_{t+1}=p_t+Kf(x_t)\,,\quad x_{t+1}=x_t+p_{t+1}\,, \tag{1}$$

where $f(x+1)=f(x)$, and K is a "stochasticity" parameter. Such maps are periodic in p when the phase space is the cylinder $-\frac{1}{2}\leq x<\frac{1}{2}$, $-\infty<p<\infty$. The unit cell is the torus $-\frac{1}{2}\leq x<\frac{1}{2}$, $0\leq p<1$. We will assume the inversion symmetry $f(-x)=-f(x)$, so that the map (1) is reversible.[5] An example of a map with this symmetry is the standard map with $f(x)=\sin(2\pi x)/2\pi$. The periodicity in p makes the Markov model analogous to a periodic crystal in solid-state physics.[10] In Eq. (8) below we give a general exact expression for D in terms of the basic parameters of the model. As a check of this theory, we calculate D explicitly for the sawtooth map,[11] a completely chaotic system with $f(x)=x$, discontinuous at $x=\pm\frac{1}{2}$. The results are compared with numerical measurements of D in Figs. 2 and 3. For K near the critical value $K_c=0$, (8) gives a scaling behavior which agrees very well with numerical

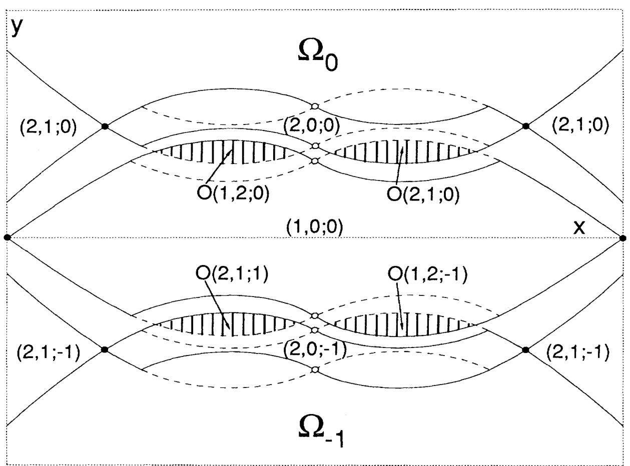

FIG. 1. Schematic illustration in symmetry coordinates of the turnstile overlap (crosshatched) of the 0/1 resonance with the 1/2 resonances in two unit cells. Notation in the text.

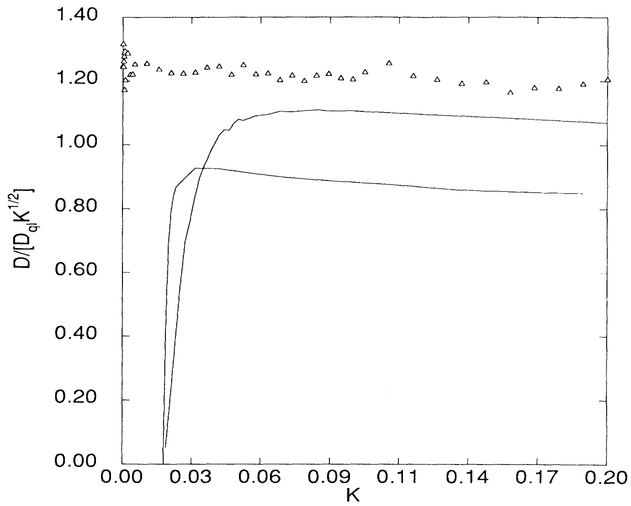

FIG. 2. $D(K)/\sqrt{K}D_{ql}$ for the sawtooth map: numerical results ($\triangle$), and results from formula (8) with use of all resonances of orders ≤ 21 for the simple resonance partition (lower curve) and from the first-refined partition described in the text (upper curve).

results. We also find that formula (8) agrees well with numerical results away from criticality, and for $K\rightarrow\infty$, provided a suitable partition is chosen. We present here the main results and outline their derivation. Details will be given elsewhere.[12]

We may define a Markov model for the dynamics by specifying a partition of the phase space into a countable number of nonintersecting subsets of the phase space, called states, and then specifying transition probabilities between states. Our Markov models are based on a partition of phase space into resonances, and subsets of resonances generated by repeated forward or inverse iterates of the map (1). We denote a unit cell in phase space by Ω_l, $l=0,\pm1,\pm2,\ldots$, $(l\leq p<l+1$ in $\Omega_l)$, and choose in Ω_0 a set of R resonances with winding numbers $\nu_r=m_r/n_r$, $r=1,\ldots,R$. The elements of the corresponding set in Ω_l are the translates (r,l) of these resonances, which have winding numbers $\nu_{r,l}=\nu_r+l$.

The states of the simplest models are the islands, n_r states in resonance (r,l). These states are labeled by $(r,s;l)$ with $s=0,1,\ldots,n_r-1$, where $s=0$ corresponds to the island in some arbitrarily chosen gap of the hyperbolic periodic orbit, and $s>0$ to the island in the sth iterate of this gap. The largest gap usually lies around some vertical line $x=\bar{x}$, called the dominant line. We choose the $s=0$ or "main" island to lie in this gap, and we associate with it lower and upper turnstiles, as shown in Fig. 1.

A more refined partition may be obtained by taking the nth forward or inverse image of each period n resonance. This will divide each island into 4 or 6 (depending on K) states, for a total of $4n$ or $6n$ states in each resonance. Each main island will be split into 4 or 6 main states, with 4 or 6 turnstiles. In this partition r will range from 1 to $4R$ or $6R$.

This process may be repeated, producing an arbitrarily fine partition of the phase space.

Given any partition in this sequence, we denote by A_r, $\Delta W_r^{(d)}$, and $\Delta W_r^{(u)}$ the areas of the connected chaotic regions in one state, in the lower and in the upper half turnstiles, respectively. Consider the overlap of the outgoing half turnstile of state (r,l), with the ingoing half turnstile of state (r',l'). The area of the connected chaotic region within this overlap may be written, by

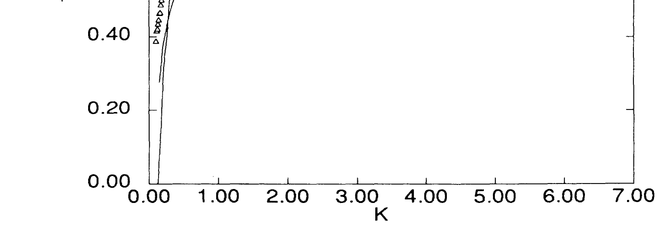

FIG. 3. D/D_{ql} vs K for the sawtooth map: numerical results ($\triangle$), converged results from formula (8) with use of the resonance partition (lower solid curve), the first-refined partition based on the same resonances (upper solid curve), and the second correlation results of Cary and Meiss (dashed line).

translational invariance of (1), as $O(r,r';l'-l)$. It gives the fraction of the flux $\Delta W_r = \Delta W_r^{(d)} + \Delta W_r^{(u)}$ which is transferred per iteration from the state $(r,0;l)$ to the state $(r',1;l')$, or $(r',0;l')$ if $n_{r'}=1$; see Fig. 1. We define $O(r,r;0) \equiv A_r - \Delta W_r$ and $\bar{A}_r \equiv \sum_{r',l'} O(r,r';l')$. Then for $K > K_c$ and finite R the phase-space partition is not complete and $\bar{A}_r < A_r$, but as $R \to \infty$, $\bar{A}_r \to A_r$. According to the Markov assumption the transition probability from $(r,0;l)$ to $(r',1;l')$ is defined by

$$P(r,0 \to r',1;l'-l) \equiv O(r,r';l'-l)/\bar{A}_r ,$$

namely by use of $\bar{A}_r$ instead of A_r. Within a given resonance (r,l), $n_r > 1$, the transition probability from $(r,s;l)$, $s>0$, to $(r,s';l)$ is given by $\delta_{s+1,s'}$. All other transition probabilities are zero. Then

$$\sum_{r',s',l'} P(r,s \to r',s;l') = 1$$

as required.

The master equation of our model is

$$b(r',s';l' \mid t+1) = \sum_{r,s,l} P(r,s \to r',s';l'-l)\, b(r,s;l \mid t) , \quad (2)$$

where $b(r,s;l \mid t)$ is the probability of being in state $(r,s;l)$ at time t. This equation, together with a particular partition, defines a Markov chain.[13] We introduce the Block quasimomentum (k) representation,[10] $\beta(r,s;k \mid t)$ of $b(r,s;l \mid t)$:

$$b(r,s;l \mid t) = \frac{1}{2\pi}\int_0^{2\pi} dk\, \beta(r,s;k \mid t) e^{-ikl} . \quad (3)$$

Let us denote by $\boldsymbol{\beta}(k \mid t)$ the vector with S components $\beta(r,s;k \mid t)$, where S is the total number of states per unit cell. Using the translational symmetry, (2) and (3), we obtain the master equation in the k representation $\boldsymbol{\beta}(k \mid t+1) = \boldsymbol{\Phi}(k)\boldsymbol{\beta}(k \mid t)$, where $\boldsymbol{\Phi}(k)$ is the $S\times S$ transition matrix (or characteristic function)[13] with elements

$$[\boldsymbol{\Phi}(k)]_{r',s';r,s} = (1-\delta_{n_r,1})(1-\delta_{s,0})\delta_{r,r'}\delta_{s+1,s'} + \delta_{s,0}\delta_{s'1}\sum_l O(r,r';l)e^{ikl}/\bar{A}_r . \quad (4)$$

Here $\delta_{s',1} \equiv 1$ for $n_{r'}=1$. For $j=1,\dots,S$, the eigenvalues $\lambda_j(k)$ of $\boldsymbol{\Phi}(k)$, defined by

$$\boldsymbol{\Phi}(k)\mathbf{e}_j(k) = \lambda_j(k)\mathbf{e}_j(k) , \quad (5)$$

form S bands, analogous to the Bloch bands in a periodic crystal with S degrees of freedom per unit cell. It follows from (4) and (5) that $|\lambda_j(k)| \le 1$ for all j and k. For R large enough the Markov chain (2) is irreducible and aperiodic,[13] and obviously the same is true for the chain corresponding to $\boldsymbol{\Phi}(0)$. We observe that there exists an equilibrium distribution given by the eigenvector $[\mathbf{e}_1(0)]_{r,s} = \bar{A}_r$. It follows[13] that $\lambda_1(0)=1$ is always a nondegenerate eigenvalue, and the chain is ergodic.

The diffusion coefficient D for the model is given by

$$D = \lim_{t\to\infty} \frac{1}{2t} \sum_{r,s,l} (p_{r,s;l} - p_{r',s';0})^2 b(r,s;l \mid t) ,$$

where $p_{r,s;l} = p_{r,s;0} + l$ is a "momentum" assigned to the state $(r,s;l)$. Independently of the choice of $p_{r,s;0}$ and $p_{r',s';0}$ we find that

$$D = -\ddot{\lambda}_1(0)/2 , \quad (6)$$

where the overdot stands for differentiation with respect to k. This follows from (3), (5), and the fact that $\dot{\lambda}_1(0)=0$. To see that $\dot{\lambda}_1(0)=0$, differentiate (5) once to find that

$$[\mathbf{I} - \boldsymbol{\Phi}(0)]\dot{\mathbf{e}}_1(0) = i\mathbf{h} - \dot{\lambda}_1(0)\mathbf{e}_1(0) , \quad (7)$$

where

$$\mathbf{h}_{r,s} = \delta_{s,1}h_r = \delta_{s,1}\sum_{r',l} lO(r',r;l) ,$$

and $\sum_r h_r = 0$ from the symmetry $f(-x) = -f(x)$. By summing over all S components the result follows. In solid-state-physics terms, we may thus interpret D in (6) as the inverse of the hole effective mass at the top of the highest Bloch band $\lambda_1(k)$.[10]

To obtain a more explicit expression for D, we differentiate (5) twice at $k=0$. Using (4) and summing over all (r,s) we find

$$D = \frac{1}{2\bar{A}_T}\left[\sum_{r,r',l} l^2 O(r,r';l) - 2i\sum_r [\dot{\mathbf{e}}_1(0)]_{r,0} g_r/\bar{A}_r\right] , \quad (8)$$

where $\bar{A}_T \equiv \sum_r n_r \bar{A}_r$ is the total area and $g_r = \sum_{r',l} lO(r,r';l)$. Since $\lambda_1(0)$ is a nondegenerate eigenvalue, we may always solve (7) for $\dot{\mathbf{e}}_1(0)$ up to an arbitrary complex constant times the vector $\mathbf{e}_1(0)$. Finally, since $\sum_r g_r = \sum_r h_r = 0$, we see that D as given in (8) does not depend on this constant.

We illustrate formula (8) in the case of the sawtooth map, for which all the overlaps may be found analytically.[12] Our numerical measurements of $D(K)$ near $K=0$ have been fitted by a power law aK^b with $a=0.0504 \pm 0.0003$ and $b=2.494\pm 0.0008$. Figure 2 shows $D(K)/\sqrt{K}D_{ql}$ ($D_{ql}=K^2/24$ is the quasilinear value of D) for small K as obtained numerically and from formula (8) with use of all resonances with $n_r \le 21$ (the lower curve), and from the refined partition generated by taking the nth inverse image of all resonances with $n_r \le 21$ (the upper curve). We see that $D(K)$ as given by (8) exhibits a threshold behavior. As we reduce K, the turnstiles of some neighboring resonances cease to overlap; as the value of K for which this happens depends on the number of resonances we denote the value by $K_c(R)$. For $K < K_c(R)$ the Markov chain is reducible and (8) gives $D=0$. For $K_c(R) \le K < K_T(R)$ our expression for D has not converged and we find that $D \sim [K - K_c(R)]^2$. The threshold value $K_T(R)$ is an estimated lower limit of convergence of (8), in the sense that the addition of more resonances does not change the value of D significantly for $K > K_T(R)$.

Both partitions predict the proper scaling exponent b, but the refined partition gives a better estimate of the prefactor a; we find $D \approx 1.15K^{2.5}$ in good agreement with the numerical result of $D \approx 1.25K^{2.5}$.

The scaling seems to arise as a collective effect of many resonances with approximately equal partial fluxes, in contrast to the standard map.[5] For very small $K - K_c(R)$ one partial flux is much smaller than the others: It scales like $[K - K_c(R)]^2$, leading to the (incorrect) scaling observed in D below threshold.

Figure 3 shows D/D_{ql} as a function of K for the resonance partition (lower solid curve) and for the refined partition (upper solid curve) together with the result of Cary and Meiss[2] (dashed line) and numerical results. In the case of the resonance partition we see just a hint of oscillations that are in phase with those of the numerical results, but their amplitude is far too small. However, refining the partition improves the theoretical estimate dramatically. The oscillations arise as the lowest part of the 0/1 resonance turnstile periodically passes through translates of itself as K increases.[12]

In conclusion, it appears that formula (8) gives good results for *all* values of K. The predictions of the Markov model are improved considerably by extending the phase-space partition to the interior of the resonances.

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