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Deterministic diffusion in one-dimensional maps—calculation of diffusion constants by harmonic inversion of periodic orbit sums

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Abstract

A method is proposed for the calculation of diffusion constants for one-dimensional maps exhibiting deterministic diffusion. The procedure is based on harmonic inversion and uses a known relation between the diffusion constant and the periodic orbits of a map. The method is tested on an example map for which results calculated by different other techniques are available for comparison. © 2001 Elsevier Science B.V. All rights reserved.

1. Introduction

Deterministic diffusion plays an important role in a variety of physical phenomena and applications, e.g., particle confinement in magnetic fields [1], conductivity in metals [2], etc. A general theory of diffusion for systems with continuous time is presented in [3]. In systems with periodic phase-space structure, diffusion may be induced by chaotic dynamics inside the elementary cells, causing an irregular jumping between the cells. The investigation of deterministic diffusion is an interesting task both from the theoretical point of view, concerning the question of how the typical stochastic properties arise from a purely deterministic dynamics, as well as with regard to its various applications in different physical contexts.

It has been observed that even the simplest model systems—one-dimensional maps—which exhibit de-

terministic diffusion are capable of explaining the behaviour of relevant physical systems [4,5]. For such maps, it has been demonstrated that the diffusive properties are related to the periodic orbits of the map restricted to an elementary cell [4–7]. In particular, the diffusion constant characterizing the diffusive spreading can be obtained from the leading zero of a zeta function consisting of a product over contributions from all periodic orbits of the reduced map. Similar to the dynamical zeta functions which appear in semiclassical quantization problems, this product usually does not converge. In former work [4–6], the convergence problem was handled by the application of cycle expansion techniques. However, cycle expansion strongly depends on the existence of a symbolic dynamics and the shadowing of long orbits by combinations of short ones.

On the other hand, it has been demonstrated [8,9] that the convergence problems of the zeta functions and corresponding response functions arising in semiclassical quantization problems can be circumvented by the application of harmonic inversion, which is a

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universal method in the sense that it does not rely on a symbolic code or other special properties of the system. The method has recently been extended from Hamiltonian systems to maps [10]. In this Letter we demonstrate that harmonic inversion can also be used for the calculation of diffusion constants of one-dimensional maps. In analogy with the procedure for semiclassical quantization, we rewrite the zeta function as a response function, from which we construct a periodic orbit signal including a finite set of periodic orbits. The analysis of the signal by harmonic inversion yields the zeros of the underlying zeta function, from which the diffusion constant is calculated. We apply this technique to an example map for which the periodic orbits can easily be calculated, and which has already been examined with the help of cycle expansion techniques [11], rendering a comparison with previous results possible.

We start by describing the general procedure. We consider one-dimensional maps $\hat{f} : \mathbb{R} \to \mathbb{R}$ defined by an anti-symmetric function $\hat{f}$,

$$\hat{x}_{n+1} = \hat{f}(\hat{x}_n), \qquad \hat{f}(-\hat{x}) = -\hat{f}(\hat{x}), \qquad (1)$$

for points $\hat{x}$ inside the elementary cell $[-1/2, 1/2)$, and a discrete translational symmetry outside the elementary cell,

$$\hat{f}(\hat{x} + n) = \hat{f}(\hat{x}) + n, \quad n \in \mathbb{Z}. \qquad (2)$$

From this map, a reduced map $f : [-1/2, 1/2) \to [-1/2, 1/2)$ can be constructed by restricting the dynamics to the elementary cell via the definition

$$x = \hat{x} - [\hat{x} + 1/2], \qquad (3)$$

$$f(x) = \hat{f}(x) - [\hat{f}(x) + 1/2], \qquad (4)$$

where $[\,\cdot\,]$ denotes the integer part of the quantity in the brackets. Each periodic orbit of the reduced map $f(x)$, consisting of a sequence of fixed points $\{x_1, x_2, \ldots, x_n\}$, corresponds to an orbit of the full map $\hat{f}(\hat{x})$ which returns to an equivalent point,

$$\hat{f}^n(x_j) = x_j + \sigma_p, \quad \sigma_p \in \mathbb{Z}. \qquad (5)$$

The diffusion constant associated with the map is determined by the lattice translation σ after n applications of the map, averaged over initial conditions in the elementary cell:

$$D = \lim_{n \to \infty} \frac{1}{2n} \langle \sigma^2 \rangle_n. \qquad (6)$$

As was shown in Ref. [6], for hyperbolic or almost hyperbolic maps, the diffusion constant can be determined from the periodic orbits of the reduced map (4) by considering the zeta function

$$Z(z, \beta) = \prod_{m=0}^{\infty} \prod_p \left(1 - \frac{z^{n_p} e^{\sigma_p \beta}}{|\Lambda_p| \Lambda_p^m} \right), \qquad (7)$$

where the second product runs over all primitive periodic orbits of the reduced map; n_p and $\Lambda_p = \sum_{i=1}^{n} f'(x_i)$ are the topological length and the stability of the orbit, respectively, σ_p denotes the lattice translation of the corresponding orbit of the full map, and β is a free parameter. According to Ref. [6], the diffusion constant D can be expressed in terms of the leading zero $z_0(\beta)$ of the zeta function as a function of β:

$$D \approx -\frac{1}{2} \left[\frac{\partial^2}{\partial \beta^2} z_0(\beta) \right]_{\beta=0}. \qquad (8)$$

Additionally, from the symmetry of the map, it follows that $[\partial z_0 / \partial \beta]_{\beta=0} = 0$. Using these relations, an expansion of $\ln z_0(\beta)$ for small β yields

$$\ln z_0(\beta) \approx -\beta^2 D, \qquad (9)$$

which can directly be used to calculate the diffusion constant from the leading zero for small β.

The problem that remains is how to actually calculate the leading zero, since expression (7) for the zeta function usually diverges. In past works, this problem has been tackled by application of cycle expansion techniques. As an alternative, we demonstrate in the following how the zeta function can be expressed in terms of a response function, and how the leading zero can then be obtained by harmonic inversion of a periodic orbit signal constructed from this response function.

2. Harmonic inversion for maps

We start by defining the quantity $w = -i \ln z$ and rewriting the zeta function (7) as a function of w:

$$Z(w, \beta) = \prod_{m=0}^{\infty} \prod_p \left(1 - \frac{e^{iwn_p} e^{\sigma_p \beta}}{|\Lambda_p| \Lambda_p^m} \right). \qquad (10)$$

The density of zeros of the zeta function (10) can be written in the form

$$\rho(w, \beta) = -\frac{1}{\pi} \operatorname{Im} g(w, \beta), \tag{11}$$

where the response function $g(w, \beta)$ is given by

$$g(w, \beta) = g_0(w, \beta) + \frac{\partial}{\partial w} \ln Z(w, \beta) \tag{12}$$

with $g_0(w, \beta)$ a smooth, slowly varying function of w. Using the definition

$$t_p^{(m)} = \frac{e^{iwn_p} e^{\sigma_p \beta}}{|\Lambda_p| \Lambda_p^m}, \tag{13}$$

we rewrite the second term of the response function as

$$\frac{\partial}{\partial w} \ln Z(w, \beta)$$

$$= \sum_{m=0}^{\infty} \sum_{p} (-in_p) \frac{t_p^{(m)}}{1 - t_p^{(m)}} \tag{14}$$

$$= \sum_{m=0}^{\infty} \sum_{p} \sum_{r=1}^{\infty} (-in_p) \left(t_p^{(m)}\right)^r \tag{15}$$

$$= \sum_{m=0}^{\infty} \sum_{p} \sum_{r=1}^{\infty} (-in_p) \frac{e^{iwrn_p} e^{r\sigma_p \beta}}{|\Lambda_p^r| \Lambda_p^{rm}} \tag{16}$$

$$= \sum_{po} (-in_0) \frac{e^{iwn_{po}} e^{\sigma_{po} \beta}}{|\Lambda_{po}|} \sum_{m=0}^{\infty} \Lambda_{po}^{-m}, \tag{17}$$

where the first sum in (17) now runs over *all* periodic orbits (po) including multiple traversals of primitive orbits, and n_0 denotes the topological length of the underlying primitive orbit. After carrying out the sum over m, the response function finally reads

$$g(w, \beta) = g_0(w, \beta) + \sum_{po} (-in_0) \frac{e^{\sigma_{po} \beta}}{|1 - \Lambda_{po}|} e^{iwn_{po}}. \tag{18}$$

On the other hand, the response function can be written in terms of the zeros w_k of the zeta function (10) and their multiplicities d_k:

$$g(w, \beta) = \sum_{k} \frac{d_k}{w - w_k(\beta)}. \tag{19}$$

Like the zeta function (10), expression (18) for the response function will usually not converge in those regions of the complex variable w, where the poles of

$g(w, \beta)$ are located, and the zeros of the zeta function cannot directly be calculated from (18). Instead, we apply harmonic inversion to obtain an analytical continuation [8,9]. The poles $w_k(\beta)$ of the analytical continuation of $g(w, \beta)$ in (18) are the zeros of the analytical continuation of the zeta function $Z(w, \beta)$ in (10). To apply harmonic inversion, we now construct a periodic orbit signal by Fourier transformation of the response function (18):

$$C(s, \beta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} g(w, \beta) e^{-isw} \, dw. \tag{20}$$

Considering only the second, oscillating part of $g(w, \beta)$, this results in

$$C(s, \beta) = \sum_{po} \frac{-in_0 e^{\sigma_{po} \beta}}{|1 - \Lambda_{po}|} \delta(s - n_{po}). \tag{21}$$

The corresponding signal resulting from Fourier transformation of Eq. (19) reads

$$C(s, \beta) = -i \sum_{k} d_k e^{-isw_k(\beta)}, \tag{22}$$

which contains the zeros $w_k(\beta)$ of the zeta function (10) as frequencies. The zeros $w_k(\beta)$ can now be determined by adjusting the periodic orbit signal (21)—including all orbits up to a maximum topological length n_{max}—to the form of the corresponding signal (22) by harmonic inversion. According to Eq. (9) and with the relation $w = -i \ln z$, the diffusion constant can be obtained from the leading frequency w_0 using the relation

$$D \approx \frac{-i}{\beta^2} w_0(\beta), \tag{23}$$

which for small β should be independent of β.

3. Results

As an example, we consider the following map, which has also been examined in Ref. [11]: For points $\hat{x}$ inside the interval $[-1/2, 1/2]$ the map is defined by

$$\hat{f}(\hat{x}) = \hat{x}(1 + 2|2\hat{x}|^{\alpha}), \tag{24}$$

where α is a free parameter with the restriction $\alpha > -1$. Outside the elementary cell, the map is continued

according to Eq. (2). Using Eqs. (3) and (4), a corresponding reduced map $f(x)$ can be constructed.

As was discussed in Ref. [11], the periodic orbits of the reduced map $f(x)$ can be described by a complete symbolic dynamics with a three-letter alphabet. For $-1 < \alpha \leqslant 0$ the dynamics is completely hyperbolic. The 0 orbit (corresponding to the fixed point $x = 0$) is infinitely unstable (i.e., $\Lambda_p = \infty$) and does not contribute to the response function (18). For $\alpha > 0$, the 0 orbit becomes marginally stable with $\Lambda_p = 1$, and the dynamics becomes intermittent. Furthermore, it was shown in [11] that at $\alpha = 1$ the system undergoes a phase transition from normal to anomalous diffusion, and the diffusion constant as defined by Eq. (6) equals 0 for $\alpha \geqslant 1$.

For $\alpha > 0$, the marginally stable 0 orbit would give a diverging contribution to the zeta function (7) as well as to the periodic orbit signal (21). As was discussed in Ref. [7], it is appropriate to simply omit this orbit from the zeta function, as was also done in Ref. [11]. In Ref. [11], the diffusion constant of map (24) as a function of α was determined using explicit cycle expansion expressions for the average in Eq. (6) rather than making use of Eq. (8). In the following, we will determine the diffusion constant by harmonic inversion as outlined above.

We calculated the diffusion constant for different values of the parameter α in the region $-0.5 \leqslant \alpha \leqslant 2$ using the periodic orbits up to topological length $N = 13$ (but omitting the 0 orbit). For each value of α, we performed calculations for different small values of β and checked the convergence of the results for the diffusion constant for $\beta \to 0$. The results for the diffusion constant are presented in Fig. 1. In the region $\alpha \lesssim 0.5$, our results are in excellent agreement with those from Ref. [11] obtained with the periodic orbits up to topological length $N = 10$. For $\alpha > 0.5$, the different techniques applied in Ref. [11] yielded quantitatively different values for the diffusion constant; here, our results show a good qualitative agreement with the different cycle expansion results. This is even true when we used the reduced set of orbits up to topological length $N = 10$ in our calculations: The function $D(\alpha)$ in Fig. 1 becomes slightly more flat, but still shows a good qualitative agreement with the results of Ref. [11]. As in [11], it was not possible to reproduce the theoretical value $D = 0$ for $\alpha \geqslant 1$, but one only obtains an asymptotical convergence to this value.
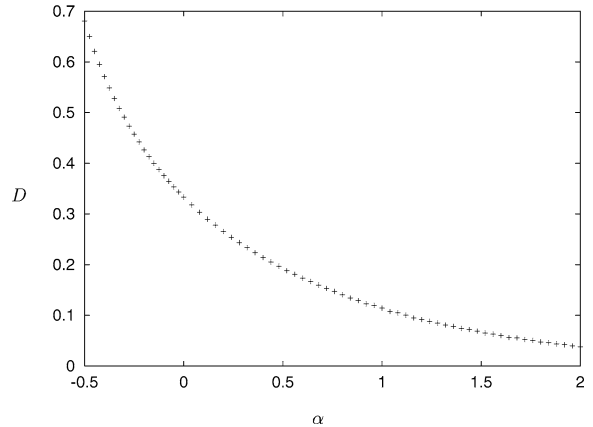

Fig. 1. Results for the diffusion constant of map (24) as a function of the parameter α, calculated by harmonic inversion of the periodic orbit signal (21) including all periodic orbits up to topological length 13 (with the exception of the 0 orbit).

In our calculations, we observed that the condition that for given α expression (23) for the diffusion constant should become independent of β for $\beta \to 0$ was well fulfilled for $\alpha < 0$. However, with increasing $\alpha > 0$, the results became numerically unstable if β was too close to zero, so that we had to extrapolate from the results for β around 0.5. The convergence of the frequencies and amplitudes in the harmonic inversion procedure itself was also very good for $\alpha < 0$, but convergence was increasingly hard to obtain for $\alpha > 0$. A criterion for the reliability of the results for a given value of α is the closeness of the leading frequency for $\beta = 0$ to its theoretical value $w_0 = 0$, as well as the closeness of the corresponding amplitude d_0 (see Eq. (22)) obtained by harmonic inversion to its theoretical value 1 (the multiplicity of the leading zero of the zeta function). The absolute value of the leading frequency for $\beta = 0$ and the corresponding amplitude as a function of α are presented in Fig. 2. The absolute value of the leading frequency was smallest for $\alpha < 0$ but stayed below $|w_0| \approx 10^{-3}$ for all values of α. The corresponding amplitudes were nearly exactly equal to their theoretical value 1 for $\alpha < 0$, but began to deviate from their theoretical value for $\alpha \gtrsim 0.3$, indicating that the harmonic inversion results became less well converged. A possible reason for the deviations may be that the density of frequencies becomes too large for the signal length chosen. It can be expected that the
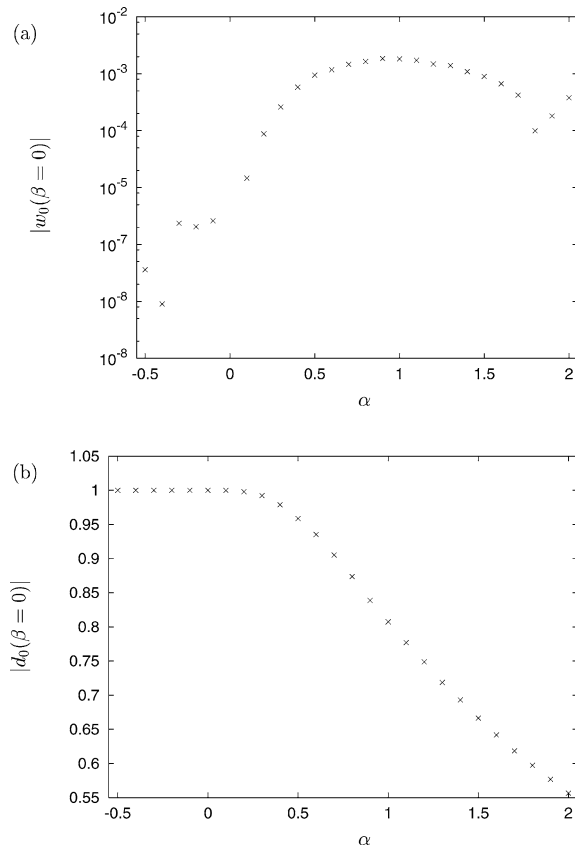
Fig. 2. Test of the convergence of the harmonic inversion procedure: Absolute value of the leading frequency w_0 for $\beta = 0$ and the corresponding amplitudes d_0 obtained by harmonic inversion, as a function of the parameter α. The closeness of these values to their theoretical values $w_0(\beta = 0) = 0$ and $d_0(\beta = 0) = 1$ are a measure for the reliability of the results for the diffusion constant obtained for the respective value of α.

accuracy of the results will be improved by including longer orbits.

In Ref. [11] it was proposed to truncate the periodic orbit sum by introducing a stability cutoff and to use the stability as an ordering parameter for the cycle expansion. It is worth noting that the harmonic inversion procedure has the advantage that no discrete ordering parameter is needed at all. However, a stability cutoff can also be used with the harmonic inversion technique because very unstable orbits give only a small contribution to the signal which can be neglected.

4. Conclusion

In conclusion, we have demonstrated how the diffusion constant of one-dimensional diffusive maps can be determined from a finite set of periodic orbits using harmonic inversion techniques. Starting from a zeta function whose leading zero possesses a known relation to the diffusion constant, we have constructed a periodic orbit signal which was analysed by harmonic inversion. The diffusion constant could then be determined from the leading frequency of the signal. Since, in contrast to other methods such as cycle expansion, harmonic inversion does not depend on any special properties of the map, the general procedure should work in the same way for all chaotic maps. We have tested the method for a simple map whose periodic orbits can easily be determined and for which results for the diffusion constant obtained by cycle expansion techniques are available in the literature. Our results are in excellent agreement with the ones from cycle expansion.

Acknowledgements

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