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LETTER TO THE EDITOR

New universal aspects of diffusion in strongly chaotic systems

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Abstract. We study some new universal aspects of diffusion in chaotic systems, especially those having very large Lyapunov coefficients on the chaotic (indecomposable, topologically transitive) component. We do this by discretizing the chaotic component on the surface-of-section (SOS) in a (large) number N of simplectically equally big cells (in the sense of equal relative invariant ergodic measure, normalized so that the total measure of the chaotic component is unity). By iterating the transition of the chaotic orbit through the SOS, where j counts the number of iterations (discrete time) and assuming complete lack of correlation, even between consecutive crossings (which can be justified due to the very large Lyapunov exponents) we show the universal approach of the relative measure of the occupied cells, denoted by $\rho(j)$, to the asymptotic value of unity, in the following way: $\rho(j) = 1 - (1 - \frac{1}{N})^j$, so that in the limit of big N, $N \to \infty$, we have, for j/N fixed, the exponential law $\rho(j) \approx 1 - \exp(-j/N)$. This analytic result is verified numerically in a variety of specific systems: for a plane billiard (Robnik 1983, $\lambda = 0.375$), for a 3D billiard (Prosen 1997 $a = -\frac{1}{5}, b = -\frac{12}{5}$), for an ergodic logistic map (tent map), for a standard map ($k = 400$) and for the hydrogen atom in a strong magnetic field ($\epsilon = -0.05$) the agreement is almost perfect (except, in the latter two systems, for some long-time deviations on very small scales). However, for Hénon–Heiles system ($E = \frac{1}{6}$) and for the standard map ($k = 3$) the deviations are noticeable though not very big (only about 1%). We have tested the random number generators (Press *et al* 1986), and confirmed that some are almost perfect (ran0 and ran3), whilst two of them (ran1 and ran2) exhibit big deviations.

One of the major open problems in the mathematics of nonlinear Hamiltonian (conservative) chaotic systems of the KAM type is the proof of the so-called coexistence problem (Strelcyn 1991), i.e. the proof that the chaotic components have positive measure. (The KAM Theorem guarantees that the set of invariant tori has positive measure, whose complement is small with the perturbation parameter (Kolmogoroff 1954, Arnold 1963, Moser 1962, Benettin

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et al 1984, Gutzwiller 1990).) The chaotic component could be defined e.g. by the positivity of the (largest) Lyapunov exponent, which is a sufficient but not necessary criterion†. We shall define a chaotic component as the closure of a dense chaotic orbit, which is thus assumed to be an indecomposable invariant component (topologically transitive, i.e. containing a chaotic dense orbit).

There are really no serious doubts about the positivity of the measure of the chaotic components, and so in physics we rely on heuristic arguments to actually assume positivity. Then the question is how to calculate the symplectic (invariant and ergodic) measure of the chaotic component.

We have approached this problem in a recent extensive work (Dobnikar 1996, Robnik and Dobnikar 1997) on the dynamics in a plane-billiard system, defined as the quadratic conformal map of the unit disk (in the complex z-plane) onto the physical (complex) w-plane, $w(z) = z + \lambda z^2$. This system has been introduced by Robnik (1983) and recently extensively studied for many different values of λ by many authors, in a variety of contexts and even in experimental set-ups such as quantum dots (Bruus and Stone 1994, Stone and Bruus 1993a, b), optical models (Nöckel and Stone 1997, Nöckel *et al* 1996) and microwave cavities (Rehfeld *et al* 1997, Richter 1996, Stöckmann *et al* 1997). Further dynamical details were corrected in Hayli *et al* (1987).

At $\lambda = 0$ we have the integrable case of the circle billiard, for $0 < \lambda < \frac{1}{4}$ the billiard is convex, and since the boundary is analytic, the KAM theory applies (Lazutkin 1981, 1991), at $\lambda = \frac{1}{4}$ we get the first point of zero curvature at the boundary point $w = w(z = -1) = -\frac{3}{4}$, allowing for the breaking of Lazutkin caustics (invariant tori associated with the boundary glancing orbits), and for $\frac{1}{4} < \lambda < \frac{1}{2}$ the billiard is non-convex, largely and strongly chaotic (very tiny islands of stability) probably becomes rigorously ergodic at some $\lambda \geqslant 0.2775$ (Li and Robnik 1994) and is definitely proven to be rigorously ergodic for $\lambda = \frac{1}{2}$ (the so-called cardioid billiard, having the cusp singularity at $w = w(z = -1) = -\frac{1}{2}$) (Markarian 1993). The cardioid billiard has also been studied by Bäcker *et al* (1995) and by Bäcker and Dullin (1997).

Our main problem was to calculate numerically, accurately and reliably, the measure of chaotic components. Working in the KAM regime ($0 < \lambda < \frac{1}{4}$) we were observing the typical KAM hierarchy of smaller and smaller islands of stability surrounded by chaotic components, the details of which will be reported in a separate paper (Robnik and Dobnikar 1997), and are reported already in Robnik (1983).

The main objective was to calculate the fractional measure (the relative area on the SOS, the latter being defined by the Poincaré–Birkhoff coordinates; see e.g. Berry (1983), Robnik (1983) of the largest chaotic component at given λ, which we traditionally denote by ρ_2.

This parameter is also important in treating the related quantum mechanical problem (solutions of the Helmholtz equation with the Dirichlet boundary conditions on the billiard boundary) (Berry and Robnik 1984, Prosen and Robnik 1993, 1994a, b, Li and Robnik 1995).

We have discovered, to our surprise, that this numerical calculation is extremely difficult, and as a consequence, some of the previous results had to be revised. By dividing the SOS into a large number of rectangular grid cells of equal relative (normalized) measure we have calculated the relative measure of the chaotic component ρ_2 by three different methods: **(M1)** calculating the Lyapunov exponent for a trajectory starting in a given cell

† For example, in nonrational plane polygonal billiards all Lyapunov exponents are strictly zero (Sinai 1976) yet they can be ergodic. Strong evidence for this has recently been published by Artuso *et al* (1997).

and summing up the area of cells having the positive Lyapunov exponent; **(M2)** calculating two nearby trajectories, separated by an infinitesimal distance (e.g. single precision e-8 while all calculations were in double precision e-16) and summing the cells exhibiting macroscopic divergence in a reasonable time; and **(M3)** starting the chaotic trajectory and counting (summing up) the area of the cells visited (black cells).

It turns out that the third method **(M3)** is the fastest and most reliable. To improve the result one has to enlarge the number of cells N on the chaotic component. However, then the time j (of iterating the map on the SOS, the discrete time) has to be taken much larger (by at least several orders of magnitude) than N, otherwise the statistics of visiting cells (black cells) would be insignificant. Even after calculating as many as 10^9 iterations, with $N = 1000$–2000, the result was no better than within 1%. One reason is that the boundary of the chaotic component turned out to have relatively large fractal dimension around 1.56. The difficulties of estimating the asymptotic value of the relative area ρ_2 of the chaotic component led us to the careful investigation of the evolution of the relative area of occupied (black) cells $\rho_2(j)$ as time j proceeds. We wanted to understand this theoretically, in order to make better estimates of the limiting asymptotic value $\rho_2 \equiv \rho_2(j=\infty)$. From here onwards we shall use the notation $\rho(j) \equiv \rho_2(j)/\rho_2(j=\infty)$.

In general, this time evolution $\rho(j)$ with j is quite complex and specific, nonuniversal, depending on many features appearing in the phase space (SOS), e.g. the existence of sticky objects like cantori can affect a temporary but quite persistent trapping of the orbit near such an object, which is then manifested in a transient plateau of the curve $\rho(j)$, which sometimes might be mistakenly interpreted as final and definite convergence of the cumulative area/volume $\rho_2(j)$. However, if the system is really strongly chaotic, having a large maximal positive Lyapunov exponent, then due to the bound motion and conservation of the phase-space volume, we find a very strong stretching and folding in the phase space. In such a limiting case, therefore, one small phase-space cell (SOS cell) becomes uniformly distributed, in the coarse-grained sense, all over the allowed chaotic component. Thus, in such extreme cases, the probability of entering a given cell belonging to the same chaotic component in SOS is just equal to the relative measure of the cell, i.e. there are no correlations, not even between two consecutive SOS iterations: complete randomness of deterministic motion.

While the behaviour in such an ideal extreme case is quite obvious, it is far from obvious that the conditions of the complete randomness are actually satisfied in specific chaotic deterministic dynamical systems. Therefore, to make things precise we have developed the following theoretical model.

Suppose we have N cells, where their order and geometry of arrangement is completely irrelevant and perhaps not even known. We are filling the cells with balls, one at the time. At each step j (discrete time) we have equal probability of choosing any cell, equal to $a \equiv 1/N$. (Thus there are absolutely no correlations between any moves, including the consecutive ones, and therefore e.g. the repetition of falling into a given, already filled, cell is allowed.) We define by $P_j(k)$ the probability that at the jth step k cells are occupied, keeping in mind that $a = 1/N$ is the model parameter implicit in the mathematical formulae. We shall refer to this model as *the random model* (of strongly chaotic deterministic diffusion). The probabilities must be normalized, therefore

$$\sum_{k=1}^{k=N} P_j(k) = 1 \qquad \forall j = 1, 2, \ldots. \tag{1}$$

We shall calculate $P_j(k)$, and their moments, in particular the first moment, namely the average (normalized) measure of the occupied cells,

$$\rho(j) \equiv \sum_{k=1}^{N} ka P_j(k) = \langle ka \rangle \tag{2}$$

where by $\langle \cdots \rangle$ we denote the averaging operation.

Before explicitly calculating $P_j(k)$ we observe the physically (probabilistically) quite obvious recursion relation, namely

$$P_{j+1}(k+1) = P_j(k+1)\frac{k+1}{N} + P_j(k)\left(1 - \frac{k}{N}\right) \qquad \forall 0 \leqslant k \leqslant j \tag{3}$$

where we also define the boundary conditions

$$P_j(0) \equiv 0 \qquad P_1(1) = 1 \qquad P_j(k > j) = 0 \qquad P_j(k > N) = 0. \tag{4}$$

The interpretation of equation (3) is: the probability of having $(k+1)$ cells occupied at time $(j+1)$ is equal to the sum of the following probabilities: either at time j the $(k+1)$ cells were already occupied, and we add the next ball into the black cells with probability $(k+1)/N$, or at time j only k cells are occupied (black), and we add the next ball (the $(j+1)$st one) into the empty (not-yet occupied) cells with probability $(1 - k/N)$. With the boundary conditions (4) the recursion relation (3) solves the problem, in principle. We show the explicit solution below, using a different approach. However, for a practical (numerical) evaluation of $P_j(k)$ (on the computer) it is much better to use the recursion formula (3) than the explicit result which we shall derive below.

First note that the summation of the recursion equation (3) on each side from $k = 0$ to $k = N - 1$ confirms the preservation of normalization (1), for all j.

Next, we can immediately find the solution for $\rho(j)$ by the following trick: multiply the recursion relation (3) on the left and on the right by $(k+1)/N$ and sum it from $k = 0$ to $k = N - 1$. By denoting $S(j)$ the second moment,

$$S(j) \equiv \langle (ak)^2 \rangle = \sum_{k=1}^{k=N} P_j(k)(ak)^2 \tag{5}$$

we obtain in a straightforward manner,

$$\rho(j+1) = S(j) - (S(j) - P_j(N)) + (1-a)(\rho(j) - P_j(N)) + a(1 - P_j(N)) \tag{6}$$

and therefore after cancellation of the $S(j)$ we get the simple recursion equation for $\rho(j)$, namely

$$\rho(j+1) = a + (1-a)\rho(j) \tag{7}$$

with the explicit solution, which is quite easy to find,

$$\rho(j) = 1 - (1-a)^j = 1 - \left(1 - \frac{1}{N}\right)^j \tag{8}$$

which in the limit of large N, for j/N fixed, becomes a simple exponential law

$$\rho(j) \approx 1 - \exp\left(-\frac{j}{N}\right). \tag{9}$$

We see that in the limit of sufficiently large N, for j/N fixed, we have the universal scaling of the relative measure of the chaotic region ρ, normalized to unity, such that $\rho(j) \to 1$, when $j \to \infty$, as a function of the scaled discrete time, namely j/N. We shall show below, that this law is obeyed by a surprising variety of deterministic dynamical systems.

Our *random model* is a probabilistic (statistical) model and therefore we can calculate all moments of $P_j(k)$, systematically, using the same trick as above: multiply the recursion relation (3) by $(k+1)^2/N^2$ on both sides, sum it up from $k=0$ to $k=N-1$ on both sides, and uncover the recursion relation for the second moment $S(j)$, namely

$$S(j+1) = \frac{1}{N^2} + \left(\frac{2}{N} - \frac{1}{N^2}\right)\rho(j) + \left(1 - \frac{2}{N}\right)S(j) \tag{10}$$

and by using the exact result for $\rho(j)$ from equation (8) we have

$$S(j+1) = 2a - a(2-a)(1-a)^j + (1-2a)S(j) \qquad a \equiv 1/N. \tag{11}$$

This equation can be solved either by standard techniques or by using the definition of $S(j)$, equation (5), to yield the explicit result

$$S(j) = 1 - (2-a)(1-a)^j + (1-a)(1-2a)^j \qquad a \equiv 1/N \tag{12}$$

so that the predicted dispersion $\sigma^2(j)$ according to our model is exactly

$$\sigma^2(j) = S(j) - \rho^2(j) = a(1-a)^j + (1-a)(1-2a)^j - (1-a)^{2j} \qquad a \equiv 1/N. \tag{13}$$

In the asymptotic limit of a sufficiently large number of cells $N = 1/a \to \infty$, but keeping j/N fixed, we find the simple exponential laws:

$$\rho(j) \approx 1 - \exp(-j/N) \qquad S(j) \approx [1 - \exp(-j/N)]^2 \approx \rho^2(j) \tag{14}$$

and therefore

$$\sigma^2(j) \approx N^{-1}[\exp(-j/N) - \exp(-2j/N)] \to 0. \tag{15}$$

Now we show the explicit and exact result for $P_j(k)$, for the sake of completeness. In fact the quantity we seek is the subject of the classical problem from combinatorial analysis, treated e.g. in Vinogradov (1979) volume 2, p 973, Riordan (1978) p 48, table 2 and Graham *et al* (1994). The question is how many possibilities are there to distribute j different things into N different cells under the condition that $N-k$ cells are empty (i.e. precisely k cells are occupied): the answer is well known, namely in the literature denoted by $C_{Nj}(N-k)$,

$$C_{Nj}(N-k) = \binom{N}{N-k} k!\mathcal{S}(j,k) = \frac{N!}{(N-k)!}\mathcal{S}(j,k) \tag{16}$$

where $\mathcal{S}(j,k)$ are the so-called Stirling numbers of the second kind (Vinogradov 1979, Riordan 1978, Graham *et al* 1994)

$$\mathcal{S}(j,k) \equiv \frac{1}{k!}\sum_{i=0}^{k}\binom{k}{i} i^j (-1)^{k-i} \tag{17}$$

which are known to satisfy the triangular recursion relation $\mathcal{S}(j,k) = k\mathcal{S}(j-1,k) + \mathcal{S}(j-1,k-1)$, where $\mathcal{S}(0,0) = 1$, $\mathcal{S}(j,0) = 0$, $\mathcal{S}(0,k) = 0$ $(j,k) > 0$. Of course, having the N cells and j things, as in our *random model*, the total number of possibilities to distribute j things (balls) into N cells is just N^j, and therefore we have the final and complete explicit solution to the *random model*, namely

$$P_j(k) = \frac{C_{Nj}(N-k)}{N^j} = \frac{N!\mathcal{S}(j,k)}{(N-k)!N^j}. \tag{18}$$

Now we proceed by analysing specific dynamical systems from the point of view of the statistical theory presented in our *random model*, to see to what extent we find agreement in real systems. The really big surprise is that the behaviour was found to be in excellent or even perfect agreement with theory in a large variety of deterministic dynamical systems, sufficiently far from a pronounced KAM regime, by which we mean either close to ergodic

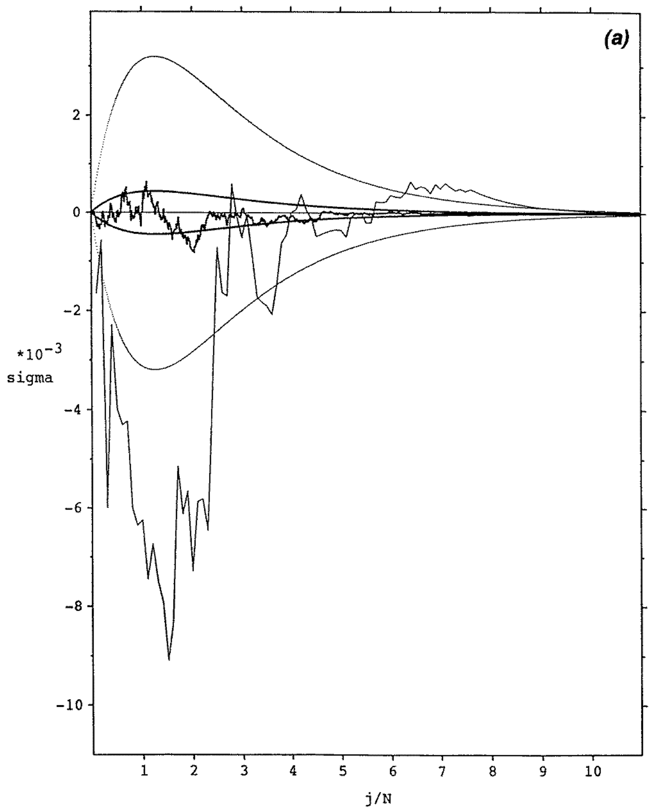

Figure 1. (a)–(c) We show the plots of $\rho_{\text{numerical}}(j) - \rho_{\text{theory}}(j)$ versus the scaled discrete time j/N. The more noisy curve is the numerical result for a chaotic orbit with a certain representative initial condition, whilst the less noisy one is the average over 50 evenly distributed initial conditions. We also show the $\pm\sigma(j)$ standard deviation (pairs of smooth curves) as predicted theoretically in equation (13), for one initial condition (outer curves) and for the average over the 50 initial conditions (the inner curves). It is clear that for the 2D billiard in (a) the agreement is almost perfect, in the sense that the fluctuations are within the predicted range, whilst for the 3D billiard in (b) we see systematic deviations, obviously caused by some, perhaps unexpected, long time correlations. Such correlations are even stronger in the case of the hydrogen atom in a strong magnetic field, shown in (c). In all cases the deviations are predominantly negative: the orbit tries to stick to some of the already occupied cells.

(big $\rho_2(j = \infty) \approx 1$), or strongly chaotic (big Lyapunov exponent but not necessarily very large $\rho_2(j = \infty)$).

We have investigated the plots $\rho(j)$ versus j/N for the following systems: **(a)** the 2D billiard (Robnik 1983) at $\lambda = 0.375$, **(b)** the 3D billiard (Prosen 1997a,b, def. geom.: $a = -\frac{1}{5}, b = -\frac{12}{5}$), **(c)** the hydrogen atom in strong magnetic field diamagnetic Kepler problem (DKP) with the *scaled energy* $\epsilon = -0.05$ (see e.g. Hasegawa *et al* 1989), **(d)** the Hénon-Heiles system at the escape (dissociation) energy $E = \frac{1}{6}$ (see Hénon and Heiles 1964), **(e)** the standard map on a torus (Chirikov 1979) with $k = 3$, **(f)** the standard map on a torus (Chirikov 1979) with $k = 400$, and **(g)** for the logistic map at $\lambda = 4$ (the ergodic tent map).

In the case of smooth systems **(c)** and **(d)** we have used special symplectic integration routines, devised by Yoshida (1990). This enabled a fast and extremely accurate calculations,

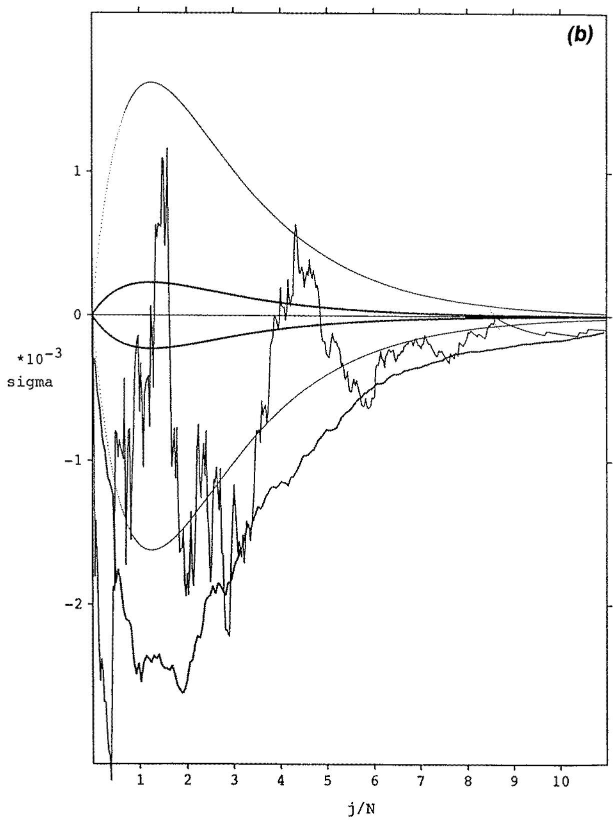

Figure 1. (Continued)

allowing us to compute to an order of magnitude of about 10^5 iterations on the SOS.

The agreement for all systems was perfect (deviations much smaller than 1%), except in **(d)** and **(e)**, where the deviations fluctuated about up to 1%. Therefore we do not show these plots, since all curves practically overlap with the theoretical curve (8) and (9) within the graphical resolution. (In fact the agreement was better still than in the case of the ergodic-only system (the irrational triangle) whose results we show in figure 3, which is another reason for not showing the plots for **(d)–(g)**.)

The small deviations stem from the fact that the Lyapunov coefficients are still not big enough, and also that there might be significant episodes of transient behaviour in the relationship of $\rho(j)$ with respect to the discrete time j/N. Such transient episodes are typically caused by the sticky objects in the phase space, e.g. by cantori, where the classical orbit spends a long time before resuming the chaotic random filling of the remaining empty cells. They are very well manifested in systems with more pronounced KAM structure, such as the 2D billiard ($\lambda = 0.15$) or 3D billiard (for sufficiently small a and b, e.g. $a = -0.1$, $b = 0$). In order to describe such systematic effects in a statistical way we have developed a *multicomponent random model*, where orbital transitions inside each component are random as in our *random model*, however, they may jump (rarely) from one into another component. Some of the dynamical features are well described by such a model, whose detailed description will be published in a separate paper (Robnik *et al* 1997).

In cases **(a)–(c)** the agreement is so good, surprisingly, that it is necessary to magnify the

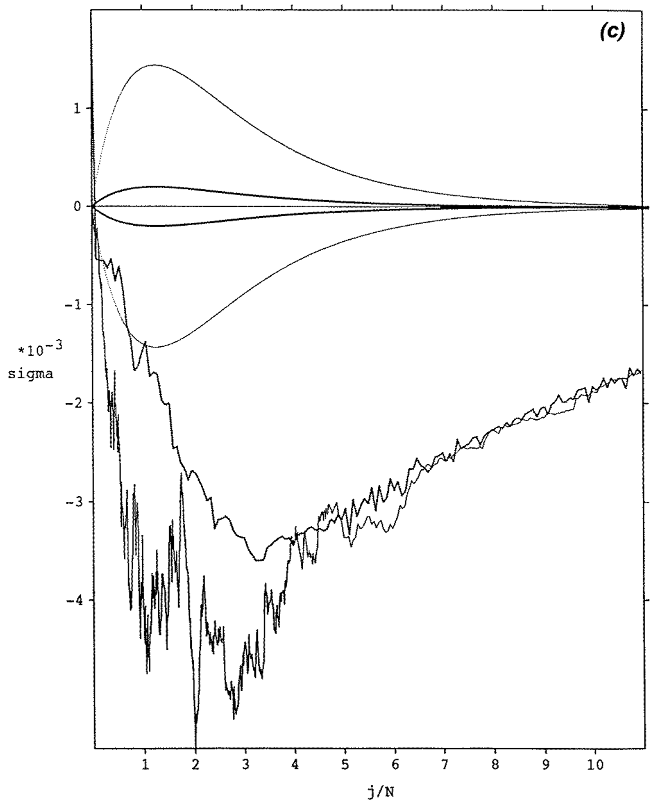

Figure 1. (Continued)

scale so that the details of deviations become clearly visible. This is done in figures 1(a)–(c) for the systems, respectively. We plot the fluctuation (difference) $\rho_{\mathrm{numerical}}(j) - \rho_{\mathrm{theory}}(j)$ (the noisy curves) to be compared with the theoretically expected standard deviation $\sigma(j) = \pm\sqrt{S(j) - \rho^2(j)}$ (smooth curves), again as a function of the scaled discrete time j/N. We do this in each of the plots for one initial condition (the pair of outer smooth curves) and for the average over 50 randomly (uniformly over the chaotic component) chosen initial conditions (the pair of inner smooth curves) which suppress the dispersion by a factor of 50 and the standard deviation by $\sqrt{50}$. In each of these plots, figures 1(a)–(c), the more noisy curve corresponds to one initial condition, and the less noisy one to the average over 50 initial conditions.

Our conclusion on inspection of these plots is that the 2D billiard perfectly obeys the law of our *random model*, whilst for the hydrogen atom in a strong magnetic field and the 3D billiard we uncover systematic deviations from the theory for sufficiently large scaled discrete times j/N: the deviations are orders of magnitude bigger than the prediction of our *random model* for the DKP, but somewhat smaller in the 3D billiard. It should be noted that the deviations are almost strictly *negative*, reflecting the fact that the physical orbits like to stick to already occupied cells (in the vicinity of the sticky objects in the phase space, such as cantori, whose structure could be identified and uncovered). The same behaviour was observed in the systems **(d)**, **(e)** and **(f)** defined above. We could see the plateaux in the curves $\rho(j)$ versus j/N, and then identify the relevant objects in the SOS.

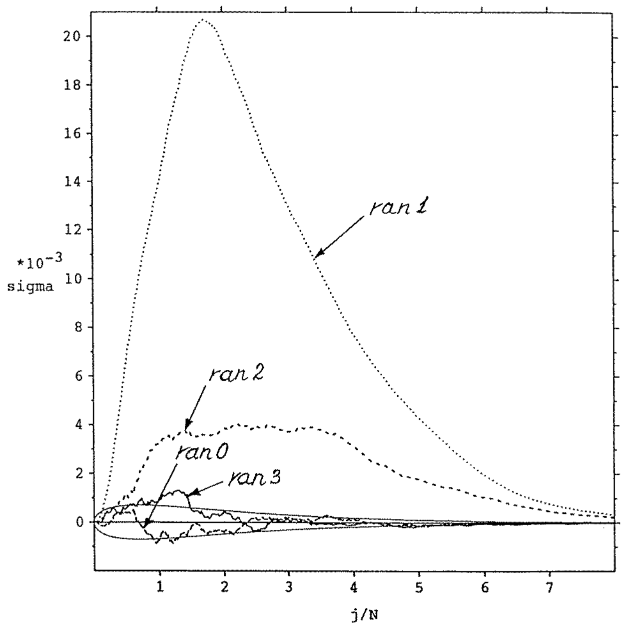

Figure 2. We show the results $\rho_{\rm numerical}(j) - \rho_{\rm theory}(j)$ versus j/N for the random number generators, compared with the theoretical $\pm\sigma(j)$ curves according to equation (13) (Press *et al* 1986): for ran0 and ran3 the agreement is excellent, while for ran1 and ran2 the deviations are so big and mainly positive, that they are actually not random: they seem to repel from the occupied cells.

It is interesting to look at the results for random number generators. Cells are 'randomly' chosen, using different random-number-generator algorithms. One such algorithm was devised by Finocchiaro *et al* (1993) in the context of nuclear physics. The agreement was perfect, so we do not show the fluctuations plots.

Also, we have checked and tested some well known algorithms for random-number generators, such as ran0, ran1, ran2 and ran3 devised and described in Press *et al* (1986 ch 7, and the references therein). The results are shown in figure 2. As we see ran0 and ran3 are in excellent agreement with our *random model*, whilst for ran1 and ran2 random generators the deviations clearly become very large. Thus, for example, our dynamical deterministic 2D billiard systems, the logistic map or the standard map at $k = 400$, are in fact better random-number generators than some of the most familiar random-number generators used in computers.

Finally, we have looked at the irrational triangle (the angles are $\alpha = (\sqrt{5} - 1)\pi/4$, $\beta = (\sqrt{2} - 1)\pi/2$) as one ergodic system with strictly zero Lyapunov exponents (Sinai 1976, Artuso *et al* 1997). Even there, agreement with our *random model* is surpringly good on the largest scale (figure 3), while the fluctuation diagram exhibits large deviations, again negative, showing that the real billiard orbits like to stay in the already occupied regions (sticky objects in phase space).

In conclusion, we have developed *the random model* of stochastic diffusion of dynamical systems with invariant measure on their SOS, which is supposed and confirmed to apply very well in strongly chaotic systems (for which the Lyapunov coefficients on the chaotic component are sufficiently large). We have discovered and explained the universal scaling behaviour of the normalized chaotic measure ρ as a function of the scaled discrete time

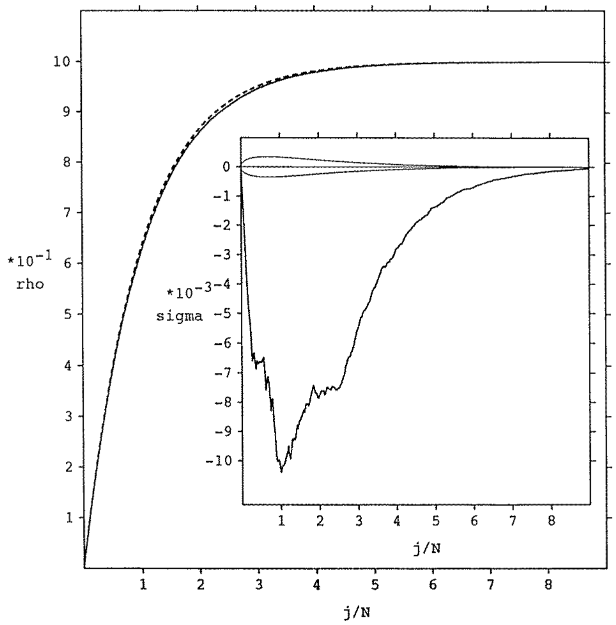

Figure 3. We show the global plot, $\rho_{\rm numerical}(j)$ (full curve) and $\rho_{\rm theory}(j)$ (broken curve), for the irrational triangle, where the agreement is surprinsingly good, in spite of strictly vanishing Lyapunov exponents. In the fluctuations diagram we plot $\rho_{\rm numerical}(j) - \rho_{\rm theory}(j)$ versus j/N, together with the $\pm\sigma$, where we see the same trend to negative deviations due to the sticky objects in the phase space. Only one initial condition was used in this calculation.

j/N, where N is the number of cells: namely, in the limit of sufficiently large N, for j/N fixed, we have a simple exponential law $\rho(j) = 1-\exp(-j/N)$. We also predict the higher moments, especially the dispersion given in equation (13). The model is solved completely in the sense that we have calculated the probabilities $P_j(k)$ of having exactly k nonempty cells at time j. Therefore, all the moments can be calculated. The deviations from the predictions of the random model are qualitatively understood, but will be treated in detail together with a new, more general theory (the multicomponent model) in a separate work (Robnik *et al* 1997). The work is in a sense an extension of the theory of transport in Hamiltonian systems by MacKay *et al* (1984).

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