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Modular smoothing of action

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Abstract. The central quantity in the theory of transport for Hamiltonian systems, and in particular the area-preserving twist maps, is the action of rotational periodic orbits. Usually this is a complicated discontinuous function of two arguments: some perturbation parameter k and a rational rotation number m/n, denoted by $A(k; m/n)$. We applied the idea of modular smoothing to this complicated fractal. Our main result is that all the information contained in the fractal $A(k; m/n)$ can be retrieved from a set of continuous or smooth functions of one variable.

1. Introduction

One of the most exciting and important problems in the modern theory and applications of Hamiltonian dynamical systems is a development of detailed and computationally effective theory of transport in phase space [1, 2]. Many applications of Hamiltonian dynamics, ranging from celestial mechanics to chemistry, require such detailed description of the transport. Let us list just a few historically important examples. In the design of supercolliders or magnetic confinement systems [3] a good understanding of the stability and transport in nonlinear Hamiltonian systems would lead to a substantial improvement of efficiency. Also, in fluid mechanics, this knowledge is essential for understanding mixing flows [4]. Calculation of rates and probabilities of chemical reactions, which can be formulated as Hamiltonian systems, is actually a problem in the transport theory [5]. In many problems in astronomy and astrophysics, such as the gaps in the distribution of asteroids or the structure of the rings of Neptune, Hamiltonian stability and transport is central [6].

Typical Hamiltonian systems are neither completely integrable nor strongly chaotic, and for such systems the study of transport properties is particularly difficult [1]. The main problem is that for mixed systems, the regular and chaotic motions coexist on intertwined domains in the phase space. The boundary between the two qualitatively different behaviours, and consequently all other important quantities in the transport theory are exceedingly complicated fractals. The method of modular smoothing [7] has been developed in order to encode these fractal functions in terms of much simpler, continuous and smooth functions. In this paper we shall extend the method of modular smoothing to demonstrate that the central object in the theory of twist maps and the transport theory, namely the action along various periodic orbits, although being a complicated fractal

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function of two arguments, can be approximated using only a few continuous and smooth functions of one argument. This paper is organized as follows. Section 2 serves to recapitulate the necessary definitions and fix the notation. In section 3 we briefly illustrate the main idea of the method of modular smoothing. Sections 4 and 5 contain our main results concerning the modular smoothing of the action. In section 6 we present an application of the new algorithm for calculating the action and illustrate various ways of reducing the errors. In section 7 we discuss potential applications of the modular smoothing method to calculate the flux and areas of resonances, which are the objects of direct interest in the theory of transport. Our results are summarized and a list of problems is given in section 7.

2. The basic definitions and notation

Most typical features of the fractal phase space are already exhibited by the systems with two degrees of freedom, which, after reduction on an energy hypersurface, are equivalent to a one-parameter family of nonautonomous Hamiltonian systems with periodic time dependence and with one degree of freedom. By taking stroboscopic plots at time $t = 2\pi \mathrm{i}$ the latter are reduced to area-preserving (symplectic) maps of the cylinder. In addition, the momentum coordinate for such maps is usually a monotonic function of the average velocity on an orbit, which is called the twist property of the map. The most studied example of these maps is the Taylor–Chirikov standard map (SM), which is given by the following equations:

$$T : \begin{cases} p_{t+1} = p_t - \dfrac{k}{2\pi}\sin(2\pi q_t) \\ q_{t+1} = q_t + p_{t+1} \end{cases} \qquad q_t \in \mathbb{S}^1,\ p_t \in \mathbb{R} \tag{1}$$

where k is the perturbation parameter and t is an integer. It is generally believed that the SM contains all essential features related to the fractal structure of the chaotic boundary. Our results will be illustrated using this system. The SM represents a symplectic (canonical) transformation of the phase space with an additional property that is given by a generating function $S(q_t, q_{t+1})$ by the formulae:

$$p_t = -\partial S/\partial q_t \qquad p_{t+1} = \partial S/\partial q_{t+1} \tag{2}$$

where

$$S(q_t, q_{t+1}) = (q_t - q_{t+1})^2/2 + \frac{k}{4\pi^2}\cos(2\pi q_t). \tag{3}$$

Area-preserving twist maps can always be generated by equations (2) and the corresponding generating function $S(q_t, q_{t+1})$ [1]. The generation function is used to define action functionals on sequences of real numbers. Various regular orbits, such as periodic, quasiperiodic and homoclinic orbits of the map are given by stationary points of the corresponding action functionals. The periodic and quasiperiodic orbits are parametrized by the frequency (or the rotation number) defined as follows

$$\nu := \lim_{i\to\infty} \frac{T^i(\bar{q}) - \bar{q}}{i} \tag{4}$$

where $T^i(\bar{q})$ is the ith iteration of the horizontal component of the lift of the map (1). We used $\bar{q}$ instead of q to indicate that in definition (4) we have the lift of the map on $R \times R$ instead of the map itself which acts on $\mathbb{S} \times \mathbb{R}$. The orbits can all be calculated using the

periodic action $A(k; m/n)$ whose stationary points are the periodic orbits with the rational frequency $\nu = m/n$. It is defined on the sequences of n real as follows

$$A(k; m/n)(x_0, x_1, \ldots x_{n-1}) = \sum_{t=0}^{t=n-1} S(x_t, x_{t+1})|_{x_n = x_0 + m}. \tag{5}$$

There are (at least one) minimum and minimax stationary value for for each m/n, denoted $A_{\min}(k; m/n)$ and $A_{\text{minmax}}(k; m/n)$ which correspond to the so-called minimum and minimax periodic orbits. In what follows we shall frequently omit the subscript min or max and denote the stationary points of (5) simply by $A(k; m/n)$. The quasiperiodic orbits are stationary points of the corresponding action functional, defined on infinite sequences of reals, but in practical calculations this action and the orbits are calculated as limits of the periodic action and periodic orbits.

Let us briefly recapitulate definitions of the critical values of the parameter k, relative to the periodic and quasiperiodic orbits, since these will be needed later. The standard map, for $k = 0$, has regular orbits with any real frequency, which go around the cylinder. Such orbits are called rotational. Orbits with rational $\nu = m/n$ are periodic with period n. There is a complicated pattern of bifurcations of these periodic orbits as the parameter k is increased. All stable rotating periodic orbits bifurcate into unstable at some critical value of the parameter $k_c(m/n)$, characteristic of the particular orbit. The function $k_c(m/n)$ is called the fractal diagram for the corresponding system [8]. It is defined at rationales, and is a discontinuous fractal function.

At moderate values of the perturbation parameter $k \neq 0$ there are quasiperiodic orbits for every irrational ν. Depending on the frequency and the value of k, a quasiperiodic orbit can fill an invariant circle or an invariant set with many holes. The closure of the latter orbit is a cantor set, which is called the cantorus [9]. On the other hand, there are also many invariant circles, filled by quasiperiodic orbits, which are smooth perturbations of the invariant circles of the integrable system with the same frequencies. These tori are called KAM tori, due to Kolmogorov, Arnold and Moser who first proved their existence in the now celebrated KAM theorems [10]. Usually, upon increasing the perturbation parameter some of the KAM tori will bifurcate into cantori with the same frequencies [11]. Also, in some systems the invariant circles can reappear and disappear as the parameter is increased [12].

Whether a quasiperiodic orbit fills a KAM torus depends in a very intricate way on its frequency and the perturbation k. This dependence is described by the critical function $K(\nu)$, which is defined as follows [13]. Its value at an irrational ν is the smallest value of the perturbation parameter k at which there is no KAM torus with that ν. This function also has a very complicated fractal structure. It is zero and continuous at rationales and has a nonzero value at most irrationals, where it is discontinuous.

Similarly the periodic action $A(k; m/n)$ is a discontinuous fractal function of the two arguments. However, we shall show that the information contained in $A(k; m/n)$ can be retrived from just a few continuous and smooth functions of one variable.

3. The idea of modular smoothing

The main problem with most of the existing techniques for numerical calculation of action is that they rely on the calculation of the corresponding periodic orbits. Each periodic orbit has to be calculated separately and without the knowledge of other distant orbits. Artuso *et al* [14] developed a method to express long periodic orbits via the short ones, however, their

method works for hyperbolic systems which are not typical in Hamiltonian dynamics. The calculations of periodic orbits are usually based on some form of the Newton method, and are relatively easy only in the case of the orbits with small periods [15]. Recently Vrahatis [16] proposed a procedure based on a generalized bisection method. In any case the calculations of long periodic orbits close to the bifurcation points are quite time consuming, and the efficiency of the methods depends on special techniques to determine the good initial guess for the Newton method [17], or a good choice of the initial characteristic polihedra [16]. For example, although renormalization group methods have produced some strong results they are still local, and difficult to apply on realistic systems [18]. However, a few years ago the method of modular smoothing for an efficient and relatively accurate calculations of fractal objects in Hamiltonian mechanics was reported [7, 19]. The method is based on the transformation properties of these objects under the action of the unimodular group on the frequencies. It has been applied for the calculation of the critical functions [7], fractal diagrams [21] and on the KAM tori [20]. Also, the method has been used to analyse the typical fractal properties of the critical functions [22] and the fractal diagram [23]. We shall only briefly recapitulate the basic idea and the main results.

Detailed analysis of the perturbation expansion suggests that the transformation properties of, for example $K(\nu)$, can be described by a sequence of successively smoother functions $L_i(\nu)$ of the critical function and its transformations, with $L_0(\nu) = -\ln K(\nu)$. The method is based on the cancellation of the singularities in $L_i(\nu)$ and $L_i(M\nu)$, where M is an element of the unimodular group

$$M\nu = \frac{a\nu + b}{c\nu + d} \tag{6}$$

with a, b, c and d integers satisfying $|ad - bc| = 1$.

The function L_0 has infinite singularities at all rationals, but the function L_1 defined for the standard map by the following formula:

$$L_1(\nu) = L_0(\nu) - \nu L_0(\nu') \tag{7}$$

where $\nu' = \nu^{-1} - \{\nu^{-1}\}$ is the Gauss transform of ν, which is continuous everywhere and bounded (except at zero and infinity). An analogous continuous function $l_1(m/n) = \ln k_c(m/n) - (m/n)\ln k_c(m'/n')$ describes the fractal diagram $k_c(m/n)$. Here $\{\nu\}$ stands for the integer part of ν. Notice that the critical function of the standard map is invariant under integer translations of the frequency, so that $L_0(\nu) = L_0(\nu - \{\nu\})$ for any $\nu \in \mathbb{R}$. In this paper we shall always denote the Gauss transformation of the frequency ν or m/n by ν' or m'/n'. The function

$$L_2(\nu) = (\nu + 1)L_1(\nu + 1) - \nu L_1(\nu) \tag{8}$$

seems to be continuously differentiable, etc. Furthermore, values of the functions L_i, $i > 0$ at rationals can be calculated using the perturbation expansion of a finite order. For example, for $L_1(m/n)$ we need perturbation expansion of the order n. A smooth interpolation $L_{1\text{app}}$ through only a few points $L_1(m/n)$ then allows one to reconstruct the original fractal function with a bounded maximal error of just a few per cent. In summary, the method of modular smoothing enables one to approximate a discontinuous fractal object in Hamiltonian dynamics by continuous and smooth functions.

4. Modular smoothing of actions

We shall now present a series of mainly numerically supported arguments which lead to our main conclusion, stated as follows. *Although $A(k; m/n)$ is a complicated fractal function it*

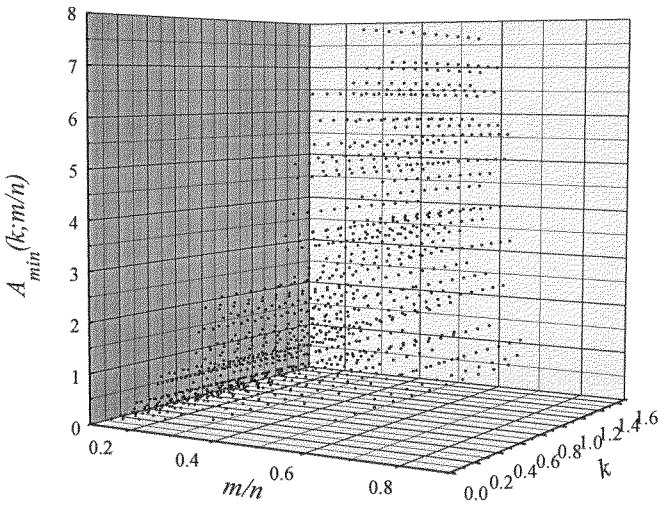

Figure 1. The action of minimizing periodic orbits $A_{\min}(k; m/n)$.

has well-defined transformation properties under the action of the Gauss transformation on m/n*, accompanied by a suitable change in* $k \to k' = k'(k; m/n)$*. These transformation properties are expressible in terms of continuous and smooth functions, and determine* $A(k; m/n)$ *completely*. So, in order to approximate $A(k; m/n)$ quite accurately and efficiently for any combination of k and m/n one needs to know A at only relatively few values of k and m/n, for small n.

The action $A(k; m/n)$ for the SM is illustrated in figure 1. Figure 2 gives various sections of figure 1. The figures were obtained by tedious numerical calculations of periodic orbits at various values of k. There are actually $A_{\min}(k; m/n)$ and $A_{\text{minmax}}(k; m/n)$, but all our conclusions will be the same for both. In what follows we shall illustrate our results using $A_{\min}(k; m/n)$ and denote it simply by $A(k; m/n)$. It is a complicated fractal object with a nontrivial self-similar structure. At zero perturbation $A(0; m/n)$ is also fractal but can be calculated analytically, since the map is integrable at $k = 0$. However, for $k \neq 0$ no simple smooth (or continuous) approximation is possible.

Let us first examine $A(k; m/n)$ along the lines $m/n =$ constant. These functions are presented in figure 3. $A(k; m/n =$ constant$)$ is a smooth monotonic function of k, which can be approximated by, let us say, polynomials of a certain fixed degree. However, the approximating polynomials have coefficients which depend in a discontinuous fractal way on m/n, so that $A(k; m/n)$ is not a simple product of a fractal and a smooth function.

Our guiding idea is to use the singularities of the function $A(k; m/n)$ at m/n and the Gauss transformation m'/n' in order to obtain functions with weaker singularities. The problem is to find an appropriate relation between the values of the first argument k such that $A(k; m/n)$ and $A(k'; m'/n')$ are, at least, continuously related.

In the case of the zero perturbation, since the map is integrable, the actions of m/n and m'/n' orbits should be related by a smooth function. The fractal function $A(0; m/n)$, which can be calculated analytically, and is given by the following simple formula:

$$A(0; m/n) = \frac{m^2}{2n} \tag{9}$$

should be smoothly related to the function $A(0; m'/n')$. Indeed, the ratio between $A(0; m/n)$

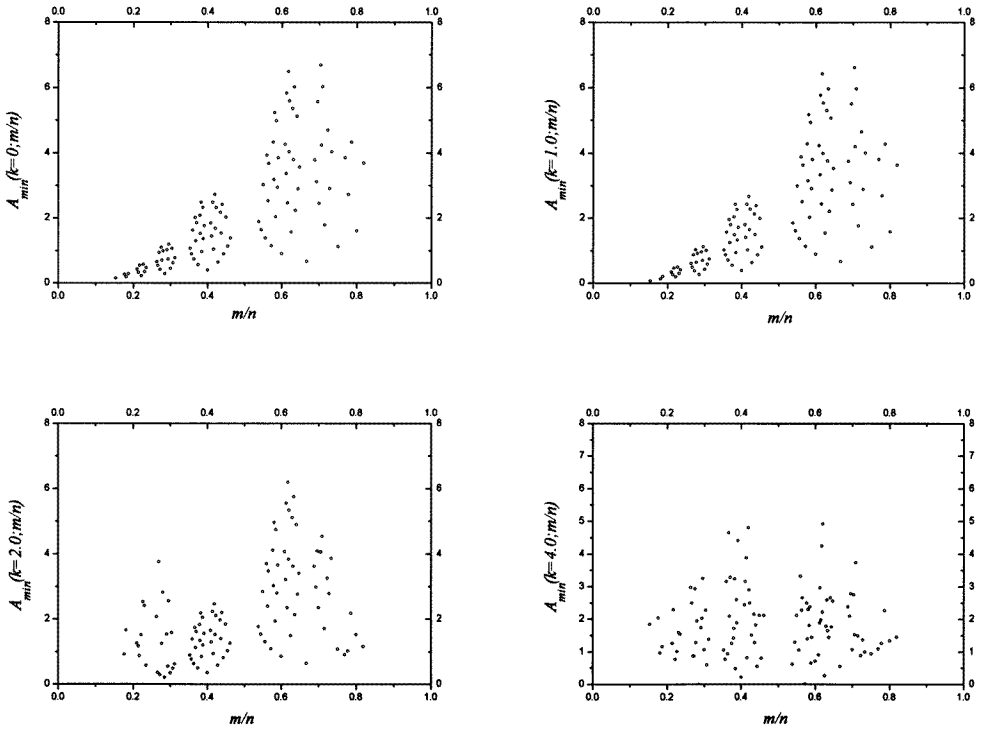

Figure 2. The action $A_{\min}(k; m/n)$ as a function of the frequency m/n, for fixed values of (a) $k = 0$, (b) 1, (c) 2, (d) 4.

and $A(0; m/n)$ is given by the following function:

$$\frac{A(0; m/n)}{A(0; m'/n')} = \frac{m}{m'}\frac{m/n}{m'/n'} \equiv \frac{m}{m'}g(m/n) = \frac{(m/n)^3}{(1 - a_1 m/n)^2} \tag{10}$$

where a_1 is the first coefficient in the continued fraction expansion of the rational $m/n = [0, a_1, a_2, \ldots a_d]$. This is a smooth function except for the singularities at $m/n = 1/l$, $l = 1, 2 \ldots$. So our problem is easily solved in the case of zero perturbation. Guided by this result we shall analyse the ratio between $A(k; m/n)$ and $A(k'; m'/n')$ when $k \neq 0$. However, the proper relation between k and k' still has to be found.

Motivated by the common belief that the map should behave qualitatively the same in a neighbourhood of any periodic orbit at the corresponding critical $k_c(m/n)$, we first consider the values $A(k_c(m/n); m/n)$ on the fractal curve $k_c(m/n)$. This is also a fractal function of m/n, presented in figure 4. Furthermore, we know that $k_c(m/n)$ and $k_c(m'/n')$ are related by the continuous function $l_1(m/n)$. The numerical evidence shows that the following ratio:

$$\frac{A(k_c(m/n); m/n)}{A(k_c(m'/n'); m'/n')} \equiv J(k_c(m/n); m/n) \tag{11}$$

is a piecewise continuous function of m/n (this is illustrated in figure 5). As in the case of $k = 0$, the discontinuities at $1/l$, $l = 1, 2 \ldots$ are only due to the use of the Gauss transformation in definition (11).

Thus, an approximation of the fractal $A(k_c(m/n); m/n)$ is given by only a few values, which are needed to interpolate the continuous branches of $J(k_c(m/n); m/n)$, and by the

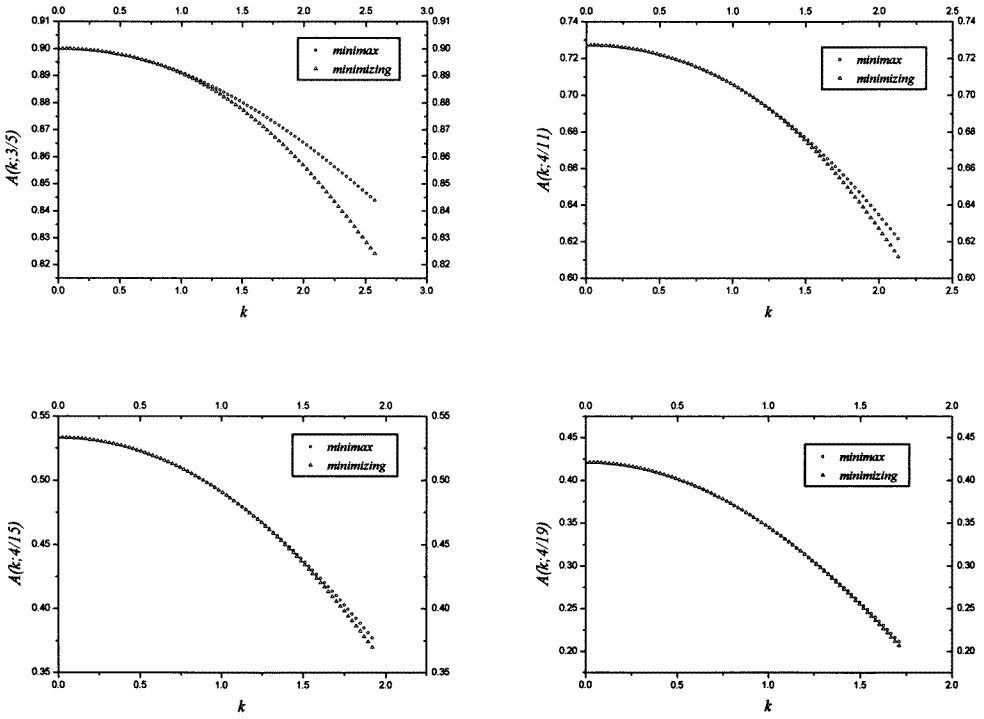

Figure 3. The actions $A(k; m/n = \text{constant})$ of minimum and minimax orbits as functions of k for several fixed m/n.

continuous function $l_1(m/n)$. The latter can also be approximated by a few values of $k_c(m/n)$ for small n.

In order to proceed further we shall consider the ratio:

$$\frac{A(k; m/n)}{A(k'; m'/n')} \equiv \mathcal{J}(k, k'; m/n, m'/n') \tag{12}$$

as a function of four independent arguments: $k, k', m/n$ and m'/n'. As we have seen, if m'/n' is the Gauss transformation of m/n, and if $k = k_c(m/n)$ and $k' = k_c(m'/n')$ this expression is a piecewise continuous function of m/n. This is also true when $k = 0 = k'$. We expect that m'/n' should always be the Gauss transform of m/n, and would like to find out whether there are other combinations of k and $k' = k'(m/n)$ which would render $\mathcal{J}(k, k'(m/n); m/n, m'/n'(m/n))$ a continuous or smooth function of m/n.

The following observation is crucial for further analysis. The expression $l_1(m/n) = \ln k_c(m/n) - (m/n) \ln k_c(m'/n')$ (as well as the analogous one for $L_1(\nu)$) is defined using the critical values: $k_c(m/n)$ and $k_c(m'/n')$. However, $l_1(m/n)$ is simply related to the same expression in which $k_c(m/n)$ and $k_c(m'/n')$ are replaced by $ak_c(m/n)$ and $ak_c(m'/n')$ respectively, where a is an arbitrary positive real number. The relation is:

$$l_{1a}(m/n) \equiv \ln(ak_c(m/n)) - (m/n) \ln(ak_c(m'/n')) = (1 - m/n) \ln a + l_1(m/n). \tag{13}$$

This indicates that $A(ak_c(m/n); m/n)$ and $A(ak_c(m'/n'); m'/n')$ might also be related by a simple relation. Indeed, numerical evidence shows that the function of two arguments:

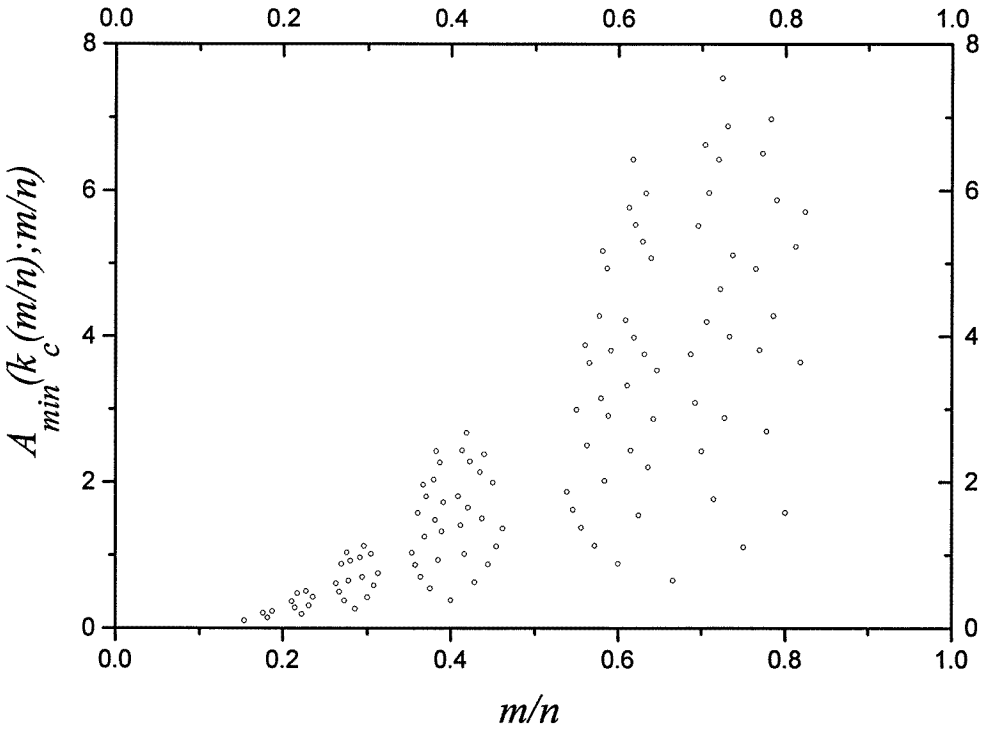

Figure 4. Representation of the fractal function $A_{\min}(k_c(m/n); m/n)$.

k and m/n defined by the following relation:

$$J(k; m/n) := \mathcal{J}\left(k, \frac{k_c(m'/n')}{k_c(m/n)}k; m/n\right) \tag{14}$$

is certainly a piecewise continuous function of m/n along any fractal curve: $k(m/n) = ak_c(m/n)$. Thus, we obtain a one-parameter family of functions of one variable $J_a(m/n)$, defined in the following equation, which completely describes the fractal $A(k; m/n)$

$$J_a(m/n) \equiv J(ak_c(m/n); m/n). \tag{15}$$

The functions $J_a(m/n)$, same as $J_0(m/n)$, are continuous except at the singularities at each $m/n = 1/l$, $l = 1, 2\ldots$ due to the Gauss transformation used in their definition.

These functions on the interval $(\frac{1}{2}, 1)$ are illustrated in figure 6 for various values of a. Note that the fractal function:

$$k'(k; m/n) := \frac{k_c(m'/n')}{k_c(m/n)}k \tag{16}$$

which appears in definition (14) can be calculated from the continuous function $l_1(m/n)$. In what follows $k'(k; m/n)$ will always denote the function (16).

Thus, we see that $A(k; m/n)$ is continuously related to $A(k'(k; m/n); m'/n')$. The strongest singularity of the action at arbitrary $(k, m/n)$ has been cancelled out by the singularity of A at $(k'(k; m/n), m'/n')$. This is precisely the idea of the modular smoothing as applied on the action: $A(k; m/n)$. The next step in the method of modular smoothing would be to consider the transformation properties of the piecewise continuous functions $J_a(m/n)$, in order to remove the singularities in the first derivatives. However, at this stage,

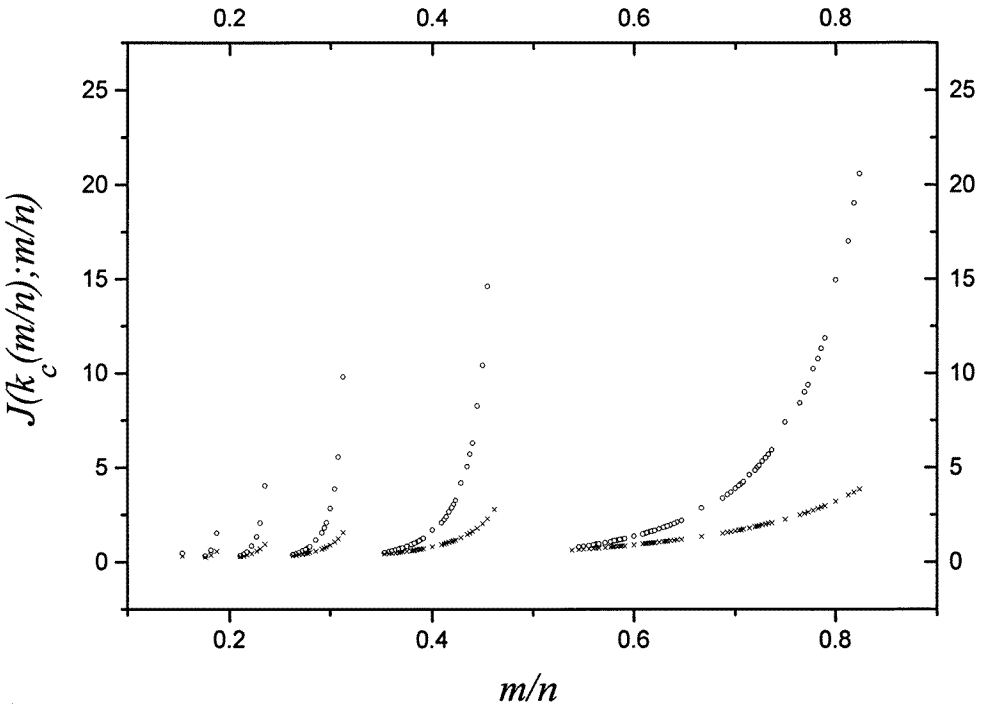

Figure 5. Representation of the function $J(k_c(m/n); m/n)$ on the whole interval $(0, 1)$. For later purposes we also present the graph of $g \equiv mn'/nm'$ (cross).

due to insufficient numerical accuracy, we shall not proceed any further with the modular smoothing programme. Instead, in order to approximate the fractal $A(k; m/n)$ we shall use only the piecewise continuous functions $J_a(m/n)$.

The continuous branches of the functions $J_a(m/n)$, for each fixed a, at the intervals $(1/l, 1/l + 1)$, $l = 1, 2 \ldots$ are all similar. Numerical evidence indicates that they all have singularities in the first derivatives. These are clearly seen only at the resonances which are dominant in the corresponding intervals. However, the relation between the different branches of $J_a(m/n)$, although probably smooth, is not given only by the simple rescaling of the argument m/n.

The same structure of the discontinuities in the functions $J_a(m/n)$ and the graph of the Gauss transformation, illustrated in figure 5, suggests another useful representation of these functions. Figure 7 presents ratios

$$\frac{J(ak_c(m/n); m/n)}{(mn'/nm')} \tag{17}$$

as functions of $g \equiv mn'/nm'$, for several values of a. The singularities in the first derivative are illustrated better in this representation than in figures 5 and 6. Each of the continuous branches of the function $J_a(m/n)$, for any fixed a, can be approximated by a polynomial in $g = mn'/nm'$ of a low degree. Furthermore, there is a simple rescaling relation of the argument g so that all continuous branches of one $J_a(m/n)$ can be presented on the single interval, let us say, $(\frac{1}{2}, 1)$. However, this change of argument is not enough to describe the relation between the continuous branches, and that is expressed by the fact that also the coefficients of these polynomials depend on the interval. This is illustrated in figure 8. The

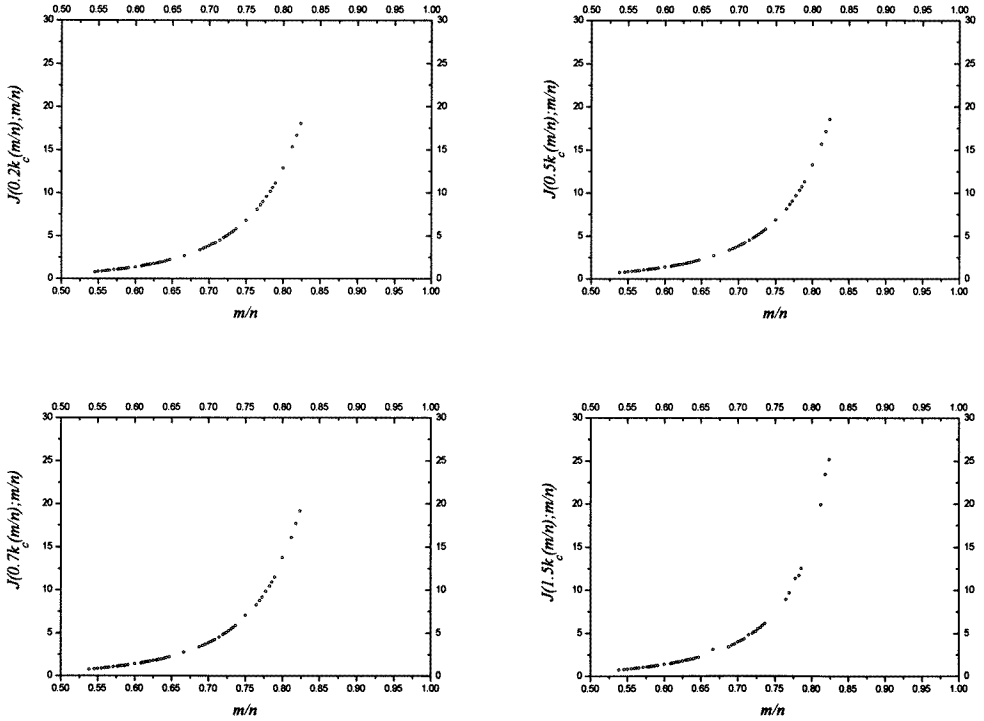

Figure 6. The functions $J_a(m/n)$ on the interval $(\frac{1}{2}, 1)$ for the following values of $a = 0.2, 0.5, 1.0, 1.5$.

curves represented by crosses give the numerically calculated function $J_a(m/n)$, $a = 1$. The curves represented by circles give the approximation of J_1 at the interval $(\frac{1}{2}, 1)$ by the polynomial of the fifth degree in g, and the polynomials which are obtained from this one by the substitution of the argument g, which describes the rescaling of the interval. The fact that crosses and circles do not coincide (except for J_1 on $(\frac{1}{2}, 1)$ and its polynomial approximation) shows that the coefficients of the polynomial approximations also depend on the interval. As was pointed out, the relation between the different branches of one of the functions $J_a(m/n)$ is not trivial. However, one can use the approximation by polynomials of a fixed low degree, and extrapolate the dependence of the coefficients on the interval by extrapolating from the values of the coefficients at the first few intervals.

In our sample calculations, described in the next section, we used the simplest approximation of J_a/g by a linear function: $J_a/g \approx A_a(n)g + B_a(n)$ on each interval $(1/l, 1/l + 1)$. The coefficients $A_1(l)$ and $B_1(l)$ are given in figure 9, and their values can be extrapolated from the values at the first few intervals. Even such a crude approximation gave results with a quite small error in the approximated values of $A(k; m/n)$ at many frequencies and for a range of k up to $k \leqslant 1.5$.

5. The modular smoothing algorithm for the calculation of actions

We shall now describe an algorithm for approximating $A(k_0; m_0/n_0)$ at an arbitrary point $(k_0; m_0/n_0)$ by using only smooth functions, and a small number of initial, directly calculated, values of the action at orbits with small period. We shall first develop the

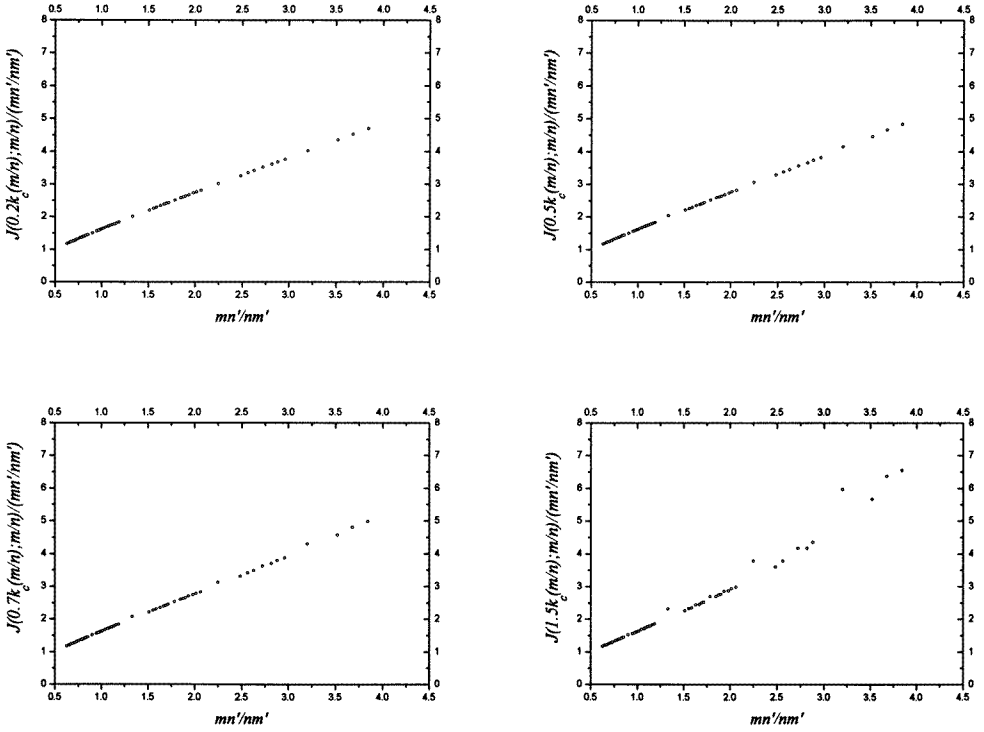

Figure 7. Representation of several continuous functions J_a divided by mn'/nm', for the same values of a as in figure 6, but as functions of mn'/nm'.

general procedure and then describe our sample calculations with specific details. Let us suppose that we have calculated $A(k; m/n)$ at the following $r \times s$ grid of points:

$$(k_i, m_j/n_j) \qquad i = 1 \ldots r \qquad j = 1 \ldots s \tag{18}$$

where m_j/n_j are the first s numbers in the Farey tree, and where k_i is always of the form: $k_i = a_i k_c(m_j/n_j)$ with arbitrary a_i, $i = 1 \ldots r$. We shall also need $A(k; m/n)$ at the Gauss transformation of m_j/n_j and at the corresponding $k = k'(k_i; m_j/n_j)$, but these points are already in the grid. Note that we need to know the values of the fractal diagram $k_c(m_j/n_j)$. Generally in the following procedure we shall have to know the fractal diagram at arbitrary m/n, which can be approximated from an interpolation through $l_1(m_j/n_j)$.

Before we proceed with the algorithm let us recall that the functions $J_a(m/n)$ have an infinite number of continuous branches defined on the intervals $(1/l, 1/l + 1)$, $l = 1, 2 \ldots$. In principle, a knowledge of a certain number of points on each of these branches is required in order to obtain an approximation of $J_a(m/n)$ on the whole interval $(0, 1)$. However, due to the self-similarity of the continuous branches of $J_a(m/n)$ on different intervals, which we shall need to know only approximately, only a finite and small number of points will be needed. For example, as we shall see, the linear approximations with extrapolated coefficients gave excellent results. Here we want to stress again that only quite a small number of input values $A(a_i k_c(m_j/n_j); m_j/n_j)$ are needed.

The algorithm uses the set of $s \times r$ values of the action as input, and is split into two parts. In the first part of the algorithm we use only the input values of $A(k; m/n)$ to obtain r smooth approximations $J_{a_i}^{\mathrm{app}}(m/n)$ of r functions $J_{a_i}(m/n)$. For example, the following

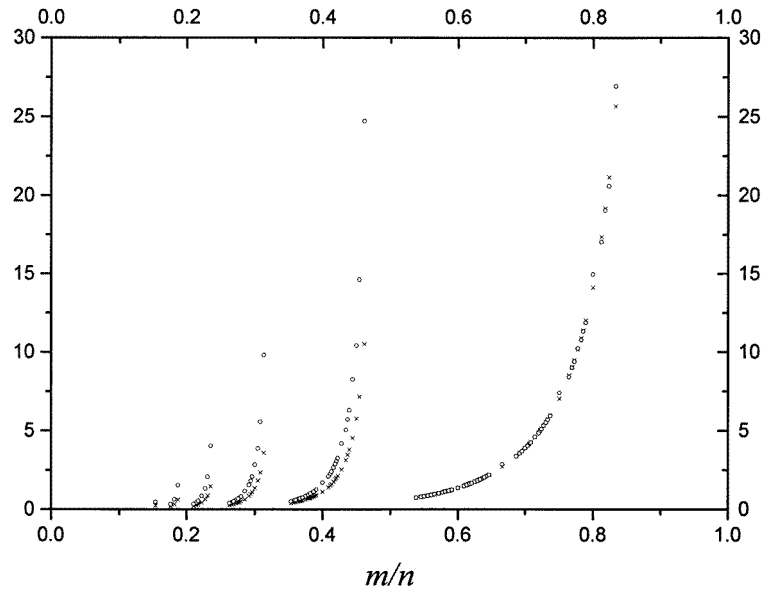

Figure 8. Ilustration of the nontrivial scaling relation between the different continuous branches of the function $J_1(m/n)$ (see also the text!).

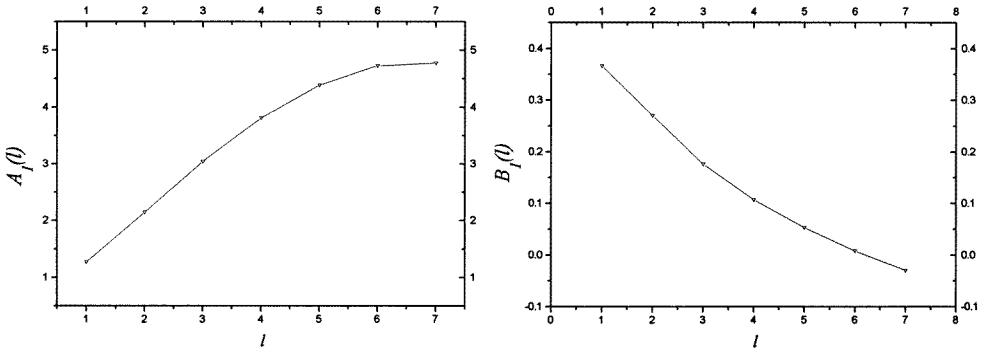

Figure 9. The coefficients $A_1(l)$, $B_1(l)$, $l = 1, 2\ldots$ in the linear approximations of the branches of $J_1(g)/g$.

values:

$$\begin{aligned} &A(k_c(m_1/n_1); m_1/n_1), \ldots, A(k_c(m_s/n_s); m_s/n_s) \\ &A(k_c(m_1'/n_1'); m_1'/n_1'), \ldots, A(k_c(m_s'/n_s'); m_s'/n_s') \end{aligned} \tag{19}$$

give $J(k_c(m/n); m/n)$ at the points: $m_1/n_1, \ldots m_s/n_s$. These can be interpolated by some smooth function $J^{\text{app}}(k_c(m/n); m/n)$. Similarly, the following points:

$$\begin{aligned} &A(a_i k_c(m_1/n_1); m_1/n_1), \ldots, A(a_i k_c(m_s/n_s); m_s/n_s) \\ &A(a_i k_c(m_1'/n_1'); m_1'/n_1'), \ldots, A(a_i k_c(m_s'/n_s'); m_s'/n_s') \end{aligned} \tag{20}$$

with $a_i \neq 1$ give $J_{a_i}(m/n)$ at the points: $m_1/n_1, \ldots, m_s/n_s$. These can also be interpolated by some other smooth function $J_{a_i}^{\text{app}}(m/n)$.

In this way we obtain r smooth functions $J_{a_i}^{\text{app}}(m/n)$, $i = 1\ldots, r$. We can add to these functions one more which can be calculated exactly, namely the function: $J(0; m/n)$,

so that we end up with $r+1$ smooth functions of m/n. This part of the algorithm does not depend on m_0/n_0. Once we have interpolated $J(a_i k_c(m_j/n_j); m_j/n_j)$ we can use the functions $J^{\text{app}}_{a_i}$ to calculate the action at any $(k; m/n)$.

In order to continue to the second part of the algorithm we now note that $A(k; m_0/n_0)$ is a smooth function of k, which we shall approximate by a polynomial of order r:

$$A(k; m_0/n_0) = b_0(m_0/n_0) + b_1(m_0/n_0)k \cdots + b_r(m_0/n_0)k^r + \cdots. \tag{21}$$

The coefficients $b_i(m/n)$ are fractal functions of m/n, but they can be approximately calculated at any m/n in terms of smooth functions. In order to calculate $b_0(m_0/n_0), \ldots, b_r(m_0/n_0)$ we use the values:

$$A(a_1 k_c(m_0/n_0); m_0/n_0), \ldots, A(a_{r+1} k_c(m_0/n_0); m_0/n_0) \tag{22}$$

which are not known in advance but can be approximated from various values of the smooth functions:

$$J^{\text{app}}_{a_1}(m/n), \ldots, J^{\text{app}}_{a_r}(m/n). \tag{23}$$

The procedure is as follows. Express $A(a_i k_c(m_0/n_0); m_0/n_0)$, for each $i = 1, \ldots, r$, in terms of $A(a_i k_c(m_0^d/n_0^d); m_0^d/n_0^d)$ and an appropriate sequence of values of the functions J^i_{app} using the sequence of Gauss transformations. The formula is as follows

$$\begin{aligned} A(a_i k_c(m_0/n_0); m_0/n_0) &\approx A_{\text{app}}(a_i k_c(m_0/n_0); m_0/n_0) \\ &= J^{\text{app}}_{a_i}(m_0/n_0) A(a_i k_c(m_0'/n_0'); m_0'/n_0') \\ &= \cdots = J^{\text{app}}_{a_i}(m_0/n_0) \ldots J^{\text{app}}_{a_i}(m_0^{d-1}/n_0^{d-1}) A(a_i k_c(m_0^d/n_0^d); m_0^d/n_0^d). \end{aligned} \tag{24}$$

The sequence of transformations $m_0/n_0 \to m_0'/n_0' \to m_0''/n_0'' \to m_0^d/n_0^d$ is the sequence of Gauss transformations leading from m_0/n_0 up to one of the s initial m/n at which the values of the action are calculated directly, for example $m_0^d/n_0^d = \frac{1}{2}$.

These numbers $A_{\text{app}}(a_i k_c(m_0/n_0); m_0/n_0)$, $i = 1, \ldots, r$ together with $A(0; m_0/n_0) = b_0(m_0/n_0)$ are used to approximate the coefficients: $b_1(m_0/n_0), \ldots, b_r(m_0/n_0)$ by $b_1^{\text{app}}(m_0/n_0), \ldots, b_r^{\text{app}}(m_0/n_0)$. The latter are the solutions of the following set of $r+1$ linear algebraic equations:

$$\begin{aligned} A_{\text{app}}(a_i k_c(m_0/n_0); m_0/n_0) &= b_0^{\text{app}}(m_0/n_0) + b_1^{\text{app}}(m_0/n_0) a_i k_c(m_0/n_0) \\ &\quad + \cdots + b_r^{\text{app}}(m_0/n_0)(a_i k_c(m_0/n_0)^r \end{aligned} \tag{25}$$

where $i = 1, \ldots, r+1$ and $a_{r+1} \equiv 0$.

We can now plug the numbers $b_0^{\text{app}}(m_0/n_0), \ldots, b_r^{\text{app}}(m_0/n_0)$ back into the polynomial (21) and finally calculate it at $k = k_0$, which gives the desired approximate value of $A(k; m/n)$ at $(k_0; m_0/n_0)$. In order to approximate $A(k; m/n)$ at any other point only the second part of the algorithm has to be repeated, this time for the new point $(k_0; m_0/n_0)$.

The algorithm which we have just explained can be easily programmed on a computer. As input it requires $r \times s$ values of $A(k; m/n)$ at specified points $(a_i k_c(m_j/n_j); m_j/n_j)$, and s values of the fractal diagram $k_c(m_j/n_j)$ which are needed to interpolate $l_1(m/n)$. These require explicit calculations of only s periodic orbits, with small period, at r prescribed values of the parameter k. As the output it gives an approximate value of the action $A(k; m/n)$ for any value of k and m/n. At the beginning of the procedure a subroutine for interpolation of continuous functions of one variable has to be applied in order to obtain the functions $J^{\text{app}}_{a_i}$ and $l_{1\text{app}}$. The subroutine has to be invoked only once for each desired function, and these smooth interpolations can then be used to approximate $A(k; m/n)$ at any $(k; m/n)$. The interpolation algorithm could be any of the standard subroutines and the choice is not essential for our arguments. What is essential is that we have reduced the

problem of interpolating a fractal function $A(k, m/n)$ is replaced by the simple problem of interpolating only a few continuous or smooth functions of one variable.

6. Calculations and errors

The modular smoothing algorithm was tested by comparing the values of the action calculated directly, using the numerical calculations of periodic orbits, with the values of the action obtained by the algorithm. We shall first illustrate the calculations which use only the most simple approximations of the involved functions. Such crude approximations lead to the results with an error in the values of action of about 5% on the set of all frequencies up to the eighth level in the Farey tree. We shall then discuss the main sources of errors and show how the accuracy can be improved.

In all our calculations we needed the fractal diagram $k_c(m/n)$, so we first obtained an approximation of the function $l_1(m/n)$. Actually, we used an approximation of the function $l_2(m/n)$, which was obtained earlier [7], using a finite perturbation expansion of order $n = 8$.

In the first step of the algorithm we had to obtain the smooth approximations $J_{a_i}^{\text{app}}(m/n)$. Here we used the representation in terms of the variable $g \equiv mn'/nm'$, discussed at the end of the last section, and the linear approximations. In order to obtain the approximations $J_(a_i^{\text{app}}(m/n)$ we needed to calculate numerically only the periodic orbits with frequencies $m_j/n_j = \frac{1}{2}, \frac{2}{3}, \frac{1}{3} \ldots$ for values of k equal to $a_i k_c(m_j/n_j)$ where $a_i = \frac{1}{2}, 1$.

Furthermore, each $J(k; m/n = \text{constant})$ as a function of k for fixed m/n is approximated over a large interval of values of k by a polynomial of the second order. The system of the three linear equations for the coefficients of the polynomial approximation were solved algebraically and the solutions were expressed in terms of values of the functions J_a^{app}; $a = 0, \frac{1}{2}, 1$.

We then applied the algorithm to calculate $A(k; m/n)$ at all points $(a_i k_c(m_j/n_j); m_j/n_j)$ where m_j/n_j were all rationals up to and including the eighth level of the Farey tree, and $a_i = 0.2, 0.5, 0.7$. These values are compared with direct calculations of $A(k; m/n)$ through numerical computations of the periodic orbits. The errors are illustrated in figure 10.

Figure 10 indicates the main sources of errors. First, the continuous functions $J_a(m/n)$ are approximated by smooth (very simple) functions, so that the singularities in the first derivative are neglected. This is the most obvious source of errors, near and at the dominant resonance inside each of the intervals $(1/l, 1/l + 1)$; $l = 1, 2, \ldots$. This error is inherent to the method of modular smoothing. Other sources of errors, which we mention below, can be reduced by applying finer approximations of various continuous and smooth functions, which have to be approximated. For example, each continuous branch of $J_a(g)$, for any fixed a, significantly departs from the linear approximation as $g \to \infty$, which corresponds to m/n approaching the right endpoint of the corresponding interval. Consequently the errors are increased as m/n approaches the resonances of the form $1/l$, $l = 1, 2, \ldots$. Furthermore, the coefficients of the linear approximations are extrapolated from the first few values, so that we expect larger errors at frequencies which have a large continued fraction coefficient, which corresponds to higher-order resonances close to the most dominant resonances of lower orders. Finally, the smooth function $A(k; m/n = \text{fixed})$ is approximated by a polynomial at $k = 0$ of only the second order in k. All these errors are larger at larger values of k, but they can be reduced by taking the polynomial approximations of higher orders. Also, if one is interested in the values of $A(k; m/n)$ for larger k, then, instead of expansion (21) at $k = 0$, an expansion at, let us say, $k = 1$ would be more appropriate.

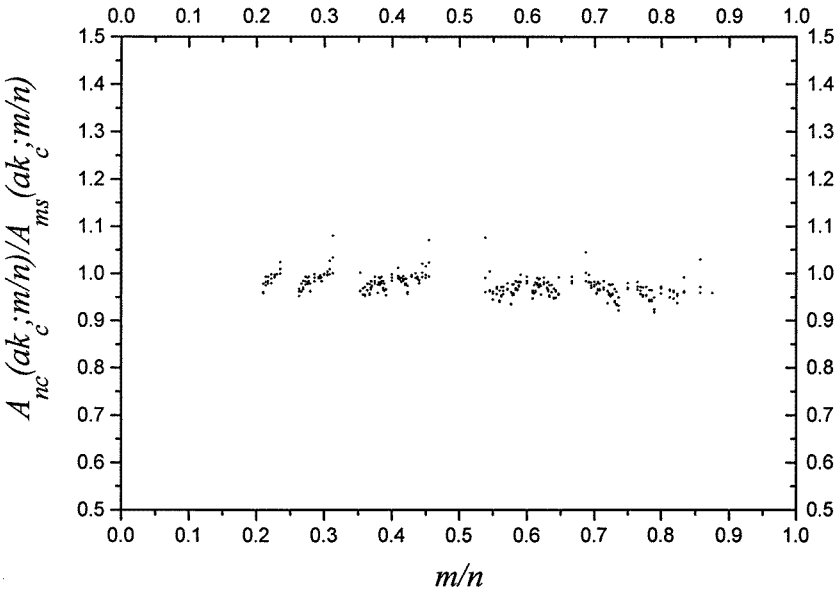

Figure 10. The figure represents the ratio between $A(k;m/n)$ calculated by numerical calculation A_{nc} of periodic orbits and by applying the algorithm of modular smoothing A_{ms}. The error is of the order of a few per cent.

7. Calculations of the flux and the areas of resonances

We have seen that the crude approximations used in section 6 gave an error of about a few per cent in the values of the action for the minimal periodic orbits. Calculations of the minimax action with the same type of approximations give the errors of the same order. Once the actions have been calculated these results should be used to compute the flux and the area of resonances, which are the quantities of direct interest in the transport theory.

The flux and the areas are given as differences of actions for minimum and minimax periodic orbits which are used to calculate the partial barriers and separatrices, and are also complicated fractals. As is indicated in figure 4, the actions of minimum and minimax periodic orbits with the same frequency are of the same order, so that their difference is usually quite small. An error of a few per cent in the actions renders an error of at least a few hundred per cent in the flux.

To achieve a reasonable accuracy of the calculations of the flux one could either improve the accuracy of the action calculations or try to smooth out the singularities directly in the flux, as it is done for the actions. Numerical evidence partially indicates that the smoothing of the flux $F(k;m/n)$ could be done in the same way as for the actions, that is, the ratio of the flux at $ak_c(m/n)$ and m/n and at $ak_c(m'/n')$ and m'/n' seems to be piecewise continuous (see figure 11). However, since the values of the flux are quite small, the ratio of the two small values is rather sensitive to the errors in the calculations of the numerator and denominator. The numerical accuracy of our computations was not enough to render any definite results in this direction.

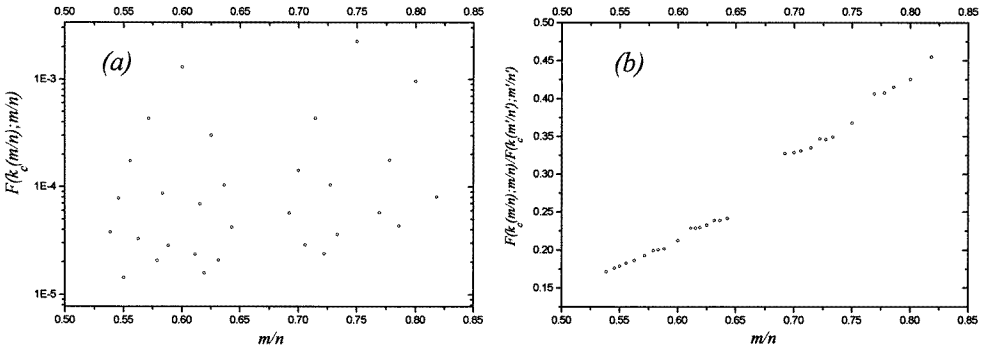

Figure 11. (*a*) The flux at the critical values of the minimizing periodic orbit and (*b*) the ratio of the flux at m/n and m'/n'.

8. Summary and discussion

In this paper we presented a nontrivial extension of the method of modular smoothing which enables one to calculate the action of the rotational periodic orbits $A(k; m/n)$ relatively effectively and accurately. The main result is the algorithm for interpolation of the discontinuous fractal function $A(k; m/n)$ which requires interpolating only a few continuous or smooth functions of one variable. The algorithm is based on the fact that the ratio of actions $\mathcal{J}(k, k'; m/n m'/n')$, given by (12), gives continuous or smooth functions of m/n if m'/n' is the Gauss transform of m/n and $k = ak_c(m/n)$ and $k' = ak_c(m'/n')$, for any fixed a.

We have used the action at frequencies related by the Gauss transformation in order to smooth out only the strongest singularities, and obtain piecewise continuous functions. Numerical evidence indicates that the functions $J_a(m/n)$ are not smooth (except for $a = 0$), so that even better approximations would be obtained if the singularities in the first derivative of $J_a(m/n)$ could be cancelled out by some modular transformation. Further research in this direction requires extremely accurate calculations of long periodic orbits in a neighbourhood of the strongest resonances, which is a difficult numerical problem.

The algorithm described in section 4 can be improved in many ways, which, however, are not crucial in this paper. We shall mention only a couple of important possibilities. First, one should adopt the most suitable interpolation algorithm to obtain the functions $J_{a_i}^{\mathrm{app}}$ and $l_{1\mathrm{app}}$. In our sample calculations the approximations $J_{a_i}^{\mathrm{app}}$ were obtained by rewriting $J_a(m/n)/g$ as a functions of $g(m/n) = mn'/n'm$, which made these functions almost linear and vary easy to interpolate and extrapolate the coefficients. This requires only a few input values of the action. Also we used the smooth approximation of the function $l_2(m/n)$, which was obtained earlier using some prior knowledge of the type of singularities. This is indeed not essential, and one could use just the piecewise linear interpolation to obtain $l_{1\mathrm{app}}$.

Our results are presented for the action along the minimum periodic orbits $A(k; m/n) \equiv A_{\mathrm{min}}(k; m/n)$, but the same conclusions are true for $A(k; m/n) \equiv A_{\mathrm{minmax}}(k; m/n)$. Once the actions are calculated at sufficiently many points $(k; m/n)$ using the algorithm of modular smoothing, one would like to calculate the flux and the areas of resonances, and thus obtain all necessary elements for the Markov model of the transport in phase space. To achieve a reasonable accuracy of the calculated values of the flux one needs very accurate calculations of the actions. However, due to the difficulties of the numerical calculations of the flux, we

cannot say anything definite about the modular smoothing as the method that could provide us with accurate calculations of the flux and the areas of the resonances at many frequencies and various values of the perturbation, which would be the ultimate goal of the theory.

Our investigations were carried out using the standard map as a typical system. The idea of modular smoothing and in particular its applications to the theory of transport have to be extended onto other area-preserving maps and Hamiltonian systems with two degrees of freedom.

The results in this paper are supported mainly by controlled numerical calculations. Problems with numerical calculations of periodic orbits with long periods are well known, and we had to be very careful in checking continuity or smoothness of the functions $J_a(m/n)$. We suspect that it would be extremely difficult to rigorously prove our results, but we believe that the numerical evidence is sufficiently convincing.

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