J. Phys. A: Math. Gen. 23 (1990) L715-L720. Printed in the UK

LETTER TO THE EDITOR

Diffusion in Hamiltonian chaos and its size dependence

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Received 23 April 1990

Abstract. The diffusion process of Hamiltonian map lattice models is numerically studied. For weak non-integrability, the diffusion coefficient of the model has stretched exponential dependence on the non-integrability, which is consistent with Nekhoroshev's bound. Up to a certain size, the exponent of the stretched exponential decreases with the system size, showing that diffusion is enhanced with the increase of the size. As the size gets larger than the correlation length the exponent approaches a finite value. The diffusion coefficient of a model with global interaction is also studied. It again is enhanced with the system size.

Studies on Hamiltonian chaos have a great importance in fundamental physics as a basis of classical statistical mechanics, as well as in application to plasma confinement, solid state physics, etc [1-7]. Chaotic motion of a Hamiltonian system with many degrees of freedom is essential to lead the system to thermal equilibrium.

Some important facts are known on the chaotic motion of Hamiltonian systems with many degrees of freedom. When the dimension of the phase space ($=2N$) is larger than 2, every part of stochastic sea is topologically and dynamically connected even if KAM tori exist [3, 4, 8]. Our dynamics wanders around various states in a stochastic sea, leading to ergodic motion.

This wandering motion is, however, extremely slow when the order of non-integrability is small. The slowness is characterised by an inequality by Nekhoroshev [9-11], sketched as follows. Suppose that we have a nearly integrable $2N$-dimensional Hamiltonian system

$$H(I,\varphi)=H_0(I)+\varepsilon V(I,\varphi) \qquad |\varepsilon|\ll 1,\ I\in \boldsymbol{R}^N,\ \varphi\in \boldsymbol{T}^N \tag{1}$$

then the motion of action variables I is bounded in a small region for a long time T_N as

$$\|I(t)-I(0)\|\leqslant c\varepsilon^{\alpha} \qquad \text{for } |t|\leqslant T_N \stackrel{\text{def}}{=} c'\varepsilon^{-1}\exp(\xi(1/\varepsilon)^{\beta}) \tag{2}$$

where c, c', ξ, α, β are positive constants. We see from (2) that T_N is a tremendously long time for small non-integrability ε. If the diffusion is really slow, we may have to wait until the end of the universe to observe a bunch of gas particles relaxed into thermal equilibrium.

In Nekhoroshev's estimate the exponent β decreases as the system size gets large as

$$\beta=\frac{1}{(\text{polynomial of } N)}. \tag{3}$$

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0305-4470/90/150715+06$03.50

This suggests that the diffusion can be enhanced by increasing the system size, thus supporting the belief that we have thermodynamical behaviour within a non-astronomical timescale.

In this letter we give for the first time numerical examples that the exponent β decreases as N gets large for small N. We also show that β is unchanged if we increase N far beyond the spatial correlation length. The exponent β appears to remain finite when $N\to\infty$.

Numerical calculation is carried out with the use of coupled map lattice models, which are defined on discrete space and time [12-20];

$$[x_i(t), p_i(t)] \mapsto [x_i(t+1), p_i(t+1)] \qquad i=1,2,\ldots,N \tag{4}$$

where the subscript i represents an index of the lattice site. Numerical simulation of Hamiltonian chaos requires long time computation, and coupled map lattices are particularly suitable for such problems.

We study the following models.

(*a*) One-dimensional chain with nearest-neighbour interaction.

$$\begin{aligned} p_i(t+1) &= p_i(t) + \frac{K}{2\pi}\{\sin[2\pi(x_{i+1}(t)-x_i(t))] - \sin[2\pi(x_i(t)-x_{i-1}(t))]\} \qquad K>0 \\ x_i(t+1) &= x_i(t) + p_i(t+1) \end{aligned} \tag{5}$$

where we take periodic boundary condition $x_{i+N}=x_i$, $p_{i+N}=p_i$.

(*b*) Global interaction.

$$\begin{aligned} p_i(t+1) &= p_i(t) + \frac{K}{2\pi\sqrt{N-1}}\sum_{j=1}^{K}\sin[2\pi(x_j(t)-x_i(t))] \qquad K>0 \\ x_i(t+1) &= x_i(t) + p_i(t+1). \end{aligned} \tag{6}$$

In both models the following symplectic condition is satisfied:

$$\sum_{i=1}^{N} \mathrm{d}x_i(t)\wedge \mathrm{d}p_i(t) = \sum_{i=1}^{N} \mathrm{d}x_i(t+1)\wedge \mathrm{d}p_i(t+1). \tag{7}$$

Total momentum $\Sigma_j p_j$ is conserved in both models. Thus the degrees of freedom in our model is not N but $N-1$. For $N=2$, our models are reduced to the standard map by Chirikov and Taylor. In the globally coupled model (6), the coupling constant K is scaled by $\sqrt{N-1}$ so that the model is expected to show extensive behaviour in a strongly chaotic regime $K\gtrsim 1$. In the regime spatial correlation is negligible and the force term $(2\pi\sqrt{N-1})^{-1}K\,\Sigma_{j=1}^{N}\sin[2\pi(x_j(t)-x_i(t))]$ can be approximated by a stochastic term independent of the system size N. This approximation leads to the proportionality of diffusion coefficient to K^2, which is numerically confirmed for $K\gtrsim 1$.

These two models are intended to be typical examples of two different size dependences. Suppose we look at a particular site variable (x_m, p_m) of the model (5). When the spatial correlation decays quite rapidly (and this is so in our case), the number of variables relevant to diffusion is not the total degrees of freedom $2N$ but the variables that are within the spatial correlation length from our variable (x_m, p_m). Thus we expect that, as $N\to\infty$, the model (5) will show size independent i.e., extensive behaviour. Size independence in the behaviour of locally interacting systems are pointed out in several works [21, 22].

In the model (6), on the other hand, all variables directly interact with each other and the enhancement of diffusion by size effect is expected to remain as $N\to\infty$.

The Nekhoroshev bound (2) has a natural relation to diffusion coefficients of action variables. Chirikov [2] showed that under the bound the diffusion coefficient, if it exists, also behaves as

$$D < D' \exp(-\xi(1/\varepsilon)^{\beta}) \qquad \text{where } 0 < D'. \tag{8}$$

Here we examine the K dependence of the diffusion coefficient defined as

$$D \overset{\text{def}}{=} \left\langle \lim_{t\to\infty} \frac{1}{N} \sum_{i=1}^{N} \frac{|p_i(t) - p_i(0)|^2}{t} \right\rangle \tag{9}$$

where $\langle\ldots\rangle$ represents an average taken over independent orbits. In practical calculation the number of paths is typically 10 to 100.

It is known that many Hamiltonian systems exhibit anomalous diffusion

$$|p(t) - p(0)|^2 \propto t^a \qquad a < 1. \tag{10}$$

We have confirmed that our models show anomalous diffusion *only up to a finite interval.* After the interval the diffusion coefficient (9) converges to a finite value [23]. All the diffusion coefficients of our data are taken after the convergence is achieved†.

We calculate the diffusion coefficients for the models (5), (6) for several sizes; $N = 3, 4, 5, 6, 128$ for the locally interacting model (5) and $N = 3, 4, 5, 6$ for the globally interacting model (6).

The raw results of diffusion coefficients D of the models (5) and (6) are summarised in figure 1 and figure 2, respectively.

For the locally interacting model (5) D decays faster than any power law function, and it is fitted by a stretched exponential by changing the value of β;

$$D \propto K \exp(-\xi(1/K)^{\beta}). \tag{11}$$

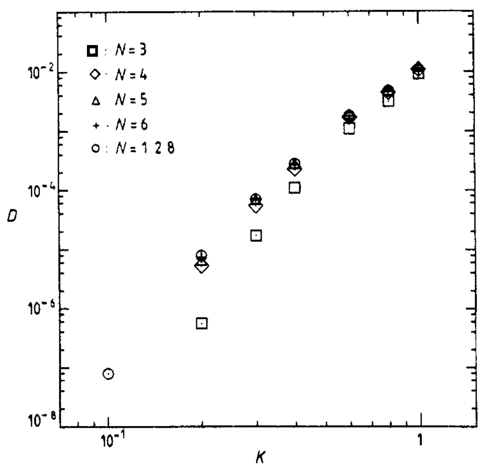

Figure 1. Diffusion coefficient of locally interacting model (5). System size $N = 3, 4, 5, 6, 128$.

† The steps necessary for the convergence are inversely proportional to the diffusion coefficients and are quite long for small K. See figure 1 of [23].

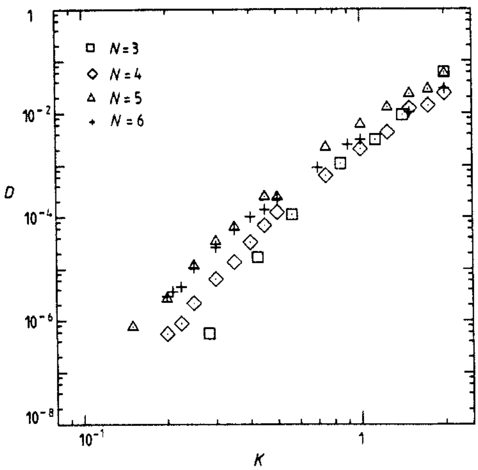

Figure 2. Diffusion coefficient of globally interacting model (6). System size $N = 3, 4, 5, 6$.

An example is shown in figure 3. The values of β in (11) which give best fit are summarised in table 1.

For the model (5) we see that:

(a) when the system size N is small compared to the spatial correlation length, β decreases as N gets large. This means that diffusion is enhanced as the system size is increased;

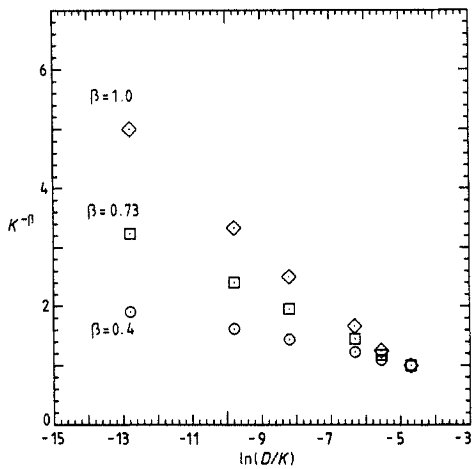

Figure 3. Fitting the diffusion coefficients by stretched exponential function. Here we show the case for the model (5) with $N = 3$. Points $(\log(D/K), K^{-\beta})$ are plotted for three values of β, i.e., $\beta = 0.4$, 0.73, 1.0. If (11) holds the plot should be linear.

Table 1. Exponent β and system size for locally interacting model.

	$D \propto K \exp(-\xi(1/K)^{\beta})$				
N	3	4	5	6	128
$\beta(\pm 0.05)$	0.73	0.46	0.50	0.47	0.43

(*b*) when $N \geqslant$ (correlation length) the value of β seems to converge to a finite value†. In our model this convergence is achieved when $N \geqslant 8$. The convergence is contrary to original estimation (3), where $\beta \to 0$ as $N \to \infty$.

Saturation of the exponent β in the model (5) reminds us of the bound by Wayne [22]. He has obtained a size independent bound on the motion of action variables for locally interacting rotators. The essential point in his theory is that the effective 'size' is the degrees of freedom concerned in the interaction, not the total system size itself. Thus we can say that our model (5) behaves 'Nekhoroshev-like' for N small, and 'Wayne-like' for N large.

In the globally interacting model (6), discrepancy from power-law behaviour is not so evident. The data may be a finite segment of a slightly stretched exponential function. If this is the case the exponent β should be quite small. Since the fitting by stretched exponential is too inaccurate within our range of K, we fit the diffusion coefficients here following the empirical formula by two power-law functions

$$D \propto \begin{cases} K^2 & \ldots \quad K \geqslant 1 \\ K^\gamma & \ldots \quad K \leqslant 1. \end{cases} \tag{12}$$

Our data give‡

$$\gamma = \begin{cases} 5.70 & \ldots \quad N = 4 \\ 4.95 & \ldots \quad N = 5 \\ 4.83 & \ldots \quad N = 6. \end{cases} \tag{13}$$

Although the power-law fitting is done for practical purpose and has no direct theoretical background, we see in this case also that the exponent γ decreases as N gets large, which is another realisation of enhancement of diffusion by getting system size large. This suggests that the stretched exponent β, if obtained, decreases with N.

To conclude, we have shown examples of Hamiltonian map lattice models in which (i) one diffusion coefficient has stretched exponential dependence on the strength of non-integrability and (ii) it is enhanced with the increase of system size until it saturates and approaches a size independent constant as the system size gets larger than the correlation length. The increase of diffusion with the size is also found in the globally coupling model.

We would like to thank National Institute for Fusion Study at Nagoya for the computational facility of FACOM M380 and VP200.

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† In our model the correlation decays quite rapidly. Typically the correlation length is less than three or four sites.

‡ The data for $N = 3$ cannot be fitted in the form (12). A rough estimate of the slope only from $K = 0.2828$ to 0.5657 gives 7.67.

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