

Numerical Calculation of Domains of Analyticity for Perturbation Theories in the Presence of Small Divisors

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We study numerically the complex domains of validity for KAM theory in generalized standard mappings. We compare methods based on Padé approximants and methods based on the study of periodic orbits.

KEY WORDS: Greene's criterion; breakdown of tori; Padé approximants.

1. INTRODUCTION

The goal of this paper is to study numerically the complex domains of values of ε for which a standard like map from $\mathbf{R}^1 \times T^1$ to itself

$$T_\varepsilon(p, q) = (p + \varepsilon s(q), q + p - \varepsilon s(q)) \quad (1.1)$$

leaves invariant topologically nontrivial circles on which the motion is, up to a smooth changes of variables, a rigid rotation by an angle ω . The well-known KAM theorem guarantees that, provided ω is Diophantine, there is a ball of positive radius on which there is such a curve.

Unfortunately, the estimates that come out of the analytical proofs are very conservative and, given the practical importance of constants, it is of considerable interest to devise proofs without this failing or, at least, devise reliable methods for numerical computation. Problems such as (1.1) provide convenient models of the general situation.

The reason to study domains of analyticity is that, in applications, one frequently uses perturbation expansions whose behavior and usefulness are

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affected by complex singularities even if the behavior of the true answer is perfectly well behaved for real values of ε .

The case when $s(q) = (1/2\pi) \sin(2\pi q)$ (called the standard map) and $\omega = (\sqrt{5} - 1)/2$ was studied in ref. 4 by deriving a perturbation expansion in powers of ε and using a Padé approximant of the series. They obtained the surprising result that the domain of analyticity was a circle. Several other families were studied in ref. 5.

In this paper, we consider the same problem for s of the form of a trigonometric polynomial of low degree.

We reimplemented from scratch the Padé method of refs. 4 and 5 using an extended precision library—the reasons for doing so are discussed in the section about the Padé method—and we used an independent method: a complex extension of Greene's method, which seems to afford higher precision and for which some theoretical justification is recently available^(7,19) (we point out that the justification used in ref. 7 works even for the case when the parameters are complex). At the end, we propose some tentative discussion of these results from the renormalization group point of view about the phenomena of the disappearance of circles.

2. GREENE'S RESIDUE CRITERION

2.1. The Basis of Greene's Criterion

In a remarkable paper, Greene⁽⁹⁾ observed that, for the standard map, it is possible to ascertain the existence of an invariant circle with rotation number ω by computing the "residue" of periodic orbits of type M_n/N_n —that is, orbits which satisfy

$$T_\varepsilon^{N_n}(p, q) = (p, q + M_n), \quad M_n/N_n \rightarrow \omega$$

If we define $R(p, q; M_n, N_n) = \text{Tr}(DT_\varepsilon^{N_n}(p, q) - 2)$, then ref. 9 asserts that there is an invariant circle of rotation number ω if and only if $R(p, q; M_n; N_n) \rightarrow 0$.

The importance of this criterion arises from the fact that it is very easy to compute periodic orbits even of relatively high periods. Greene⁽⁹⁾ used an algorithm first described in ref. 6 that exploits the fact that maps of the form (1.1) are "reversible." There are other algorithms (see, e.g., refs. 13 and 20).

We will see later that the method generalizes to the complex case.

Unfortunately, Greene's residue criterion is difficult to justify rigorously and there are strong indications that, as stated, it is false even for standard-like mappings which are not the standard map.

Nevertheless, it is possible to prove rigorously statements that serve as justification of practical computations.

For example, it is possible to show the following.

Theorem 2.1. Let T_ε be an analytic map as before; ω is Diophantine. Assume that

$$\sup_{|\operatorname{Im} q| \leq \delta} |T_\varepsilon(p, q)| \leq \Gamma \leq \infty, \quad \sup_{|\operatorname{Im} q| \leq \delta} |T_\varepsilon^{-1}(p, q)| \leq \Gamma \leq \infty$$

and that there is a mapping $K: \mathbf{T}^1 \rightarrow \mathbf{R} \times \mathbf{T}^1$ with $f(K(\varphi)) = K(\varphi + \omega)$ and that $\sup_{|\operatorname{Im} \varphi| \leq \delta} |K(\varphi)| \leq \Gamma$.

Then, there exists a constant $D > 0$ —depending on the Diophantine properties of the number ω —such that for every periodic orbit x of type M/N with $|\omega - M/N| \leq 1/N$

$$|R(x)| \leq D e^{-D\delta|\omega - M/N|^{-1/\nu}}$$

We observe that the proof of Theorem 2.1 in ref. 7 consists in computing normal forms up to high enough order around the invariant circle and observe that, as a corollary of the proof, one obtains also upper bounds for the residues of orbits whose rotation number is similar to ω . This justification, as stated in ref. 7, carries over without any change to the case that the parameters, and hence the circles, take complex values.

We also emphasize that the justification implies that all periodic orbits with a certain rotation number close to ω will have a small residue. In general, we expect to have many periodic orbits with the same rotation number. We refer to ref. 22 for a discussion of the combinatorics of the calculation of periodic orbits based on critical lines. If, for any of them, the residue is large, we can take it as an indication that the invariant circle has disappeared.

Notice that if the residue of an orbit is not zero, the eigenvalues of the derivative are not 1. Hence, applying the implicit function theorem, we conclude that if for some ε_0 we can find x_{ε_0} such that $T_{\varepsilon_0}^N x_{\varepsilon_0} = x_{\varepsilon_0} + (0, M)$ and $|R(x_{\varepsilon_0}; M, N)| = \alpha \neq 0$, we can find a neighborhood $|\varepsilon - \varepsilon_0| \leq \rho$ on which we can find a unique x_ε satisfying $T_\varepsilon^N(x_\varepsilon) = x_\varepsilon + (0, M)$. Moreover, $R(x_\varepsilon; M, N)$ will be an analytic function of ε . One then expects that the equation $|R(x_\varepsilon; M, N)| = \alpha$ will define a smooth curve in the ε plane in the neighborhood where it is defined. [It seems that $R(x_\varepsilon; M, N)$ has very large derivatives in the cases of interest, hence, the curve has reasonably small derivatives.]

This remark and the partial justification of the residue criterion suggest the following algorithms.

Algorithm 2.2. Fix $\alpha > 0$.

1. Find a real number ε_0 and a periodic orbit for T_{ε_0} satisfying

$$|R(x_{\varepsilon_0}; M, N)| = \alpha$$

2. Given that we know $\varepsilon_n = r_n e^{i\theta_n}$ satisfying $|R(x_{\varepsilon_n}; M, N)| = \alpha$, fix $\theta_{n+1} > \theta_n$, $|\theta_{n+1} - \theta_n|$ small, and then find r_{n+1} such that $\varepsilon_{n+1} = r_{n+1} e^{i\theta_{n+1}}$ satisfies $|R(x_{\varepsilon_{n+1}}; M, N)| = \alpha$.

Algorithm 2.3. Fix $\alpha > 0$ and a family of paths $\varepsilon = P_\theta(t)$ with $t \in \mathbb{R}$ being the parameter along the path and θ being an index for the paths [e.g., $P_\theta(t) = te^{2\pi i\theta}$ or $P_\theta(t) = \theta + it$].

1. If we fix θ , t , we find one periodic orbit $x_{\theta,t}$ of type M/N of a certain topological type. Then, $R(x_{\theta,t}; M, N)$ is a function of θ , t .
2. For fixed θ , we can consider $R(x_{\theta,t}; M, N) - \alpha$ as a function of t and feed it to a reliable zero finder. This gives us a critical value t_θ^* .
3. Cycling over different θ 's, we can obtain a curve $\varepsilon = P_\theta(t^*(\theta))$ of critical points.

Notice that Algorithm 2.2 is just a version of the well-known continuation methods and it is quite well understood how to write safeguards which examine that the conditions of the implicit function theorem apply. Therefore, if the program runs without detecting an error, we may be confident that indeed there is a curve $\gamma(x_{\varepsilon_0}; M, N)$ in the complex plane for which the residue of the orbit (of the given topological type) takes the value α .

The method of Algorithm 2.3 is somewhat more delicate to implement, and is slower to run. The main reason is that, for fairly high values of the parameter, there are different orbits of type M/N and it is necessary to take special precautions to ensure that all the evaluations of $R(x_{\theta,t}; M, N)$ required by the zero finder are on the same family, especially if the evaluations are on fairly separate values.

We avoided this problem by ensuring that the intervals for t were not very large, (they were centered in the last successful value) and we kept the last found periodic orbit as a guess.

We have said that Algorithm 2.3 is somewhat slower. Nevertheless, we found it useful to have several algorithms so that comparing their results could give us confidence on their reliability. As discussed later, we also compared the results obtained by using different algorithms for finding zeros and computing orbits.

We emphasize that, given the justification outlined in Theorem 2.1 for reasonably high M , N , we should consider the critical lines produced by the algorithm as lying outside the domain of analyticity, so that the most

sensible approximation of the true domain of analyticity we can form is the intersection of the regions bounded by the computed curves. Even if each of the curves is smooth, the final domains obtained taking intersections could very well have cusps. Taking the limit of a finite number of intersections allows that the final result is very complicated.

Algorithms 2.2 and 2.3 depend on having reliable methods for computing periodic orbits. We have used two. First, we observe that the Greene–DeVogelere method can be generalized to complex maps. We quickly review Appendix A of ref. 9 to check that the method described there only involves algebraic manipulations that are valid for complex numbers.

This method is based on the observation that T_ϵ in (1.1) can be written $T_\epsilon = I_{2,\epsilon} \circ I_{1,\epsilon}$ with $I_{1,\epsilon}^2 = I_{2,\epsilon}^2 = Id$:

$$I_1(p, q) = (p + \epsilon s(q), -q)$$

$$I_2(p, q) = (p, -q + p)$$

We denote by Ω_1 the set of points left fixed by I_1 . If one point $(p_0, q_0) \in \Omega_1$ and $T_\epsilon^N(p_0, q_0) \in \Omega_1$, then $T_\epsilon^{2N}(p_0, q_0) = (p_0, q_0)$. In effect,

$$T_\epsilon^{2N}(p_0, q_0) = T_\epsilon^{N-1} \circ I_{2,\epsilon} \circ I_{1,\epsilon} \circ T_\epsilon^{N-1} \circ I_{2,\epsilon} \circ I_{1,\epsilon}(p_0, q_0)$$

$$= T_\epsilon^{N-1} \circ I_{2,\epsilon} \circ T_\epsilon^{N-1} \circ I_{2,\epsilon}(p_0, q_0)$$

Since $I_{2,\epsilon} \circ T_\epsilon = I_{2,\epsilon}^2 \circ I_{1,\epsilon} = I_{1,\epsilon}$ and $T_\epsilon \circ I_{1,\epsilon} = I_{2,\epsilon} \circ I_{1,\epsilon}^2 = I_{2,\epsilon}$, we obtain that $T_\epsilon^{2N}(p_0, q_0) = (p_0, q_0)$.

The set Ω_1 can be calculated explicitly, since, using the form of I_1 , we obtain $(p_0, q_0) \in \Omega_1$ if and only if

$$p_0 - \epsilon s(q_0) = p_0$$

$$q_0 = -q_0 + k$$

When $s(0) = s(1/2) = 0$, which is the case for the trigonometric polynomials we have considered, the above equations are equivalent to $q_0 = 0, q_0 = 1/2$. We will refer to these two vertical lines as the “critical lines.”

The algorithm for searching for periodic orbits consists in searching along a critical line for the points that, after a certain number of iterations, come back to another critical line. This amounts to finding the zeros of a function of one variable.

In the case that the variable is real there are excellent zero finders that exploit the mean value property. In the complex case, however, one has to use other methods, such as the secant method. We found, however, that

one obtains better results in one tries to minimize the target function using a Powell method⁽⁸⁾ considering the complex variable as two real variables.

Notice that the secant method requires a reasonably good guess to converge to the solution, especially in the case that the function whose zeros we are computing is very rapidly oscillating. For our purposes this can be achieved by taking as a guess for the location of the periodic orbit for one value of the parameter the location of the periodic orbit for a previously computed similar value and then increasing. Nevertheless, the method becomes delicate to use and we preferred to use Powell's method for most of the calculation.

Another algorithm we used was based on the variational principle for periodic orbits that plays an important role in Aubry–Mather theory.

Lemma 2.4. A sequence of angles $\{q_1, \dots, q_n\}$ is the projection of a periodic orbit $\{(p_1, q_1), \dots, (p_n, q_n)\}$ of type M/N for (1.1) if and only if (q_1, \dots, q_n) is a critical point of the function

$$\mathcal{S}(q_1, \dots, q_n) = \sum_{i=1}^{n-1} \left[\frac{1}{2} (q_i - q_{i+1})^2 + \varepsilon S(q_i) \right] + \frac{1}{2} (q_n - q_1 - M)^2 + \varepsilon S(q_n)$$

where $S'(q) = s(q)$. [Notice that the condition $\int s(q) dq = 0$ ensures that we can find such an S defined on the circle.]

We observe that this variational principle generalizes to the complex case if we consider

$$\tilde{\mathcal{F}}(q_1, \dots, q_n) = \mathcal{S}(q_1, \dots, q_n) \overline{\mathcal{S}(q_1, \dots, q_n)}$$

because then we obtain, considering q_i, \bar{q}_i as independent variables,

$$\begin{aligned} \frac{\partial \tilde{\mathcal{F}}(q_1, \dots, q_n)}{\partial q_i} &= \overline{\mathcal{S}(q_1, \dots, q_n)} \frac{\partial \mathcal{S}(q_1, \dots, q_n)}{\partial q_i} \\ \frac{\partial \tilde{\mathcal{F}}(q_1, \dots, q_n)}{\partial \bar{q}_i} &= \mathcal{S}(q_1, \dots, q_n) \frac{\partial \overline{\mathcal{S}(q_1, \dots, q_n)}}{\partial \bar{q}_i} \\ &= \mathcal{S}(q_1, \dots, q_n) \overline{\left(\frac{\partial \mathcal{S}(q_1, \dots, q_n)}{\partial q_i} \right)} \end{aligned}$$

If we add a large enough constant to \mathcal{S} that ensure that $\mathcal{S}(q_1, \dots, q_n) \neq 0$, we see that the variational equations for $\tilde{\mathcal{F}}$, with q_i, \bar{q}_i as independent variables, are equivalent to the corresponding equations for \mathcal{S} .

Inspired by ref. 11, which uses the gradient flow of the action as a

functional in the space of orbits to prove the existence of critical points, we implemented the system of differential equations

$$\frac{dq_i}{dt} = -\frac{\partial}{\partial q_i} \tilde{\mathcal{F}}(q_1, \dots, q_n) = \overline{\mathcal{P}(q_1, \dots, q_n)} \frac{\partial \mathcal{P}(q_1, \dots, q_n)}{\partial q_i} \tag{2.1}$$

The solutions of these equations—implemented using, e.g., a standard Runge-Kutta solver—converge rather quickly to approximate solutions, especially if we take as initial conditions points which are close to being a solution (e.g., the solutions for similar parameter values). Notice that the RHS of the equations is very easy to evaluate since most of the terms that are obtained taking the derivative of \mathcal{P} vanish.

In this case, the periodic orbits can be compared with those obtained using the secant method and verified directly to be x orbits.

3. THE PADÉ METHOD

Berretti and Chierchia⁽⁴⁾ suggested the use of Padé approximants to study the analyticity domain of the expansion in powers of ε of the solutions of

$$A_\omega u_\varepsilon(x) + \varepsilon s(x + u_\varepsilon(x)) = 0 \tag{3.1}$$

where A_ω is the operator defined by

$$A_\omega u_\varepsilon(x) = u_\varepsilon(x + \omega) - 2u_\varepsilon(x) + u_\varepsilon(x - \omega)$$

and where $u_\varepsilon: T^1 \rightarrow \mathbf{R}$ satisfies

$$u_\varepsilon(x + 1) = u_\varepsilon(x) \tag{3.2}$$

The function u_ε is called the “hull function” by Aubry and if we define

$$K_\varepsilon(x) = \begin{pmatrix} u_\varepsilon(x) - u_\varepsilon(x - \omega) - \omega \\ u_\varepsilon(x) + x \end{pmatrix} \tag{3.3}$$

then

$$T_\varepsilon \circ K_\varepsilon(x) = K_\varepsilon(x + \omega) \quad \text{with} \quad K_\varepsilon(x + 1) = K_\varepsilon(x) \tag{3.4}$$

so that K_ε semi-conjugates the motion on an invariant circle to a rotation ω . The quantity $u_\varepsilon(x) + x$ gives the conjugacy of a rotation of the motion of the first component.

Hence, finding solutions of (3.1) for a fixed ε implies that there is indeed a circle with the motion on it being conjugate to a rotation.

Conversely, finding a solution of (3.4) implies that there is a solution of (3.1), as can be verified by direct calculation.

Hence, we define the domain of validity of the KAM theorem as the domain of ε for which it is possible to find a solution of (3.4) or (3.1).

Using the Birkhoff theorem⁽¹⁶⁾ and Herman's theorem on conjugacy to rotations of smooth diffeomorphisms of the circle for Diophantine rotation numbers,⁽¹²⁾ one can show that, for real ε and Diophantine ω , the existence of analytic solutions of (3.1) is equivalent to the existence of topologically nontrivial invariant circles for (1.1) with rotation number ω .

However, for complex ε , we do not know any version of the Aubry–Mather theorem that could show that invariant circles are graphs. Nevertheless, Herman's theorem still applies, so that, in the complex case, that (3.4) is equivalent to the existence of topologically invariant circles.

It is not excluded that (3.1) does not admit a solution, but that, nevertheless, (3.4) does. That will happen, for example, if the invariant circle is not a graph.

We point out that if $u_\varepsilon(x)$ is a solution of (3.1), so is $u_\varepsilon(x + \eta_\varepsilon) - \eta_\varepsilon$, but, except for this, the solution is unique. We can, and will, always choose a solution satisfying a normalization condition

$$\int u_\varepsilon(x) dx = 0 \tag{3.5}$$

A power series expansion for $u_\varepsilon(x) = \sum_{i=1}^\infty \varepsilon^i u^i(x)$ can be computed by matching powers of ε if we have a way of computing the expansion in powers of $s(x + u_\varepsilon(x)) = \sum_{i=0}^\infty \varepsilon^i s^i(x)$ in terms of the expansion in powers of ε for u . Similar methods have been used in refs. 4, 10, and 21.

Then, Eq. (3.1) becomes

$$\mathcal{A}_\omega u^i(x) + s^{i-1}(x) = 0; \quad u_0(x) = 0 \tag{3.6}$$

Notice that s^{i-1} can be computed in terms of u^0, \dots, u^{i-1} , so that (3.6) should be considered as an equation that allows the computation of u^i given that we know u^0, \dots, u^{i-1} .

The theory of inversion of the operator \mathcal{A}_ω is worked out in detail in several places, for example, ref. 23, §32. We just recall that, if ω is Diophantine and s^{i-1} is analytic and satisfies

$$\int s^{i-1}(x) dx = 0 \tag{3.7}$$

it is possible to find a unique u^i solving (3.6) and (3.5).

To complete the proof of the claim that (3.6) can be solved by matching orders, we only have to show that if u^0, \dots, u^{i-1} solve (3.6), then s^{i-1} satisfies (3.7). To prove that, we observe that if u is a periodic function and $\Delta_\omega u(x) + s(u(x) + x) = R(x)$, then

$$\begin{aligned} \int R(x)[1 + u'(x)] &= \int u(x + \omega) + \int u(x - \omega) - 2 \int u(x) \\ &+ \int u(x + \omega) u'(x) + \int u(x - \omega) u'(x) - 2 \int u(x) u'(x) \\ &+ \int s(x + u(x))(1 + u'(x)) \end{aligned}$$

The first three terms cancel out and, realizing that integrating by parts we have $\int u(x + \omega) u'(x) = \int u(x) u'(x - \omega)$, we can write the last four terms as

$$\int \frac{d}{dx} u(x) u(x - \omega) - \int \frac{d}{dx} (u(x))^2 + \int \frac{d}{dx} s(x + u(x))$$

Hence, the integral vanishes as claimed.

If we denote

$$u_\varepsilon^{[\leq i-1]}(x) = \sum_{j=0}^{i-1} u^j(x) \varepsilon^j$$

and, analogously,

$$s_\varepsilon^{[\leq i-1]}(x) = \sum_{j=0}^{i-1} s^j(x) \varepsilon^j$$

we observe that

$$s(x + u_\varepsilon^{[\leq i-1]}(x)) = s_\varepsilon^{[\leq i-1]}(x) + O(\varepsilon^i)$$

Hence

$$\begin{aligned} \Delta_\omega u_\varepsilon^{[\leq i-1]}(x) + \varepsilon s(x + u_\varepsilon^{[\leq i-1]}(x)) \\ \times \Delta_\omega u_\varepsilon^{[\leq i-1]}(x) + \varepsilon s_\varepsilon^{[\leq i-2]}(x) + \varepsilon^i s^{i-1}(x) + O(\varepsilon^{i+1}) \end{aligned}$$

If the u^i are determined by solving (3.6),

$$\Delta^\omega u^{[\leq i-1]}(x) - \varepsilon s_\varepsilon^{[\leq i-2]}(x) = 0$$

Hence, applying the previous argument, we obtain

$$\int [\varepsilon^i s^{i-1}(x) + O(\varepsilon^{i+1})][1 + u_\varepsilon^{\llbracket i-1 \rrbracket}(x)'] = 0$$

Hence

$$\varepsilon^i \int s^{i-1}(x) dx = O(\varepsilon^{i+1})$$

and therefore $\int s^{i-1}(x) dx = 0$ as claimed.

We furthermore claim that it is possible to implement very efficient algorithms that use the recursion described above.,

We observe that

$$A_\omega \exp(2\pi i k x) = 2[\cos(2\pi k \omega) - 1] \exp(2\pi i k x)$$

so that if we discretize the u^i in terms of Fourier series, the linear equations (3.6) to be solved are diagonal.

The s^i can be computed in terms of the u^i very efficiently if we use a trick that is described in ref. 15, Vol. 2, p. 507.

We denote

$$\begin{aligned} E(\varepsilon, x) &= \exp[2\pi i k u_\varepsilon(x)] \\ \frac{\partial}{\partial \varepsilon} E(\varepsilon, x) &= 2\pi i k \exp[2\pi i k u_\varepsilon(x)] \frac{\partial}{\partial \varepsilon} u_\varepsilon(x) \\ &= 2\pi i k E(\varepsilon, k) \frac{\partial}{\partial \varepsilon} u_\varepsilon(x) \end{aligned} \tag{3.8}$$

If we expand $E(\varepsilon, x) = \sum_{j=0}^N E^j(x) \varepsilon^j$, we obtain, matching the coefficients of ε^N in (3.8),

$$(N + 1) E^{N+1}(x) = 2\pi i k \sum_{j=0}^N E^{N-j}(x)(j + 1) u^{j+1}(x) \tag{3.9}$$

Together with the initial condition $E^0(x) = 1$, (3.9) allows one to recursively compute E^{N+1} once one knows $E^0(x), \dots, E^N(x)$.

Of course, once we have computed the complex exponential, it is quite easy to compute trigonometric functions. Notice that the recursion relations (3.9) only require multiplication and addition of Fourier series and multiplication of Fourier series by a scalar.

By examining the recursion relations (3.9) and (3.6), it is possible to show the following.

Proposition 3.1. If $s(x)$ in (1.1) is a trigonometric polynomial of degree d , then

$$\deg u^i = 2di - d \quad i \geq 1$$

$$\deg s^i = 2di + q \quad i \geq 0$$

Proof. Proceeding inductively, we assume that the conclusions are true for $i \leq N$. Then, (3.9) shows $\deg E^N = 2Nd$.

Using the usual addition formulas for trigonometric functions, we see that $\deg s^N = 2Nd + d$ and observing that (3.6) is diagonal on Fourier series, $\deg U^{N+1} = 2Nd + d$, which is the inductive hypothesis for $i = N + 1$. A small calculation shows that the hypothesis is satisfied for $i = 1$. ■

Remark. We emphasize that the existence of a KAM torus for a value of ε is equivalent to the existence of a function satisfying (3.1), to that we should consider the expansion $u_\varepsilon = \sum \varepsilon^j u^j(x)$ as an expansion taking place in a certain space of functions.

This is obviously related, but in principle not equivalent, to considering the domains of analyticity of the functions obtained by specializing the expansion for values of x .

For example, for the standard map, $u'(1/2) = 0$, so that for $x = 1/2$ the series expansion vanishes identically and, in particular, converges.

If we denote by $\Omega_{\varepsilon, \theta}$ the domain of convergence of $K_\varepsilon(\theta)$, solving (3.4), the domain of validity of the KAM theorem is

$$\Omega_\varepsilon = \{ \varepsilon \mid \exists \delta > 0, \{ \varepsilon \} \times \{ |\operatorname{Im} \theta| < \delta \} \subset \Omega_{\varepsilon, \theta} \}$$

In practice, however, it is more practical—following ref. 4—to compute $\Omega_\varepsilon(\theta)$, which is the domain of convergence of $u_\varepsilon(\theta)$, for a fixed θ .

Notice that (3.4) implies that if x is in the domain of K_ε , so is $x + \omega$. It follows that the domain of K_ε in the θ variable should be strip.

On the other hand, from (3.3) it follows that for a fixed ε , $\Omega_\theta^\varepsilon$, the domain of u_ε in the θ variable, is related to Ω_θ^K , the domain of K in the θ variable, by

$$\Omega_\theta^K = \Omega_\theta^j \cap \Omega_\theta^\varepsilon - \omega$$

In the examples we have considered the numerical results suggests that $\Omega_\theta^K = \Omega_\theta^\varepsilon$ and, hence, each is a strip around the real axis.

Notice that the domain of convergence in the θ variable can be computed for fixed ε also using the Padé method.

This could be considered a check of the computation of the perturbation expansion and of the Padé method, especially because there are

renormalization group predictions about the scaling behavior of the domain of convergence of the function K .

Given a series $S(\varepsilon) = \sum \varepsilon^i S_i$, we define the Padé approximant of type $[N:M]$ as the polynomials $P(\varepsilon)$, $D(\varepsilon)$ such that

$$\begin{aligned} \deg P = N, \quad \deg D = M; \quad D(0) = 1 \\ P(\varepsilon)/D(\varepsilon) = S(\varepsilon) + O(\varepsilon^{N+M+1}) \end{aligned} \quad (3.10)$$

The fact that P , D exist can be obtained by observing that (3.10) is equivalent to

$$S(\varepsilon) D(\varepsilon) = P(\varepsilon) + O(\varepsilon^{N+M+1})$$

and, hence, expressing it in terms of the coefficients of the polynomials,

$$\begin{aligned} S_i + \sum_{j=1}^M S_{i-j} D_j = P_j, \quad i \leq N \\ S_i + \sum_{j=1}^M S_{i-j} D_j = 0, \quad N < i < N + M \end{aligned} \quad (3.11)$$

The second equation determines D_j and, substituting it into the first, we can obtain the P_i .

Even if it is quite possible to solve (3.11) directly, it is also possible to derive recursion relations for the Padé approximants for different M, N that allow a rapid calculation.

We have, in general, preferred to use a direct solution of the linear system (3.11) because it allows us to obtain an estimate of the condition of the problem.

It seems that $u'(1/2 - \sigma)$ converges in a finite domain, so that $K'_2(1/2)$ has a finite domain.

The basis of the Padé method lies in the observation that the Padé approximants frequently converge on much larger domains than the Taylor expansion, since the approximating class can accommodate bad behavior such as poles that cannot be accommodated by a Taylor expansion. Hence, frequently, the domains of analyticity of a function can be as ascertained by looking for the zeros of the denominator of the Padé approximant.

This can be justified in several cases (see ref. 2, Vol. I, Chapter 6, for a review of the many results about the convergence of Padé series on the full domain). Unfortunately, there are cases where the Padé approximants of type $[N:1]$ converge in a domain strictly smaller than the ball of convergence of the Taylor expansion (see, e.g., ref. 3, p. 400, or the more elaborate Gammel counterexample, ref. 2, Vol. I, p. 284).

Besides the theoretical considerations of the existence of counter-examples, there are several reasons that make the Padé approximants delicate to compute. We refer to ref. 2 for a very complete discussion, but point out some of the precautions we have taken to avoid them:

1. The system (3.11) tends to be very ill-conditioned, so that small numerical errors in the coefficients of the series could be enormously amplified.

2. The computation of zeros which have a larger magnitude than other zeros requires a large precision. This can be understood if we consider the function $S(\varepsilon) = 1/(1 - \varepsilon) + 1/(1 - a\varepsilon)$; the i th Taylor coefficient is $S_i = 1 + a^i$, so that if $a \ll 1$, the information to compute the zero $1/a$ is contained in the last decimal figures.

To these difficulties we may add the fact that polynomials with random coefficients tend to have their zeros on circles. Hence, it is difficult to assess the validity of a circle using the Padé method.

We implemented the Padé method using the high-precision library of the public domain program PARI.

A first implementation used macros to generate function calls. Significant parts of the code were tested on previous programs. Later, we produced another implementation using the FP programming language that is part of the PARI system. One advantage of doing so was that the language has primitives to manipulate polynomials so that the algorithms to compute the recursion relation could be coded very tersely. (Unfortunately, taking care of starting and final values made the programs difficult to read.)

In the C language implementation we would obtain estimates of the condition number and made sure that the precision of the numbers was enough to obtain meaningful results.

In the case that $s(q)$ in (1.1) is a trigonometric polynomial that contains only odd powers of the sine, we have $s(q + 1/2) = -s(q)$. Hence, $T_\varepsilon(p, q) = T_{-\varepsilon}(p, q + 1/2) - (0, 1/2)$. Using this symmetry, we can conclude that the domain in the ε plane for which circles exist should be invariant under reflections across the origin. It is possible to use this symmetry to decrease the number of coefficients in the expansion to be handled and hence increase the speed and accuracy. We decided not to do that so that we can study s 's which contain even frequencies with the same programs. Also, the consequences of the symmetry can be used as a verification of the accuracy achieved.

A simple trick that seems to increase the precision of the calculation is to use instead of power series in the variable ε power series in the

variable ε/ρ , where ρ is a number chosen phenomenologically so that the series has a radius of convergence of about 1. The choice of ρ was done by performing the calculation once, estimating the radius, and restarting the calculation with ρ chosen to be the value suggested by the first calculation.

We also point out that the zeros of the denominator need not be a singularity of the approximant if they are a zero of the numerator also. Hence, we implemented a second pass which eliminated the zeros that also correspond to an approximate zero of the numerator.

In many practical applications of Padé methods, it is also customary to consider as spurious the zeros that are far away from those of other approximants. We have not implemented these methods.

4. RESULTS

Our results are summarized in the accompanying figures.

In Fig. 1 we represent the zeros of the Padé approximants of type $[95:95]$ for the angles $\theta = i/10 + 0.034546$ as well as the curve of the critical residue for orbits of type $8/13$ evaluated for the standard map. Figure 2 represents the same calculation with the zeros of the denominator corresponding to a very small numerator removed.

The map used, the degree of the Padé approximant, and the type of the periodic orbit are indicated on the line above the circle.

In Fig. 3 we represent several critical curves corresponding to different orbits for the standard map.

Figures 4–6 present the results of similar calculations performed for the standard-like map with

$$s(x) = \frac{1}{2\pi} \sin(2\pi x) + \frac{1}{20 \cdot 2\pi} \sin(2 \cdot 2\pi x)$$

while Figs. 7–9 present the calculations for

$$s(x) = \frac{1}{2\pi} \sin(2\pi x) + \frac{1}{30 \cdot 2\pi} \sin(3 \cdot 2\pi x)$$

We draw attention to the fact explained in the previous discussion that the zeros of largest modulus violate the symmetry requirements. Nevertheless, those of small modulus satisfy it to a very high accuracy. As expected, the zeros of high modulus do not seem to be reliable.

Let us highlight some important points.

A. The results seems to suggest that the domain of analyticity of the ε expansion of K_ε for fixed θ is independent of θ . The analyticity domain for u_ε seems to be constant except in $\theta = 1/2$.

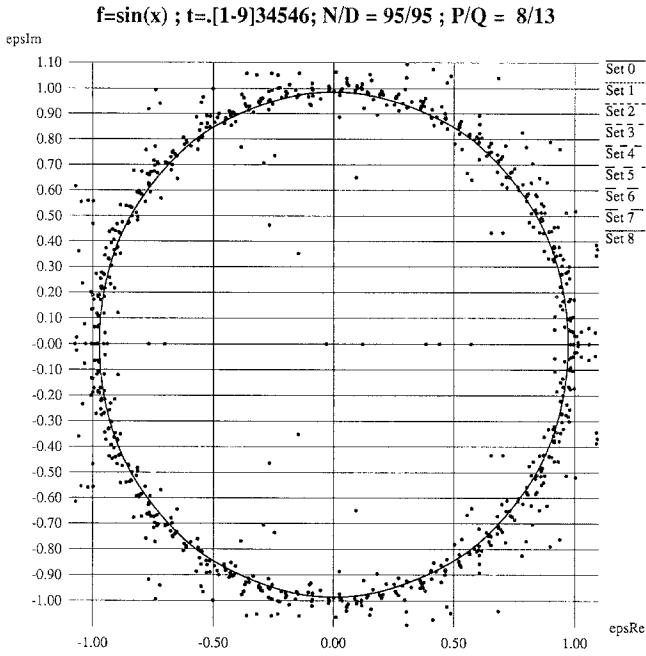


Fig. 1.

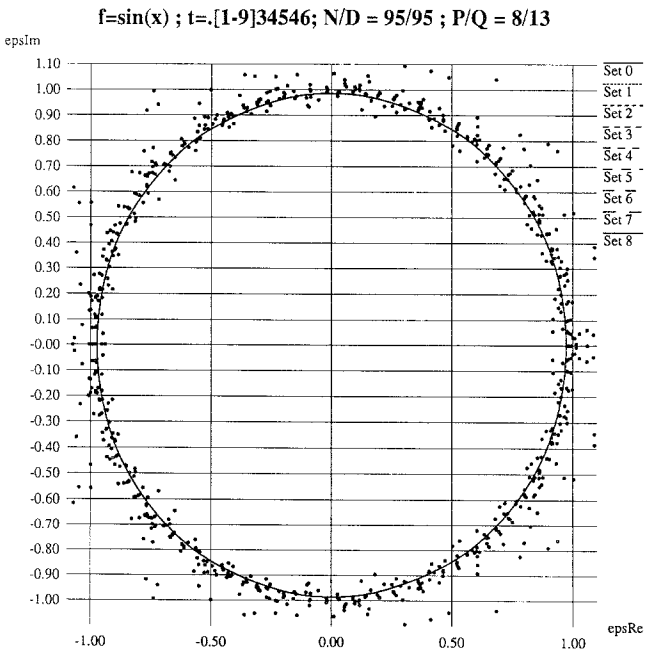


Fig. 2.

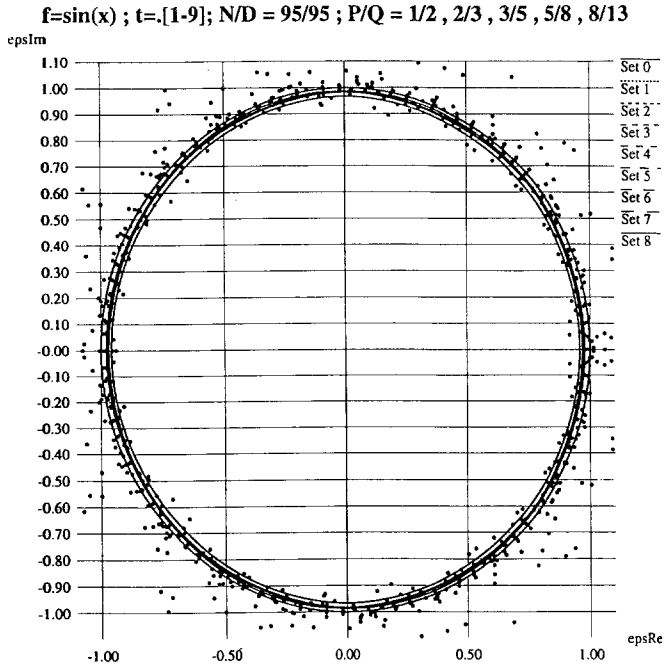


Fig. 3.

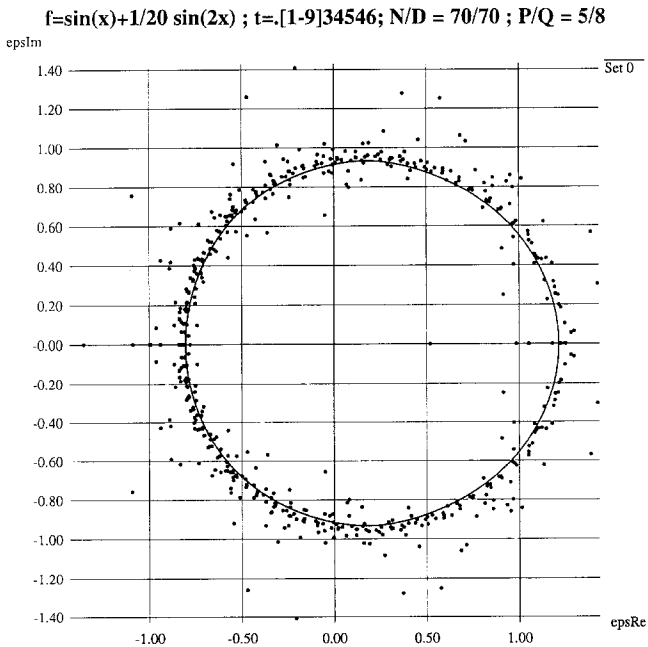


Fig. 4.

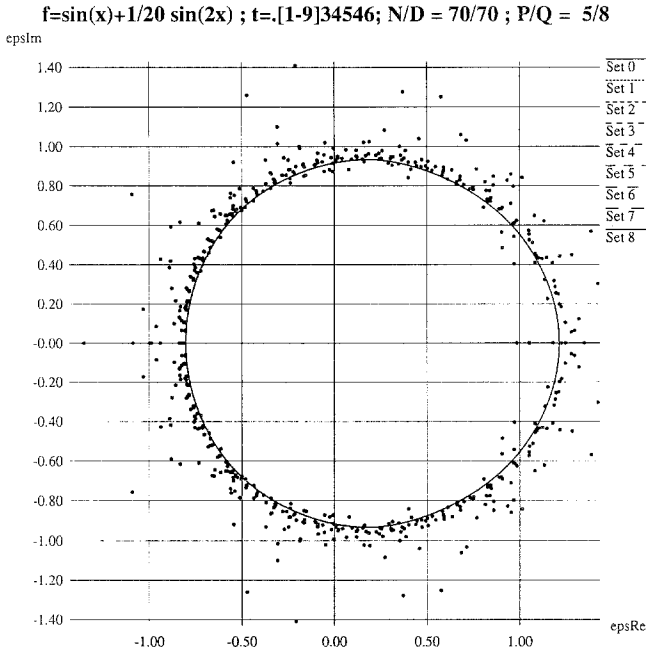


Fig. 5.

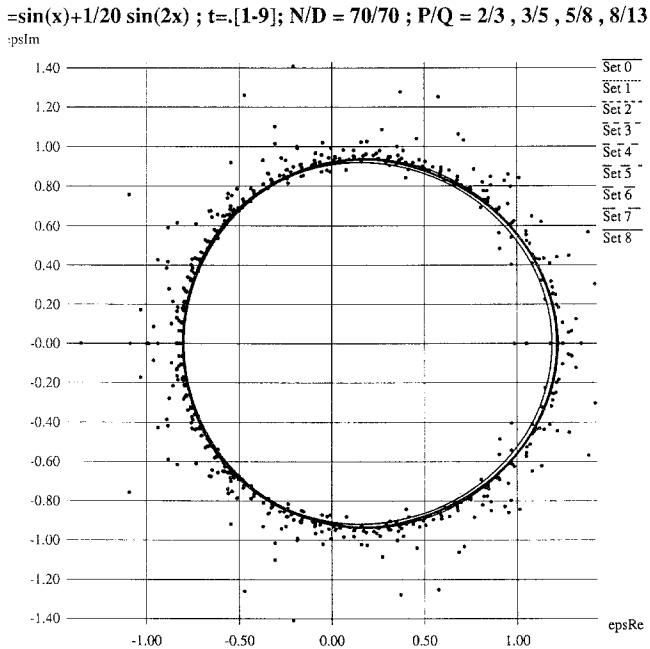


Fig. 6.

$f = \sin(x) + 1/30 \sin(3x)$; $t = .[23789]34546$; $N/D = 70/70$; $P/Q = 8/13$
epsIm

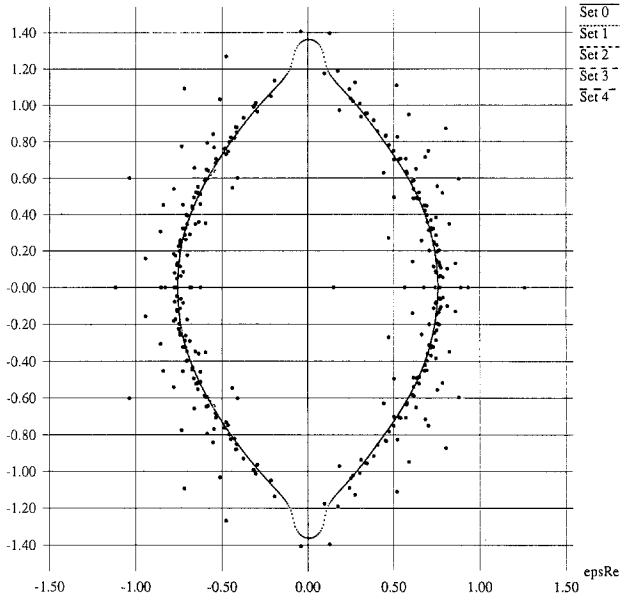


Fig. 7.

$f = \sin(x) + 1/30 \sin(3x)$; $t = .[23789]34546$; $N/D = 70/70$; $P/Q = 8/13$
epsIm

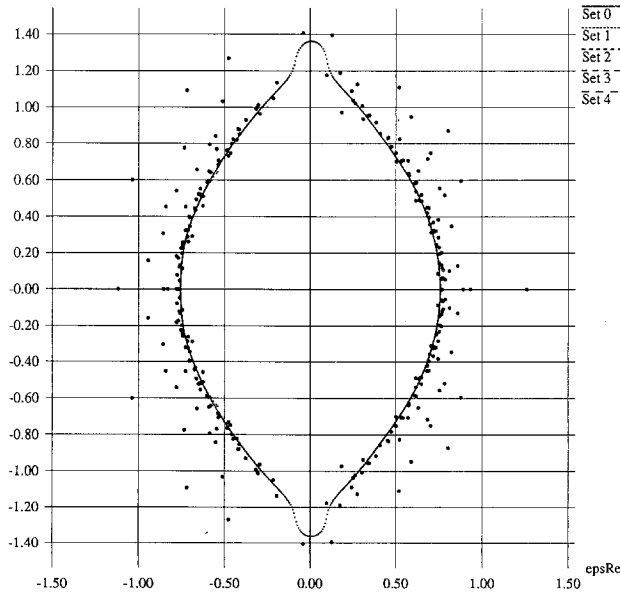


Fig. 8.

$$f = \sin(x) + 1/30 \sin(3x); t = .[23789]; N/D = 70/70; P/Q = 2/3, 3/5, 5/8, 8/13$$

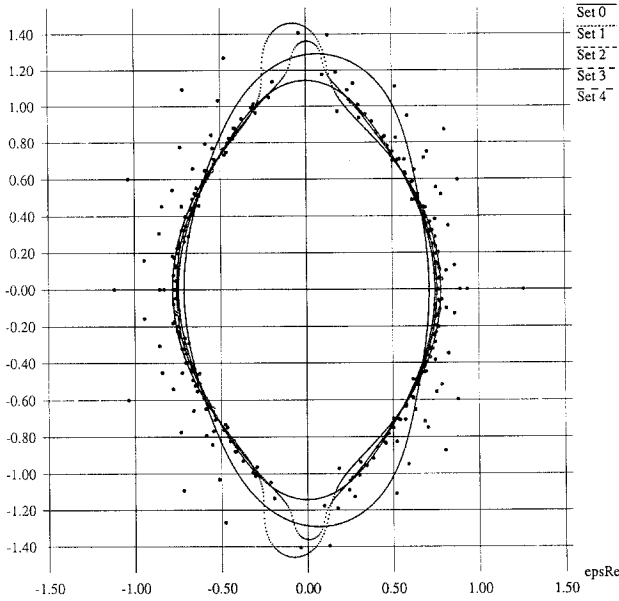


Fig. 9.

B. For the standard map, the domains of critical residue are nested onto each other in the same way that they intersect on real line. That is, the domains of critical residue do not intersect.

C. The results seems to indicate that the domains of analyticity computed by the Padé method and by taking the intersections of the domains bounded by the critical residue curves seem to agree.

Point C is interesting for practical applications since the complex extension of Greene's method seems to be much easier to implement and has the capability of dealing with very asymmetrical domains.

We point out that, according to the complex Greene method, the domain of analyticity for the ϵ expansion of the standard map is *not* a circle. The vertical and horizontal diameters differ by about 1%, which internal consistency checks suggests is between one and two orders of magnitude bigger than the reliability of the complex Greene method.

Perhaps the most interesting feature uncovered by our calculations is that for some families the critical residue lines cross, so that, for certain values of the parameters, orbits of high period have not become hyperbolic, whereas some of the low-period ones have already experienced the transition.

This can be interpreted as indicating that the dynamics induced by the renormalization group in the space of maps has more complicated features than just the MacKay fixed point, so that successive iterates of the RG transformation are on different sides of the codimension-one surfaces obtained by requiring the residue of a particular orbit to have a critical value.

Notice also that, according to the simple renormalization group scenario, the codimension-one surfaces in the space of maps Σ_n defined by the condition that the periodic orbit in the critical line of period F_n becomes hyperbolic are images of each other under the renormalization group and accumulate toward the stable manifold in a well-defined order. Hence, the order in which the orbits become critical should be a universal property.

The numerical evidence presented in this paper seems to corroborate these predictions for the standard map family and for families close to it. Nevertheless, it seems to contradict both predictions for families of the form (1.1) but with noticeably different functions.

We consider this to be evidence that the standard renormalization group scenario has only a local validity and that the renormalization group operator has a dynamics with more complicated features than just a saddle point.

More evidence along these lines and theoretical discussion, from the point of view of the RG method, reaching similar conclusions can be found in refs. 14, 24, and 25.

We also point out that the fact that the domain of analyticity appears to be smooth for families such as the standard map can be explained by assuming that the domain of analyticity of the invariant circle in the unstable manifold of the renormalization group—which in the complex extension is a manifold of complex dimension 1—has a smooth boundary. Then, the fact that the boundary becomes nonsmooth is again an indication that by changing the family we change from one universality class to another. Given the fact that the order of the crossings seems to change in a quite complicated way, it is natural to conjecture that this change of universality class is also given by the fact that the renormalization group has a complicated dynamics.

If this conjecture were true, it would have profound implications for the dynamics on the unstable manifold of the fixed point. We recall that, restricted to the unstable manifold, the renormalization group transformation is an analytic map of one complex variable and that the domain of existence of the invariant circle is the domain of attraction of the fixed point. A theorem of Broliin (ref. 1, Theorem 9.1) says that for rational transformations on the Riemann sphere, the only possible boundaries of

domains of attraction for first-order fixed points that have tangents are circles or straight lines. We think it could be very useful to study in detail the global dynamics of the renormalization group restricted to the global stable manifold of MacKay's fixed point.

It is also worth remarking that, independently of the conjecture about the smoothness of the boundary, this boundary of attraction of the trivial fixed point is an invariant set. The points on it neither converge to the trivial fixed point under successive renormalizations nor escape to infinity. This suggests that the invariant circles associated with them will have rather peculiar scaling properties.

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REFERENCES

1. H. Brolin, Invariant sets under iterations of rational functions, *Ark. Mat.* **6**:103–144 (1965).
2. G. Baker and M. Graves-Morris, *Padé Approximants* (Addison-Wesley, 1981).
3. C. M. Bender and S. A. Orszag, *Advanced Mathematical Methods for Scientists and Engineers* (McGraw-Hill, New York, 1978).
4. A. Berretti and L. Chierchia, On the complex analytic structure of the golden invariant curve for the standard map, *Nonlinearity* **3**:39–44 (1990).
5. A. Berretti, A. Celletti, L. Chierchia, and C. Falcolini, Natural boundaries for area preserving twist maps, *J. Stat. Phys.*, to appear.
6. R. De Vogelaere, On the structure of symmetric periodic solutions of conservative systems, with applications, in *Contributions to the Theory of Nonlinear Oscillations*, Vol. IV (Princeton University Press, Princeton, New Jersey, 1958).
7. C. Falcolini and R. de la Llave, A rigorous partial justification of Greene's criterion, *J. Stat. Phys.* **67**:609–643 (1992).
8. W. H. Press, B. P. Flannery, S. Teukolski, and W. T. Vetterling, *Numerical Recipes* (Cambridge University Press, Cambridge, 1986).
9. J. Greene, A method for determining a stochastic transition, *J. Math. Phys.* **20**:1183–1201 (1979).
10. J. M. Greene and I. C. Percival, Hamiltonian maps in the complex plane, *Physica* **3D**:530–548 (1981).
11. C. Golé, A new proof of Aubry–Mather's theorem, ETH preprint.
12. M. Herman, Sur la conjugaison différentiable des difféomorphismes du cercle à des rotations, *Pub. Mat. IHES* **49**:5–234 (1979).
13. H.-T. Kook and J. D. Meiss, Periodic orbits for reversible symplectic mappings, *Physica* **35D**:65–86 (1989).

14. J. A. Ketoja and R. S. MacKay, Fractal boundary for the existence of invariant circles for area preserving maps: Observations and a renormalisation explanation, *Physica* **35D**:318–334 (1989).
15. D. E. Knuth, *The Art of Computer Programming*, Vol. II, 2nd ed. (Addison-Wesley, 1981).
16. J. Mather, Existence of quasiperiodic orbits for twist homeomorphisms of the annulus, *Topology* **21**:457–467 (1982).
17. R. S. Mackay, Renormalisation in area preserving maps, Thesis, Princeton University, Princeton, New Jersey (1982).
18. R. S. Mackay, A renormalisation approach to invariant circles in area preserving maps, *Physica* **7D**:283–300 (1983).
19. R. S. MacKay, On Greene's residue criterion, Preprint.
20. M. Muldoon, Ghosts of order on the frontier of chaos, Thesis, California Institute of Technology (1989).
21. I. Percival, Chaotic boundary of a Hamiltonian map, *Physica* **6D**:67–77 (1982).
22. E. Piña and L. Jimenez Lara, On the symmetry lines of the standard mapping, *Physica* **26D**:369–378 (1987).
23. C. L. Siegel and J. Moser, *Lectures on Celestial Mechanics* (Springer-Verlag, New York, 1971).
24. J. Wilbrink, Erratic behaviour of invariant circles in standard-like mappings, *Physica* **26D**:358–368 (1987).
25. J. Wilbrink, New fixed point of the renormalisation operator associated with the recurrence of invariant circles in generic Hamiltonian maps, *Nonlinearity* **3**:567–584 (1990).