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Nonergodicity, accelerator modes, and asymptotic quadratic-in-time diffusion in a class of volume-preserving maps

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Using an elementary application of Birkhoff's ergodic theorem, we give necessary and sufficient conditions for the existence of asymptotically n^2 diffusion (where n is an integer representing discrete time) in the angle variables in a class of volume-preserving twist maps. We show that nonergodicity is the dynamical mechanism giving rise to this behavior. The influence of accelerator modes on diffusion is described. We discuss how additive noise changes the diffusive behavior and we investigate the effective-diffusivity dependence on bare diffusivity and accelerator modes. In particular, we find that the dependence of the effective-diffusivity coefficient on bare-diffusivity is universal for small values of bare-diffusivity coefficient σ if asymptotic n^2 diffusion is present in the $\sigma = 0$ case.

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Consider a *volume-preserving* diffeomorphism $M : B \times T^n \to B \times T^n$, which is of the form

$$I^{n+1} = I^n + f(I^n, \theta^n),$$
$$\theta^{n+1} = \theta^n + \Omega(I^n) + g(I^n, \theta^n), \quad (1)$$

where $I \in B \subset \mathbb{R}^m$, B is a closed ball in $\mathbb{R}^m$, and $\theta \in T^n$, where T^n denotes the n torus. We assume that the functions f, g, and Ω are bounded functions measurable on $B \times T^n$, with f and g periodic in $\theta^1, ..., \theta^n$. When discussing our results in the context of the Kolmogorov-Arnold-Moser (KAM) and Nekhoroshev theorems, stronger regularity conditions are required, real analyticity is sufficient, and certain nondegeneracy conditions on the frequencies are required.

The map M can be viewed as a generalized *twist map* of the form that arises in a variety of applications. For an equal number of "action" and "angle" variables (1) (i.e., $m = n$), and for f and g small, (1) has the form of a Poincaré map of the type arising in studies of perturbations of completely integrable Hamiltonian systems (see [1]). In these studies, the KAM theorem and Nekhoroshev's theorem are important global dynamical results. Roughly speaking, Nekhoroshev's theorem states that for any initial condition the evolution of the action variables is small over exponentially long time scales: The KAM theorem states that the evolution of certain action variables corresponding to sufficiently *nonresonant* initial conditions is small over infinite time intervals. Both Nekhoroshev's theorem and the KAM theorem are deep results. However, neither result says anything about the evolution of the angle variables. On the other hand, we shall show below that relatively simple methods can be used to prove statements about the statistics of angle evolutions for a broad class of relevant maps.

For $m = 1$ and $n = 2$, (1) is of the form recently studied in [2] in an application to fluid transport in time-periodic volume-preserving three-dimensional fluid flows. Recently, generalizations of the KAM theorem to maps of the form (1) for $m \neq n$ have been made in [3–6]. Recent extensions of Nekhoroshev's theorem to maps can be found in [7–9]. For $m = 0$, (1) is a map of the n torus; for $n = m = 1$, it is of the form of the standard map on the cylinder of which there have been many numerical studies.

Our goal is to discuss the notion of "diffusion" in the individual components of the θ vector for this map. The ith component of the θ^n is given by

$$\theta_i^n = \theta_i^0 + \sum_{k=0}^{n-1} \Omega_i(I_k) + g_i(I_k, \theta_k).$$

We are not considering θ_i^n mod 2π, but θ_i^n defined on $\mathbb{R}$, which is relevant in many applications.
The mean square deviation of this quantity is given by

$$\langle (\theta_i^n - \theta_i^0 - \langle \theta_i^n - \theta_i^0 \rangle)^2 \rangle \equiv D_{\theta_i}(n),$$

where the average indicated by the angle brackets is defined as

$$\langle \theta_i^n - \theta_i^0 \rangle \equiv \int_{B \times T^n} (\theta_i^n - \theta_i^0)\, p d\mu,$$

where $p = p(I, \theta)$ is the initial distribution of points (assumed to be integrable on $B \times T^n$) and $d\mu$ denotes the measure or "volume element" on $B \times T^n$. One is then interested in the following limit:

$$\lim_{n\to\infty} \frac{D_{\theta_i}(n)}{n^\gamma},$$

for values of the exponent γ for which the limit exists and is nonzero. If $\gamma = 1$, the motion is referred to as *diffusive* and for $\gamma \neq 1$ it is referred to as *anomalous diffusion.*

We are interested in determining the asymptotic behavior of $D_{\theta_i}(n)$ as $n \to \infty$. Consider the following calculations.

$$\begin{aligned}\lim_{n\to\infty} \frac{D_{\theta_i}(n)}{n^2} &= \lim_{n\to\infty} \left\langle \left(\frac{1}{n}\sum_{k=0}^{n-1} (\Omega_i + g_i)\left(M^k(I,\theta)\right) - \left\langle \frac{1}{n}\sum_{k=0}^{n-1} (\Omega_i + g_i)\left(M^k(I,\theta)\right) \right\rangle \right)^2 \right\rangle \\ &= \left\langle \left(\lim_{n\to\infty} \frac{1}{n}\sum_{k=0}^{n-1} (\Omega_i + g_i)\left(M^k(I,\theta)\right) - \left\langle \lim_{n\to\infty} \frac{1}{n}\sum_{k=0}^{n-1} (\Omega_i + g_i)\left(M^k(I,\theta)\right) \right\rangle \right)^2 \right\rangle \\ &= \left\langle \left[(\Omega_i + g_i)^* (I,\theta) - \langle (\Omega_i + g_i)^* (I,\theta) \rangle \right]^2 \right\rangle \equiv a.\end{aligned}$$

The mathematical manipulations in these calculations are justified as follows:

(i) The passage from the first to the second line is justified, using Lebesgue's bounded convergence theorem, by the fact that the function $(\Omega_i + g_i)$ is bounded and measurable on $B \times T^n$.

(ii) In the second line, the limit

$$\lim_{n\to\infty} \frac{1}{n}\sum_{k=0}^{n-1} (\Omega_i + g_i)\left(M^k(I,\theta)\right) \equiv (\Omega_i + g_i)^* (I,\theta)$$

exists for all points in $B \times T^n$ by Birkhoff's ergodic theorem (see [10]), *with the possible exception of a set of μ-measure zero.* This limit is the time average of the function $(\Omega_i + g_i)$ along the orbit trajectory that starts at the point (I,θ).

The nature of the coefficient a gives some insight into the dynamical mechanism giving rise to n^2 diffusion. Let B_c be the set of all points (I,θ) in $B \times T^n$ such that $(\Omega_i + g_i)^* (I,\theta) = c$. Suppose further that the initial distribution $p(I,\theta)$ is such that it is not entirely contained in B_c, for some c (with the exception of a set of μ-measure zero). Then it can be shown that $a \neq 0$ (see [11]), and from boundedness of g and Ω, we can conclude $a < \infty$. This means that if we choose initial conditions such that the particles are not initially in only one B_c, then we will observe n^2 diffusion when the number of iterations is large. The converse is also true: If we observe n^2 diffusion (i.e., $a \neq 0$), then the initial distribution of particles is not entirely contained in a set B_c, for only one c. Now suppose our system is ergodic on $B \times T^n$. Then, clearly, $a = 0$ and the diffusion exponent (if it exists) $\gamma < 2$. Thus, nonergodicity is necessary (but not sufficient) for $\gamma = 2$.

The above analysis is intuitively completely clear in one direction: assuming that different initial conditions travel with different average speeds leads to n^2 diffusion. The converse question is interesting. In particular, is it possible to obtain n^2 diffusion from a map for which the time averages are equal for almost all initial conditions (an extreme example being any ergodic map)? The answer provided by the above analysis is no. The only mechanism that leads to n^2 diffusion in deterministic maps is the difference in time averages of $(\Omega_i + g_i)$. In many studies of the diffusion in maps, asymptotic n^2 behavior for diffusion was observed, but a clear association with the difference in time averages was not presented. For example, in their pioneering work on diffusion in maps Cary and Meiss [12] observed n^2 diffusion in a nonergodic regime caused by the so-called accelerator modes (see the discussion below). In a recent study of Neishtadt *et al.* [13] on the diffusion of charged particles moving at an angle to the magnetic field in the field of a wave packet, the n^2 regime is the only one observed. There are many examples of maps arising from fluid mechanical problems that exhibit n^2 diffusion. Nonergodicity is common in measure-preserving maps (see [14,15]). Therefore, the phenomenon analyzed here should be important. It is especially important in numerical studies, where the convergence of the diffusion exponent γ should be carefully tested. In particular, small nonergodic regions in the phase space may cause γ to converge to two on very long time scales, although it may seem to have a very well defined value at intermediate time scales.

Let us consider a common situation arising in two-dimensional maps of the form (1),where $M : B \times T^1 \to B \times T^1$. Maps of this form may possess so-called accelerator modes, which we now define. In many numerical studies it has been observed that there may exist an elliptic fixed point $p = (I_0, \theta_0)$ of M such that $(\Omega_i + g_i)^* (I_0,\theta_0) = c \neq 0$. This elliptic fixed point is typically surrounded by invariant curves. This structure is then usually referred to as an *accelerator mode island.* Physically, the requirement on the time average means that, when viewed on $\mathbb{R}$, the point p moves to $\pm\infty$ when $n \to \infty$, depending on the sign of the time average of $(\Omega_i + g_i)$ at that elliptic fixed point (a similar argument goes through for cycles of elliptic fixed points). Now we show that this means that there is a subset of $B \times T^1$, having nonzero measure, containing the elliptic fixed point, which has the property that almost all points in that subset have the same time average of $(\Omega_i + g_i)$ as the elliptic fixed point.

Consider $M : B \times T^1 \to B \times T^1$ as defined above, where B is an interval in $\mathbb{R}$, L is the period or "length" of T^1, and $p = (I_0, \theta_0)$ is an elliptic fixed point such that $\theta_{i+1} - \theta_i = L$, which implies that $(\Omega_i + g_i)^* (I_0,\theta_0) = L \neq 0$. Suppose further that M is sufficiently differentiable so that the KAM theorem can be applied. Then there is a set D of positive measure, with $p \in D$, such that $(\Omega_i + g_i)^* (I, \theta) = L$ for almost every $(I, \theta) \in D$.

To prove this, we first observe that by Moser's version of the KAM theorem [16] there is a closed curve Γ, invariant for M, such that Γ is the boundary of a region of the phase space containing p. We refer to this region as A. By continuity of M and the fact that p maps to $p + (0, L)$,

$$M(A) = A + (0, L),$$

meaning that the region A is just translated by the map M.

For every point p_1 starting inside A, the difference between its θ coordinate at the nth iterate and $\theta(M^n(p))$, denoted $\epsilon(n)$ is, by the above argument, bounded. We have

$$\begin{aligned}\lim_{n\to\infty} \frac{\theta(M^n(p_1))}{n} &= \lim_{n\to\infty} \frac{\theta(M^n(p)) + \epsilon(n)}{n} \\ &= \lim_{n\to\infty} \frac{\theta(M^n(p))}{n} \\ &= (\Omega_i + g_i)^* (I_0, \theta_0) = L,\end{aligned}$$

if the quantity on the left hand side exists. Since, by Birkhoff's ergodic theorem, it does exist for amost all p_1 inside Γ, we are done.

Now suppose that for M an accelerator mode island as above exists. Suppose also that a chaotic region exists, in which $(\Omega_i + g_i)^* (I_0, \theta_0) = 0$, and the initial distribution of particles is such that it occupies both the accelerator mode island and the subset of the chaotic region of positive measure. Then our results on diffusion apply, i.e., $a \neq 0$ and the long time diffusion behaves as n^2. Actually, it is enough to assume that $\langle \Omega_i + g_i \rangle \neq (\Omega_i + g_i)(p)$ to conclude n^2 diffusion.

Many studies of diffusion have been done in the context of dissipative maps, rather then volume-preserving ones (see, e.g., [17]), with n^2 diffusion observed. The general reasoning above (not the accelerator-mode example) applies to those, if we assume that the time averages exist. The necessity of such an assumption is connected to the fundamental difficulty of proving an equivalent of Birkhoff's ergodic theorem in a dissipative context.

Let us now turn to the question of how the above picture changes when a small amount of noise is added to the system. In particular, we consider the perturbation of a system (1) of the form

$$\begin{aligned}I^{n+1} &= I^n + f(I^n, \theta^n) + \delta I, \\ \theta^{n+1} &= \theta^n + \Omega(I^n) + g(I^n, \theta^n) + \delta\theta,\end{aligned} \tag{2}$$

where $\delta I, \delta\theta$ are random variables sampled from Gaussian distributions with mean zero and variance σ. We call σ a bare diffusivity. In [18], Karney *et al.* studied this problem for the case where the deterministic part was given by the standard mapping. Using heuristic arguments, they have discovered that for small σ, the diffusion coefficient,

$$\lim_{n\to\infty} \frac{D_{\theta_i}(n)}{n} \sim \frac{1}{\sigma},$$

when σ is small. Note first that as a small amount of noise is added, the exponent γ jumps from 2 to 1: the limit $\sigma = 0$ is singular in that sense. This can be shown rigorously using homogenization methods for (2) [19]. Also the following can be proven: n^2 diffusion in the $\sigma = 0$ limit is equivalent to the $\frac{1}{\sigma}$ dependence of the diffusion coefficient for small σ. Thus, the result of Karney *et al.* admits a rigorous justification.

The above provides a clear connection between a deterministic diffusion of (1) and diffusion in a stochastic map (2). As we have already mentioned, n^2 is a common result in a class of volume-preserving maps. Besides, it implies universal $1/\sigma$ scaling of the diffusion coefficient once a small amount of noise is added to a system.

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