On the singularity structure of invariant curves of symplectic mappings. [1]

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Abstract.

We study invariant curves in standard-like maps conjugate to rigid rotation with complex frequencies. The main goal is to study the analyticity domain of the functions defined perturbatively by Lindstedt perturbation expansions. We argue, based on infinite-dimensional bifurcation theory that the boundary of analyticity should typically consist of branch points of order two and we verify it in some examples using non-perturbative numerical methods. We show that this nature of the singularities of the analyticity domain can explain previously reported numerical results and also suggests other numerical methods.

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1. Introduction.

Invariant curves have been widely studied as an important landmark that organizes the long term behavior. Notably, for two dimensional systems, they completely prevent long term diffusion and, for systems of more dimensions, even if not preventing diffusion completely, are still the main obstacles.

The standard way of computing invariant curves is to introduce a parametrization that identifies curves with functions and then study the functional equation that expresses that the curve is invariant and that the motion on it is a rigid rotation in some distorted coordinates. The amount of rotation – henceforth called the *frequency* of the curve – appears as a parameter in the functional equation and can be used to label the curves.

For families of maps that contain an integrable – i.e. explicitly solvable in closed form – system, one can study the functional equation for invariant curves perturbatively and one is led to the Lindstedt expansions of classical mechanics (see [Po] and section 3).

Even if these expansions have been in use for over a century, their analytic properties have been very hard to study. For example, due to the presence of *small divisors* for diophantine frequencies (see section 3), the fact that they have a positive radius of convergence was established only in the late 50's with K. A. M. theory (see e.g. [SM]) and numerical values with the right order of magnitude have only been achieved in the 80's with the use of *computer assisted proofs* (see [R], [LR],[CC]).

The goal of this paper is to study the domain of analyticity of these series and to study the nature of the singularities at the boundary (previous papers concerned with the numerical computation of the domain of analyticity of invariant curves have been: [BC], [BCCF], [FL], [BM] [LT1], [LT2], [BT], [AB], [BMT]). Notice that once that we know qualitatively what is the nature of the singularities at the boundary it is possible to devise interpolation and extrapolation schemes that, being well adapted to the functions we are dealing with, are quite efficient.

Following [BM] and [BT] we will regularize the problem by considering complex values of the frequency. The regularized equations, as we will see, have no small divisors and one can argue what is the structure of the boundary of analyticity. These insights – theoretical and numerical – can be transferred to the physical case of purely real frequencies by taking the limit as the imaginary part of the frequency tends to zero.

Our first result is a rigorous theorem that states that, for complex frequencies with non-zero imaginary part, provided that certain non-degeneracy conditions hold, the nature of the singularities is discrete branch points of order two. The theorem is based in the theory of bifurcation of compact operators and the non-degeneracy conditions – which hold generically – can be checked à posteriori by a finite calculation.

To verify the applicability of the theorem, we implement a non-perturbative continuation method and indeed confirm that for the most standard examples, the boundary of analyticity consists of branch points of order two.

Finally, we discuss the implication of these results for the applicability of analytic extrapolation methods. By far, the most commonly used method for analytic extrapolation is the use of Padé approximants. For Lindstedt series, extrapolation Padé methods were used in [BC] and used and refined in [BCCF], [LT1]. For Lindstedt series with complex frequencies they were used in [BM]. Since the Padé method is based on rational approximation, it is rather delicate to use for functions whose singularities are branch points and not just poles. The behavior of Padé approximants for functions with branch points has been considered in [N1], [N2], [HB1], [HB2] which make very precise conjectures about their behavior and support them with analytical and numerical evidence.

We observe that the numerical results of [BM] – which we reproduce and confirm – can be explained and fit very well the conjectures of [N1] and [N2] for functions with the singularity structure obtained by our non-perturbative results.

Moreover, the knowledge of the nature of the singularities can be used to devise methods that are better adapted than the Padé rational extrapolations. In our last section, we introduce the so-called *logarithmic Padé* method [BGM] and we discuss the results of implementing it as well as the *ratio* method.

All the numerical results confirm spectacularly well that the singularities of the examples we consider are branch points of order two and that, as the real part of the frequency approaches zero, these branch points accumulate to the natural boundary that has been previously reported in the literature. The details of this accumulation, remain as a challenge. We also hope that the approximation of the natural boundaries by branch points may also be useful in other problems related to K. A. M. theory.

2. Definitions and Notation.

We will study topologically nontrivial circles, invariant under an area-preserving map belonging in an one-parameter family of maps. The maps, henceforth called "standard like" are given by

$$F_\epsilon(q,p) = (q + p + \epsilon S(q) \bmod 2\pi,\ p + \epsilon S(q)) \tag{2.1}$$

The variables p, q and the parameter ϵ will be considered complex and the function S is 2π periodic, analytic, with zero average over $[-\pi, \pi]$.

The case $S(q) = \sin(q)$, called the standard map, has been extensively studied as a qualitative model of several physical phenomena (see [A], [Ch]) and as a typical example of breakdown of invariant curves (See [Gr], [McK]). We will also study the case when $S(q)$ is an odd trigonometric polynomial that can be considered as an extension of the usual standard map.

We define the frequency $\omega = \lim_{n\to\infty} \pi_1 \tilde{F}^n(q,p)/n \mod 2\pi$, whenever the limit exists, with $\tilde{F}$ a lift of F and π_1 the projection to the first coordinate $\pi_1(q,p) = q$. Notice that for $\epsilon = 0$ the map F_0 has an invariant curve for every complex frequency ω with $p = \omega$. We will identify invariant curves by the fixed frequency ω.

As the parameter ϵ varies an invariant curve is distorted and can even disappear (as for example an invariant curve with rational frequency for $\epsilon \neq 0$).

3. Lindstedt perturbation expansions

If an invariant curve is conjugate to a rigid rotation with frequency ω,then it can be parameterized by two functions p and q of a variable θ which satisfy:

$$F_\epsilon(q(\theta), p(\theta)) = (q(\theta+\omega), p(\theta+\omega)). \tag{3.1}$$

Moreover, assuming the invariant curve is a graph

$$q(\theta) = \theta + u_\epsilon(\theta), \quad p(\theta) = \omega + u_\epsilon(\theta) - u_\epsilon(\theta - \omega)$$

The conjugating function u_ϵ is called the hull function (see [A]). Combining (2.1), (3.1)

$$\Delta_\omega u_\epsilon(\theta) = \epsilon S(u_\epsilon(\theta) + \theta) \tag{3.2}$$

where Δ_ω is the operator defined by

$$\Delta_\omega u_\epsilon(\theta) = u_\epsilon(\theta+\omega) - 2u_\epsilon(\theta) + u_\epsilon(\theta-\omega). \tag{3.3}$$

Notice that a solution of (3.2) corresponds to a solution of (3.1) but the opposite need not be the case (for the case of real variables the Birkhoff theorem ([M], [F]) guarantees that the conjugating function is a graph but we are not aware of a similar result for the case of complex variables).

If there is a solution u_ϵ, for fixed ϵ, to (3.2) then $u_\epsilon(\theta+\alpha) - \alpha$, for $\alpha \in \mathbb{C}$, is also a solution. To fix this ambiguity we choose the normalization

$$\int_{-\pi}^{\pi} u_\epsilon(\theta) d\theta = 0. \tag{3.4}$$

Under this normalization $u_0 = 0$ is the solution for $\epsilon = 0$.

To compute the unknown hull function u_ϵ we assume that it can be expanded in a power series in ϵ

$$u_\epsilon(\theta) = \sum_{n=0}^{\infty} \epsilon^n u_n(\theta). \tag{3.5}$$

The series (3.5) are called Lindstedt series. Substituting in (3.2), expanding and matching formally corresponding orders in ϵ

$$
\begin{aligned}
& u_0(\theta) = 0 \\
(3.6) \qquad & \Delta_\omega u_1(\theta) = S(\theta) \\
& \Delta_\omega u_n(\theta) = R_n(\theta) = \frac{1}{(n-1)!}\frac{d^{(n-1)}}{d\epsilon^{(n-1)}}\Big|_{\epsilon=0} S(\theta + \sum_{l=1}^{\infty} u_l(\theta)\epsilon^l), \quad n \geq 2
\end{aligned}
$$

Notice that the right hand side of (3.6) depends only on $u_1, \ldots, u_{n-1}$ so that one can solve recursively, provided that

$$\Delta_\omega u_n(\theta) = R_n(\theta)$$

has a solution, i.e.

$$\int_{-\pi}^{\pi} R_n(\theta) d\theta = 0. \tag{3.7}$$

¿From the normalization condition on the hull function (3.4) we have

$$\int_{-\pi}^{\pi} u_n(\theta) d\theta = 0, \qquad n \geq 1$$

and, using the properties of S we can show inductively that the compatibility condition (3.7) is satisfied (see also [FL]).

In effect, if we rewrite R_n as

$$
\begin{aligned}
R_n(\theta) &= \frac{1}{(n-1)!}\frac{d^{(n-1)}}{d\epsilon^{(n-1)}}\Big|_{\epsilon=0} \left\{ \sum_{m=0}^{\infty} \frac{1}{m!}\frac{d^m}{d\theta^m} S(\theta) \left(\sum_{l=1}^{\infty} u_l(\theta)\epsilon^l \right)^m \right\} \\
(3.8) \qquad &= \sum_{m=0}^{\infty} (\frac{1}{m!}\frac{d^m}{d\theta^m} S(\theta)) \frac{1}{(n-1)!}\frac{d^{(n-1)}}{d\epsilon^{(n-1)}}\Big|_{\epsilon=0} \left(\sum_{l=1}^{\infty} u_l(\theta)\epsilon^l \right)^m \\
&= \sum_{j=0}^{n-1} (\frac{1}{j!}\frac{d^j}{d\theta^j} S(\theta)) \sum_{n_1+\cdots+n_j=n-1} \frac{n_1!\ldots n_j!}{(n-1)!} u_{n_1}(\theta)\cdots u_{n_j}(\theta), \; n \geq 2.
\end{aligned}
$$

In terms of Fourier series, the operator Δ_ω is diagonal and, if

$$u_n(\theta) = \sum_{k\neq 0} \hat{u}_{n,k} e^{ik\theta}, \quad R_n(\theta) = \sum_{k\neq 0} \hat{R}_{n,k} e^{ik\theta}$$

then

$$\hat{u}_{n,k} = \frac{\hat{R}_{n,k}}{2(\cos(k\omega) - 1)}, \quad n \geq 1, \quad k \neq 0.$$

For the case of ω real, diophantine it was shown (see [SM] for an analytic proof, [CC] for a computer-aided one) using methods from KAM theory, that the Lindstedt series for the hull function, converges to an analytic function for $|\epsilon| < \rho$ for some $\rho > 0$.

When $\mathrm{Im}\,\omega \neq 0$, $2(\cos(k\omega) - 1)$ is bounded away from zero uniformly in $k \in \mathbb{Z} - \{0\}$ so that

$$\sup_{k\neq 0} |2(\cos(k\omega) - 1)|^{-1} \leq K_\omega. \tag{3.9}$$

To estimate convergence of the Lindstedt series we introduce the norm $\| \, \|_\delta$ with $\|f\|_\delta = \sup_{k\in\mathbb{Z}} e^{\delta|k|}|\hat{f}_k|$, where $\hat{f}_k$ is the k^{th} Fourier coefficient of f. This defines a norm on a Banach space of analytic functions denoted henceforth as $C^{\omega,\delta}$. Since S is a 2π periodic, analytic function, using Cauchy inequalities we can find a constant $K_\delta(= 2/\delta)$ such that $\|\frac{1}{j!}\frac{d^j}{d\theta^j}S(\theta)\|_\delta \leq K_\delta^j \sup_{\theta\in \mathrm{I}_{2\delta}} |S(\theta)|$, where $\mathrm{I}_{2\delta} \equiv \{\theta : |\mathrm{Im}\,\theta| < 2\delta\}$.

Theorem 3.1. *For $|\epsilon|$ sufficiently small, the Lindstedt series (3.5) converges uniformly to an analytic function defined on $\mathrm{I}_\delta \equiv \{\theta : |\mathrm{Im}\,\theta| < \delta\}$.*

Proof. ¿From (3.6) we have $\|u_n\|_\delta \leq K_\omega \|R_n\|_\delta$. For $n = 1, R_1(\theta) = S(\theta)$ and $\|u_1\|_\delta \leq K_\omega \sup_{\theta\in \mathrm{I}_{2\delta}} |S(\theta)|$.

For $n > 1$, from (3.8),

$$\|u_n\|_\delta \leq K_\omega \|R_n\|_\delta \leq K_\omega \sum_{j=1}^{n-1} \|\frac{1}{j!}\frac{d^j}{d\theta^j}S(\theta)\|_\delta \sum_{n_1+\cdots+n_j=n-1} \frac{n_1!\ldots n_j!}{(n-1)!}\|u_{n_1}\|_\delta \ldots \|u_{n_j}\|_\delta. \tag{3.10}$$

To estimate the size of $\|u_n\|_\delta$, we introduce the function $\phi : \mathbb{R} \to \mathbb{R}$ with $\phi(z) = \sum_{n=0}^\infty \frac{1}{n!}\|\frac{d^n}{d\theta^n}S(\theta)\|_\delta z^n$.

Since $\frac{1}{n!}\|\frac{d^n}{d\theta^n}S(\theta)\|_\delta \leq K_\delta^n \sup_{\theta\in \mathrm{I}_{2\delta}} |S(\theta)|$, ϕ is an analytic function for $|z| < K_\delta^{-1}$. We can bound $\|u_n\|_\delta$ by the coefficients σ_n of $\sigma(z) = \sum_{n=0}^\infty \sigma_n z^n$, where

$$\sigma(z) = K_\omega z\phi(\sigma(z)), \quad \sigma(0) = 0. \tag{3.11}$$

By induction we verify that $\|u_n\|_\delta \le \sigma_n,\ n \ge 1$. Moreover, since ϕ is an analytic function and $\|S(\theta)\|_\delta \ne 0$, by the implicit function theorem, σ is analytic for $|z|$ small enough and we can bound $\sigma_n \le \alpha^n$, for some $\alpha > 0$.

This implies that the Lindstedt series converges uniformly to an analytic function in I_δ, for $\epsilon < 1/\alpha$, and concludes the proof of Theorem 3.1.

■

4. Bifurcation from a simple eigenvalue

We will analyze the equation satisfied by the hull function (3.2) using methods from functional analysis and bifurcation theory. For fixed ω we define the operator $\mathcal{T} : \mathbb{C} \times C_0^0 \to C_0^0$

$$\mathcal{T}(\epsilon, u)(\theta) = \epsilon \Delta_\omega^{-1} S(u(\theta) + \theta) \tag{4.1}$$

where C_0^0 is the space of 2π periodic, continuous, complex functions with zero average on $[-\pi, \pi]$ under the supremum norm, i.e. $\|f\|_{C_0^0} = \max_{\theta\in[-\pi,\pi]} |f(\theta)|$. It is well known that under this norm C_0^0 is a Banach space. Also, since $\mathbb{C}$ is a Banach space, $\mathbb{C} \times C_0^0$ is a Banach space under the norm $\|(\epsilon, u)\|_{\mathbb{C}\times C_0^0} = |\epsilon| + \|u\|_{C_0^0}$.

Lemma 4.1. *The operator $\Delta_\omega : C_0^0 \to C_0^0$, given by (3.3) is invertible and, for $\operatorname{Im}\omega \ne 0$ the inverse is bounded.*

Proof. Decomposing Δ_ω in Fourier coefficients we have

$$(\Delta_\omega)_{k,l} = (e^{i\omega k} + e^{-i\omega k} - 2)\delta_{k,l}, \qquad k \ne 0.$$

Since $(\Delta_\omega)_{k,l}$ is a diagonal matrix we can verify that the inverse $\Delta_\omega^{-1} : C_0^0 \to C_0^0$ exists and is given by $[\Delta_\omega^{-1}]_{k,l} = [(\Delta_\omega)_{k,k}]^{-1}\delta_{k,l}, \quad k \ne 0$ (notice that zero average is essential for the existence of the inverse).

To show that Δ_ω^{-1} is bounded for $\mathrm{Im}\,\omega \neq 0$, let $\eta \in C_0^0, \|\eta\|_{C_0^0} \leq M$. Then, decomposing in Fourier coefficients

$$\begin{aligned}
\|\Delta_\omega^{-1}\eta\|_{C_0^0} &= \max_{\theta\in[-\pi,\pi]} \Big|\sum_{k\neq 0} \frac{\eta_k e^{ik\theta}}{e^{ik\omega}+e^{-ik\omega}-2}\Big| \\
&\leq \|\eta\|_{C_0^0} \sum_{k\neq 0} \Big|\frac{1}{e^{ik\omega}+e^{-ik\omega}-2}\Big| \\
&= 2\|\eta\|_{C_0^0} \sum_{k>0} \Big|\frac{1}{e^{ik\omega}+e^{-ik\omega}-2}\Big|
\end{aligned}$$

The sum is finite for $\mathrm{Im}\,\omega \neq 0$, since the denominator grows asymptotically like $e^{k|\mathrm{Im}\,\omega|}$. This concludes the proof.

■

We will now show some interesting properties of $\mathcal{T}$.

Lemma 4.2. *The operator $\mathcal{T}$, defined by (4.1), is Fréchet differentiable for all $(\epsilon, u) \in \mathbb{C} \times C_0^0$ with*

$$D\mathcal{T}(\epsilon,u)(\zeta,\eta) = \zeta\Delta_\omega^{-1}S(u+\theta) + \epsilon\Delta_\omega^{-1}[S'(u+\theta)\eta].$$

Proof. We have the following simple computation

$$\begin{aligned}
\|\mathcal{T}(\epsilon+\zeta, u+\eta) - \mathcal{T}(\epsilon,u) - &D\mathcal{T}(\epsilon,u)(\zeta,\eta)\|_{C_0^0} = \\
&= \|(\epsilon+\zeta)\Delta_\omega^{-1}[S(u+\theta+\eta) - S(u+\theta) - S'(u+\theta)\eta]\|_{C_0^0} \\
&= \|(\epsilon+\zeta)\Delta_\omega^{-1}[S''(\tilde{u}+\theta)(\eta)^2]\|_{C_0^0} \\
&\leq |\epsilon+\zeta|\|\Delta_\omega^{-1}\|_{C_0^0}\|S''\|_{C_0^0}\|\eta\|_{C_0^0}^2
\end{aligned}$$

■

Lemma 4.2 implies that $\mathcal{T}$ is complex analytic. We follow [ChH, pg. 23] in our definition of a complex analytic operator.

Definition 4.3. *Let X, Y be Banach spaces over $\mathbb{C}$ and U be a connected open set of X. A function $f : X \to Y$ is complex analytic in U if, for each $x \in U$, there is a*

$\delta(x,h) > 0$, *such that, for each* $y^* \in Y^*$, $f(x)$ *is single valued and* $< y^*, f(x+th) >$ *is an analytic function of* t *for* $|t| < \delta(x,h)$.

We state the following theorem, based on the Definition 4.3.

Theorem 4.4. *(*[ChH, pg. 23, theorem 1.10]*) If* U *is an open connected set of* X, $f : U \to Y$ *is single valued and locally bounded, then the following statements are equivalent*
(i) f *is complex analytic in* U
(ii) f *is Fréchet differentiable in* U
(iii) f *has infinitely many Fréchet derivatives*

Theorem 4.5. *For fixed* ϵ_0, u_0 *and* ω, *with* $\operatorname{Im}\omega \neq 0$, *the Fréchet derivative of the map* $u \to \mathcal{T}(\epsilon_0, u)$, *at* $u = u_0$ *is a compact operator on* C_0^0.

Proof. The Fréchet derivative of $u \to \mathcal{T}(\epsilon_0, u)$ exists and is given by

$$D_u\mathcal{T}(\epsilon_0, u_0)\eta = \epsilon_0 \Delta_\omega^{-1}[S'(u_0 + \theta)\eta].$$

To show that $D_u\mathcal{T}(\epsilon_0, u_0)$ is a compact operator, we have to show that it maps bounded sets to precompact ones.

Notice that $D_u\mathcal{T}(\epsilon_0, u_0)$ is bounded, i.e. for η such that $\|\eta\|_{C_0^0} \leq M$

$$\|D_u\mathcal{T}(\epsilon_0, u_0)\eta\|_{C_0^0} \leq |\epsilon_0| \|\Delta_\omega^{-1}\|_{C_0^0} \max_{\theta\in[-\pi,\pi]} |S'(\theta)| \|\eta\|_{C_0^0}.$$

We will show that $\{D_u\mathcal{T}(\epsilon_0, u_0)\eta : \|\eta\|_{C_0^0} \leq M\}$ is equicontinuous. We have

$$\begin{aligned}
|D_u\mathcal{T}(\epsilon_0, u_0)\eta(\theta') - D_u\mathcal{T}(\epsilon_0, u_0)\eta(\theta)| = \\
&\left|\epsilon_0 \Delta_\omega^{-1}[S'(u_0(\theta') + \theta')\eta(\theta') - S'(u_0(\theta) + \theta)\eta(\theta)]\right| \\
&= |\epsilon_0| \left|\Delta_\omega^{-1}[F(\theta') - F(\theta)]\right|
\end{aligned}$$

where $F(\theta) = S'(u(\theta) + \theta)\eta(\theta)$.

Decomposing into Fourier coefficients,

$$
\begin{aligned}
|\Delta_\omega^{-1}[F(\theta') - F(\theta)]| &= |\sum_{k\neq 0} \frac{F_k(e^{ik\theta'} - e^{ik\theta})}{e^{ik\omega} + e^{-ik\omega} - 2}| \\
&\leq \|F\|_{C_0^0} \sum_{k\neq 0} \frac{|k||\theta - \theta'| \max \theta'' \in [-\pi, \pi] |e^{ik\theta''}|}{|e^{ik\omega} + e^{-ik\omega} - 2|} \\
&\leq \|S'\eta\|_{C_0^0} |\theta' - \theta| \sum_{k\neq 0} \frac{|k|}{|e^{ik\omega} + e^{-ik\omega} - 2|}
\end{aligned}
$$

As in the proof of Lemma 4.1 the sum is finite for $\operatorname{Im}\omega \neq 0$. By the Ascoli theorem (see [Rudin, pg. 394, theorem A5]) we conclude that $D_u\mathcal{T}(\epsilon_0, u_0)$ is a compact operator.

■

Since $D_u\mathcal{T}(\epsilon_0, u_0)$ is a compact operator the spectrum of $D_u\mathcal{T}(\epsilon_0, u_0)$ is discrete and has no accumulation points, apart from zero (see [Rudin]). Based on this property of the spectrum we are able to characterize the nature of the singularities in the analyticity domain of the hull function. This characterization is based on the following theorem from bifurcation theory of operators in Banach spaces.

Theorem 4.6. *For B a Banach space over $\mathbb{C}$, let $K : \mathbb{C} \times B \to B$ be a Fréchet differentiable operator. Assume that $D_uK(0,0) = A$ (the Fréchet derivative of the map $u \to K(0,u)$ at $u = 0$) has a simple isolated eigenvalue 0, and $\operatorname{Null}(A) = \operatorname{span}(v_0)$, $\operatorname{Null}(A^*) = \operatorname{span}(w_0^*)$, for $v_0 \in B, w_0^* \in B^*$ and the co-dimension of $\operatorname{Range}(A) = 1$. If*

$$
< w_0^*, D_{uu}K(0,0)(v_0, v_0) > \neq 0, \qquad < w_0^*, D_\epsilon K(0,0) > \neq 0
$$

then, there are two distinct solutions to

$$
K(\epsilon, u) = 0 \tag{4.2}
$$

for $0 < \epsilon < \rho$, for some $\rho > 0$, analytic in $\epsilon^{1/2}$.

Proof. The proof is divided in two parts. First we will use the Liapunov-Schmidt reduction method to reduce (4.2) to an one dimensional scalar equation. Then we will apply the Newton polygon method to deduce the form of the solutions to the one dimensional equation (see [GS], [ChH] for examples and applications of these methods).

Since the null space of A is one dimensional and the co-dimension of Range(A) is one, we can decompose B into

$$B = \text{Null}(A) \oplus M, \qquad B = N \oplus \text{Range}(A).$$

Since $B = N \oplus \text{Range}(A)$, there exists (see [Rudin, pg. 133, theorem 5.16]) a continuous projection $E : B \to \text{Range}(A)$ with $\text{Range}(E) = \text{Range}(A)$, $\text{Null}(E) = N$. Then, $K(\epsilon, u) = 0$ is equivalent to

$$\begin{aligned} EK(\epsilon, u) &= 0 \\ (I - E)K(\epsilon, u) &= 0 \end{aligned} \tag{4.3}$$

Following the Liapunov-Schmidt reduction method we will use the implicit function theorem to solve the first of (4.3) and then substitute the solution in the second. Thus we will finally have to study a k-dimensional equation for a k-dimensional null space (we assumed $k = 1$).

Let $u = v + w, v \in \text{Null}(A), w \in M$. Define the map $F : M \times \text{Null}(A) \times \mathbb{C} \to \text{Range}(A)$

$$F(w, v, \epsilon) = EK(\epsilon, w + v). \tag{4.4}$$

We have that $F(0, 0, 0) = 0, D_w F(0, 0, 0) = A$. Since $A : M \to \text{Range}(A)$ is one to one and onto, and Range(A) is closed, A restricted to M is invertible. From Theorem 4.4 Fréchet differentiability is equivalent to complex analyticity. By the implicit function theorem the solution of (4.4) in a neighborhood of $(0, 0) \in \text{Null}(A) \times \mathbb{C}$ is a complex analytic function $W : \text{Null}(A) \times \mathbb{C} \to M$ such that

$$F(W(v, \epsilon), v, \epsilon) = EK(\epsilon, v + W(v, \epsilon)) = 0.$$

Substituting in the second of the equations (4.3)

$$(I - E)K(\epsilon, v + W(v, \epsilon)) = 0. \tag{4.5}$$

¿From [Rudin pg. 99, theorem 4.12]

$$\text{Null}(A^*) = \text{Range}(A)^{\perp} = \{w^* \in B^* | < w^*, u >= 0, \forall u \in \text{Range}(A)\}$$

We define $g : \mathbb{C} \times \mathbb{C} \to \mathbb{C}$,

$$g(z, \epsilon) =< w_0^*, (I - E)K(\epsilon, zv_0 + W(zv_0, \epsilon)) >=< w_0^*, K(\epsilon, zv_0 + W(zv_0, \epsilon)) > .$$

¿From the Fredholm alternative

$$g(z,\epsilon)=0 \iff (I-E)K(\epsilon, zv_0+W(zv_0,\epsilon))=0$$

The function g is analytic in a neighborhood of $(0,0)$ since K, W are complex analytic and we compute

$$\begin{aligned}
&g(0,0)=0\\
&g_z(0,0)=0\\
&g_{zz}(0,0)=< w_0^*, D_{uu}K(0,0)(v_0,v_0) >\neq 0\\
&g_\epsilon(0,0)=< w_0^*, D_\epsilon K(0,0) >\neq 0\\
&g(z,\epsilon)=\frac{1}{2}g_{zz}(0,0)z^2+g_\epsilon(0,0)\epsilon+O(\epsilon^2)+O(z^3)+O(\epsilon z)
\end{aligned}$$

The Newton polygon is a method to identify the leading singularities for solutions of $f(z,\epsilon)=0$ where f is a power series in z whose coefficients can be power series in ϵ. For $g(z,\epsilon)=0$, the leading singular behavior is $\epsilon^{1/2}$ and if we perform the change of variables $z=\epsilon^{1/2}y$ and divide $g(z(y),\epsilon)$ by ϵ we have

$$\frac{1}{2}g_{zz}(0,0)y^2+g_\epsilon(0,0)+O(\epsilon^{1/2})=0. \tag{4.6}$$

For $\epsilon=0$ (4.6) has two distinct solutions

$$y=\pm\left(-\frac{2g_\epsilon(0,0)}{g_{zz}(0,0)}\right)^{1/2}$$

By the implicit function theorem, there are two and only two solutions $y_i(\epsilon), i=1,2$, analytic in ϵ, for $|\epsilon|$ sufficiently small. This implies $z_i=\epsilon^{1/2}y_i(\epsilon)$ and, for ϵ sufficiently small, there are two solutions to $K(u,\epsilon)=0$ analytic in $\epsilon^{1/2}$, with

$$u_i=W(\epsilon^{1/2}y_i(\epsilon)v_0,\epsilon)+\epsilon^{1/2}y_i(\epsilon)v_0, \qquad i=1,2.$$

This concludes the proof of the theorem.

■

Corollary 4.7. *Suppose that for (ϵ_0,u_0) such that $\mathcal{T}(\epsilon_0,u_0)=u_0$ (where $\mathcal{T}$ defined in (4.1)), fixed ω with $\operatorname{Im}\omega\neq 0$, $D_u\mathcal{T}(\epsilon_0,u_0)$ has a simple eigenvalue 1. Let*

$$\mathrm{Null}(D_u\mathcal{T}(\epsilon_0,u_0)-I)=\mathrm{span}(v_0), \quad \mathrm{Null}\big[(D_u\mathcal{T}(\epsilon_0,u_0)-I)^*\big]=\mathrm{span}(w_0^*).$$

If $< w_0^*, D_{uu}\mathcal{T}(\epsilon_0, u_0)(v_0, v_0) > \neq 0$ and $< w_0^*, D_\epsilon \mathcal{T}(\epsilon_0, u_0) > \neq 0$ then, ϵ_0 is an isolated branch point of order 2, in the analyticity domain of the hull function.

Proof. Consider the operator

$$K(\epsilon, u) = \mathcal{T}(\epsilon + \epsilon_0, u + u_0) - I.$$

Then,

$$\begin{aligned} D_{uu}K(0,0) &= D_{uu}\mathcal{T}(\epsilon_0, u_0) \\ D_\epsilon K(0,0) &= D_\epsilon \mathcal{T}(\epsilon_0, u_0) \end{aligned}$$

¿From Lemma 4.2 $\mathcal{T}$ is Fréchet differentiable. From Theorem 4.5 $D_u\mathcal{T}(\epsilon_0, u_0)$ is a compact operator and may exhibit isolated eigenvalues. An isolated simple eigenvalue 1 for $D_u\mathcal{T}(\epsilon_0, u_0)$ corresponds to an isolated simple eigenvalue 0 for $D_u\mathcal{T}(\epsilon_0, u_0) - I$ with an one dimensional null space and range of co-dimension 1. Moreover, since $D_u\mathcal{T}(\epsilon_0, u_0)$ is compact, we have $B = \mathrm{Null}(D_u\mathcal{T}(\epsilon_0, u_0) - I) \oplus \mathrm{Range}(D_u\mathcal{T}(\epsilon_0, u_0) - I)$ (see [Rudin]). Thus K fulfills all the conditions of Theorem 4.6.

■

Remark. The dual space of C_0^0 is the space of complex measures on $[-\pi, \pi]$ with zero Fourier coefficient equal to zero. If S is an odd trigonometric polynomial, then u_0, v_0 are odd functions and the Fourier decomposition of the operator $D_u\mathcal{T}(\epsilon_0, u_0)$ is the same in C_0^0 and $(C_0^0)^*$. Thus

$$\begin{aligned} < w_0^*, D_{uu}\mathcal{T}(\epsilon_0, u_0)(v_0, v_0) > &= \int_{-\pi}^{\pi} \epsilon_0 v_0(\theta) \Delta_\omega^{-1}[S''(u_0(\theta) + \theta) v_0^2(\theta)] d\theta \\ < w_0^*, D_\epsilon \mathcal{T}(\epsilon_0, u_0) > &= \int_{-\pi}^{\pi} v_0(\theta) \Delta_\omega^{-1}[S(u_0(\theta) + \theta)] d\theta \end{aligned} \tag{4.7}$$

are integrals of even functions over an interval centered at the origin. Thus, typically, the non-degeneracy conditions of Corollary 4.7 are satisfied. This remark applies in particular to the case of the standard map and it provides an explanation on the nature of the singularities of the hull functions. Notice that in the presence of an additional parameter one expects cases where the non-degeneracy conditions are not satisfied and different bifurcations may occur. Notice that, because of the presence of the compact operator Δ_ω^{-1} in the integrand in (4.7), the high order Fourier coefficients in the expansion of u_0, v_0 do not contribute very much to the integral. Since the Newton method (see section 5) can produce error bounds for the difference between the true u_0 and the computed one and it is well known how to validate the computation of eigenvectors of compact operators, it is quite feasible to estimate the errors in the computation and conclude that indeed the conditions in (4.7) are verified for a particular model.

Remark. If S is an odd trigonometric polynomial and ϵ_0 is a bifurcation point for the hull function, then $-\epsilon_0$ is also a bifurcation point since $u_{-\epsilon_0}(\theta) = u_{\epsilon_0}(\theta-\pi)$ satisfies the conditions of Corollary 4.7. Since this symmetry is not explicitly used in the algorithms, it provides with a useful check of their accuracy.

Remark. The compactness of the operator $\mathcal{T}$ depends crucially on the condition $\mathrm{Im}\,\omega \neq 0$. When $\mathrm{Im}\,\omega = 0$, $\mathcal{T}$ is not a compact operator and the bifurcation Theorem 4.6 does not apply.

To study numerically the domain of analyticity of the map $\epsilon \mapsto u_\epsilon$, and the nature of the singularities of the map we will numerically study the domain of analyticity of maps $\epsilon \to \Gamma[u_\epsilon]$ where Γ is an entire map from the space of continuous functions to the complex numbers. Clearly the domain of analyticity of $\epsilon \mapsto \Gamma[u_\epsilon]$ is not smaller than the domain of analyticity of the map $\epsilon \mapsto u_\epsilon$. One expects also that many observables will lead to the same domain of analyticity, with singularities of the same nature. Some observables that immediately come to mind are the evaluation of the function at certain values and the Fourier coefficients.

Theorem 4.8. *Let $f : \mathbb{C} \to C^0$ (C^0 the space of continuous functions on $[-\pi,\pi]$) be a map with $\epsilon = \epsilon_0$ an isolated branch point of order 2, i.e. $f(\epsilon) = \sum_{n=0}^{\infty} f_n(\epsilon-\epsilon_0)^{n/2}$, $f_1 \neq 0$ where the series converges for $|\epsilon-\epsilon_0|$ small enough. If $\Gamma : C^0 \to \mathbb{C}$ is an analytic function in C^0, i.e. for any $g \in C^0$, there exists $\delta = \delta(g) > 0$ such that, whenever $\|h\|_{C^0} < \delta(g)$, $\Gamma(g+h) = \sum_{k=0}^{\infty} \frac{1}{k!} D^k\Gamma(g)h^k$ where the series converges uniformly in h, and $D\Gamma(f_0)[f_1] \neq 0$, then, the point ϵ_0 is an isolated branch point of order 2 of the composition map $f \circ \Gamma$.*

Proof. Since $f(\epsilon) = \sum_{n=0}^{\infty} f_n(\epsilon-\epsilon_0)^{n/2}$ converges for $|\epsilon-\epsilon_0|$ small enough, $\|(\epsilon-\epsilon_0)^{1/2}\sum_{n=1}^{\infty} f_n(\epsilon-\epsilon_0)^{(n-1)/2}\|_{C^0}$ can be made arbitrarily small, in particular less than

$\delta(f_0)$. Then, by the analyticity of Γ,

$$\begin{aligned}
\Gamma(f_0 + (\epsilon - \epsilon_0)^{\frac{1}{2}} \sum_{n=1}^{\infty} f_n (\epsilon - \epsilon_0)^{\frac{n-1}{2}}) &= \sum_{k=0}^{\infty} \frac{1}{k!} D^k \Gamma(f_0) \left[(\epsilon - \epsilon_0)^{\frac{1}{2}} \sum_{n=1}^{\infty} f_n (\epsilon - \epsilon_0)^{\frac{n-1}{2}} \right]^k \\
&= \Gamma(f_0) + D\Gamma(f_0)[(\epsilon - \epsilon_0)^{1/2} f_1] + (\epsilon - \epsilon_0) \sum_{n=0}^{\infty} \Gamma_n (\epsilon - \epsilon_0)^{n/2} \\
&= \Gamma(f_0) + (\epsilon - \epsilon_0)^{1/2} D\Gamma(f_0)[f_1] + (\epsilon - \epsilon_0) \sum_{n=0}^{\infty} \Gamma_n (\epsilon - \epsilon_0)^{n/2}
\end{aligned}$$

Since the series for $\Gamma(f)$ converges for $|\epsilon - \epsilon_0|$ small enough, and $D\Gamma(f_0)[f_1] \neq 0$, ϵ_0 is an isolated branch point of order 2 for the composition map $f \circ \Gamma$.

■

Remark. If for a map Γ, $\Gamma(f)$ is constant for all ϵ, then the composition map $\epsilon \to f \circ \Gamma$ is actually entire in ϵ, since $\Gamma(f)$ is independent of ϵ. This is the case when we take Γ to be evaluation at $\theta = 0, \pi$ for standard-like maps, with S an odd trigonometric polynomial.

Based on Theorem 4.6 and our numerical observations we formulate the following conjecture about the behavior of the singular points of the hull function as $\operatorname{Im}\omega \to 0$.

Conjecture 4.9. *If* $\operatorname{Im}\omega \neq 0$ *the singular points in the analyticity domain of the hull function for a dense set of standard-like maps are isolated branch points of order 2. As* $\operatorname{Im}\omega \to 0$, *the branch points move towards the origin, and accumulate, in the limit of* ω *real, diophantine, to a natural boundary.*

We note that a very similar phenomenon of natural boundaries being approximated by accumulation of branch points was discussed in [LT1] for a very different problem, namely, invariant curves in a dissipative system. There, irrational frequencies were approximated by rational ones and the later were shown to lead to analyticity domains bounded by branch points. The phenomena in [LT1] were, however, very different because the derivative of the operator was not compact, and indeed the spectrum was uncountable.

We also note that the Greene's criterion for complex values [FL] also suggests that, for twist mappings, the analyticity domain for invariant curves is approximated by the place at which periodic orbits lose stability. When the eigenvalues $\lambda_\pm$ of the orbit of type p/q arrive at the unit circle with a rational phase ($\lambda_\pm = e^{2\pi i \frac{N}{M}}$), one also expects that the periodic orbit of period qM expressed as a function of the parameter also experiences a branch point of order two.

5. Newton Method

In order to verify the perturbative calculations, we will use a non-perturbative method based on numerical continuation for an appropriate operator $\mathcal{R}_\epsilon$.

For fixed ϵ, let $\mathcal{R}_\epsilon : C^{\omega,\delta} \to C^{\omega,\delta}$ with

$$\mathcal{R}_\epsilon f(\theta) = \epsilon \Delta_\omega^{-1} \big[S(f(\theta) + \theta) \big] - f(\theta). \tag{5.1}$$

If u_0 fails to satisfy (3.2) by a small amount, i.e.

$$\mathcal{R}_\epsilon u_0(\theta) = R_0(\theta)$$

we can try to improve the approximate solution by setting it to $u_0(\theta) + \eta(\theta)$, where η will be chosen to make the error much smaller.

Theorem 5.1. *Let ω with $\operatorname{Im} \omega \neq 0, \mathcal{R}_\epsilon$ as in (5.1), $\epsilon, u_\epsilon \in C^{\omega,\delta}$ such that $\mathcal{R}_\epsilon u_\epsilon(\theta) = 0$. If $D\mathcal{R}_\epsilon(u_\epsilon)$ is an invertible operator with bounded inverse, then , for $|\epsilon - \epsilon'|$ sufficiently small there exists $u_{\epsilon'} \in C^{\omega,\delta}$ such that $\mathcal{R}_{\epsilon'} u_{\epsilon'}(\theta) = 0$.*

Proof. Since u_ϵ satisfies $\mathcal{R}_\epsilon u_\epsilon(\theta) = 0$ we have

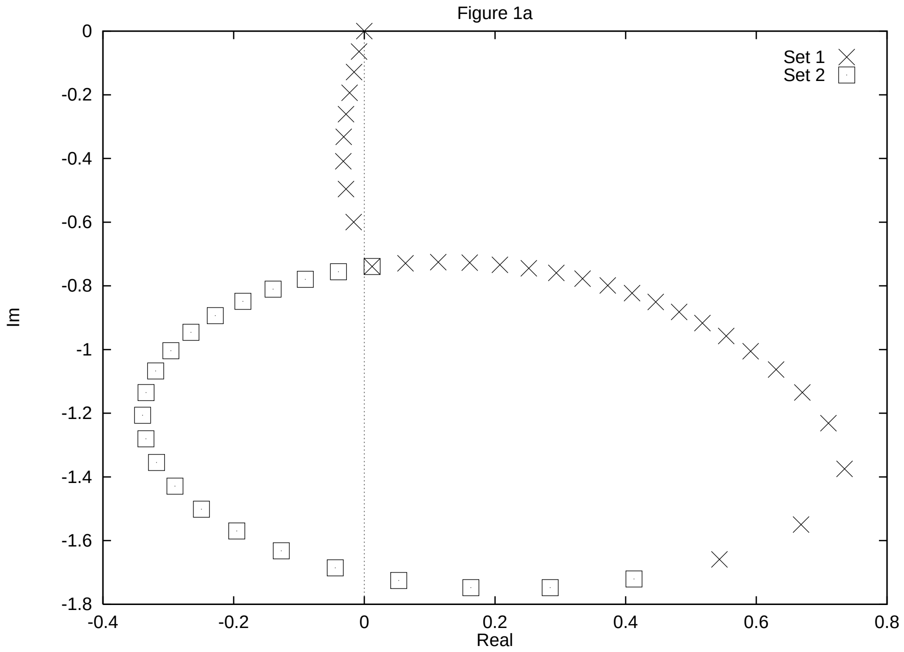
$$\|\mathcal{R}_{\epsilon'} u_\epsilon(\theta)\|_\delta = \|\mathcal{R}_{\epsilon'} u_\epsilon(\theta) - \mathcal{R}_\epsilon u_\epsilon(\theta)\|_\delta \leq |\epsilon' - \epsilon| \|\Delta_\omega^{-1} S(u_\epsilon(\theta) + \theta))\|_\delta$$

Constructing the operator

$$\Phi(f) = -\left[D\mathcal{R}_\epsilon(u_\epsilon)\right]^{-1} \mathcal{R}_{\epsilon'}(f) + f$$

Φ is a contraction in $\| \ \|_\delta$ of a factor $1/2$ in a neighborhood of u_ϵ that can be chosen uniformly for $|\epsilon' - \epsilon|$ sufficiently small. Moreover, since $\|\Phi(u_\epsilon) - u_\epsilon\|_\delta$ can be made as small as desired by choosing $|\epsilon' - \epsilon|$ small enough, we conclude, from the contraction mapping principle, that Φ has a fixed point $u_{\epsilon'}$ for all ϵ' in a neighborhood of ϵ. But a fixed point of Φ is a solution of $\mathcal{R}_{\epsilon'} u = 0$.

$\blacksquare$

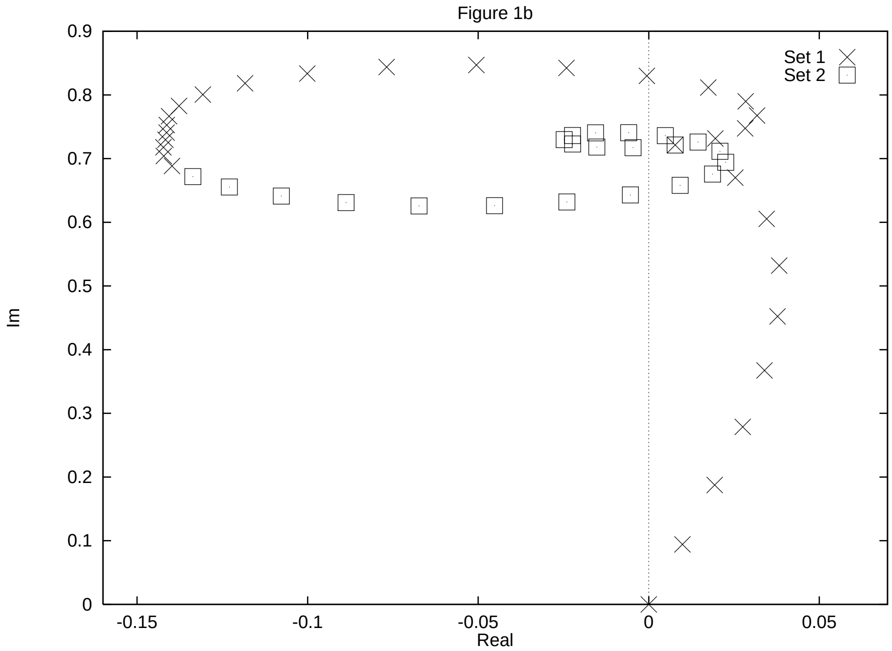


The values of the solution of (3.2) for $\theta = 0.23$ along a path in the complex plane that encircles a particular point twice. Set 1 are the values through the first turn, Set 2 the values through the second turn. After two turns we come back to the original solution. Around point $\epsilon = 0.9 + 2.39i$. $S(q) = \sin(q)$, $\omega = \frac{\sqrt{5}-1}{2} + 0.1i$.

Remark. The above theorem does not apply at values of ϵ where a branch point can occur, since $D\mathcal{R}_\epsilon(u_\epsilon)$ is not invertible at those values.

The Newton method has certain advantages over a perturbative method. A perturbative expansion only converges in a disc of radius bounded by the position of the singularity closest to the origin, and does not give any information on the nature of the singularity. Based on the Newton method, we can perform a continuation method starting from $\epsilon = 0$, when the hull function is $u = 0$, along paths in the complex plane. Initial guesses can be chosen to be either the solutions computed at points nearby or, for small values of ϵ, the Lindstedt series (3.5). On the other hand the Lindstedt series (3.5) provides more global information, that can be used to locate several singular points.

More important for our purposes is that by moving with small steps around a singularity, we can ascertain its nature.



Same as in figure 1a. Around point $\epsilon = 0.56 - 2.85i$. $S(q) = \sin(q) + \sin(3q)$, $\omega = \frac{\sqrt{5}-1}{2} + 0.1i$.

If the singularity was indeed a branch point, by going around a closed loop once, we would move to a different sheet of the Riemann surface. If the branch point was indeed of order 2, going around the closed loop twice would bring us back again to the original point. This prediction has been verified quite unmistakably in figure 1.

Note that the behavior would have been completely different should the singularity have been a pole, a branch point of some other order or an essential singularity.

Note also that, by using the continuation method along paths that wind around the singularities, we could discover the global topology of the Riemmann surface of the function defined by the Lidstedt series. We have not done that systematically since we do not have a clear idea of what we should be expecting and looking for. Nevertheless there are indications that the Riemann surface becomes increasingly complicated for large $|\epsilon|$.

6. Padé Approximations

A Padé approximant of order $[M/N]$ for an analytic function f is a rational function with numerator P of degree at most M and denominator Q of degree at most N whose Taylor expansion agrees with that of f up to order $M+N$. We also impose the normalization condition $Q(0)=1$.

We refer to [BGM], [Gi] for a survey of mathematical results about Padé approximants and applications in problems of Theoretical Physics. They have been used in almost all fields in Physics in which perturbative expansions and their breakdown play a role. Several authors have recently used Padé approximants for perturbative expansions of conjugating functions for invariant curves to estimate domains of analyticity (see [BC], [BCCF], [FL], [BM], [LT1]).

The coefficients of the numerator and denominator of a Padé approximant can be computed by

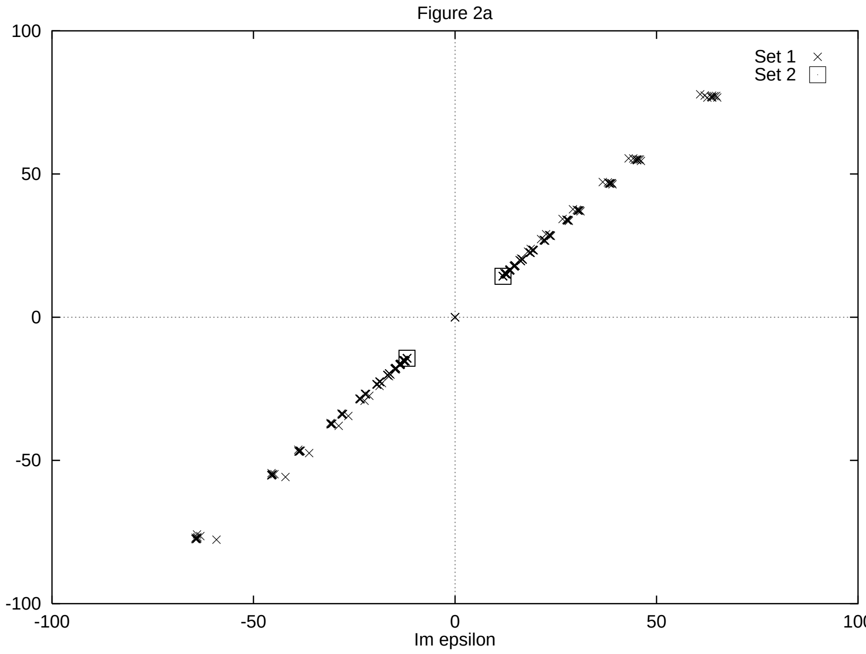
$$f(z) = \frac{P(z)}{Q(z)} + O(z^{N+M+1}), \qquad z \to 0$$

or, equivalently,

$$P(z) = Q(z)f(z) + O(z^{N+M+1}), \qquad z \to 0$$

which results to a linear system of equations for P_i, Q_i.

The standard method to examine the domain of analyticity of f is to compute the poles of the Padé approximants for f and study their behavior. According to our conjecture the domain of analyticity of f includes branch points of order 2. The presence of branch points affects the behavior of Padé approximants in ways that are numerically observable. In [N1] it was shown that for a certain class of functions with an even number of branch points of order 2 the poles and the zeros of the $[N/N]$ Padé approximants accumulate, as $N \to \infty$, along non-intersecting arcs emanating from the branch points. The position of the arcs is completely determined by the positions of the branch points.



The poles and zeros of Padé approximants [25/25] for several values of θ (Set 1) superimposed with the poles of the Padé approximant for the derivative of the logarithm of the derivative of the hull function (u') (Set 2). $S(q) = \sin(q)$, $\quad \omega = \frac{\sqrt{5}-1}{2} + 0.5i$.

Numerical investigations (see [HB1,2]) and a conjecture of John Nutall (see [N2]) suggest that for any function with a finite number of branch points the zeros and the poles of the $[N/N]$ Padé approximants accumulate on arcs emanating from the branch points. Our numerical results support the conjecture (see figures 2, 3).

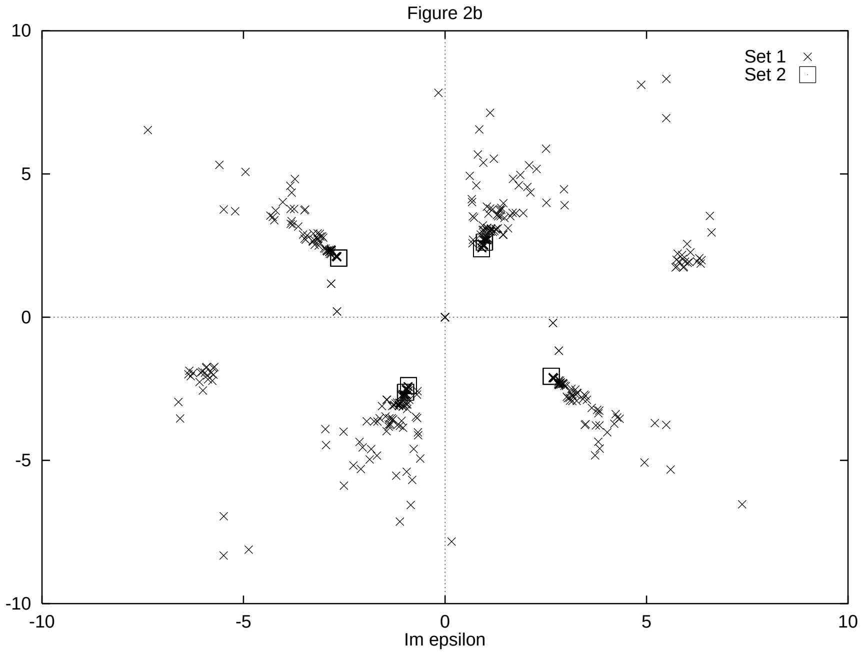
¿From the arguments in section 4, the hull function u_ϵ, for $\mathrm{Im}\,\omega \neq 0$, could have an infinite number of branch points. Notice that the influence of a singularity that is far from the origin, at $z = d_2$, on the n^{th} Taylor expansion coefficient decreases asymptotically like $O(|d_1|^n/|d_2|^n)$, where d_1 is the position of the singularity closest to the origin. In a finite precision computation only singularities close enough to the origin can be detected.

To find experimentally the accuracy necessary to distinguish branch points far from the origin we have computed Padé approximants for functions of the form

$$f(z) = \sqrt{1-\alpha_1 z} + \sqrt{1+\alpha_1 z} + \sqrt{1-\alpha_2 z}, \qquad |\alpha_1| > |\alpha_2|.$$

The $[N/N]$ Padé approximant for f gives no indication of a branch point at $1/\alpha_2$ for α_2

small enough (see figure 4 for $\alpha_1 = 1, \alpha_2 = (5i)^{-1}$) even if we use very high accuracy in the computation of the coefficients.



Same as figure 2a. $S(q) = \sin(q)$, $\quad \omega = \frac{\sqrt{5}-1}{2} + 0.1i$.

7. Improved algorithms based on the nature of the singularities

a) Logarithmic Padé approximants

To locate the position of the singularities we will construct approximants for functions related to the hull function, with different singular behavior. The advantage in altering the nature of the singularities is that certain types of approximants work better for one kind of singular behavior than another. For example, Padé approximants can better approximate functions with poles than functions with branch points.

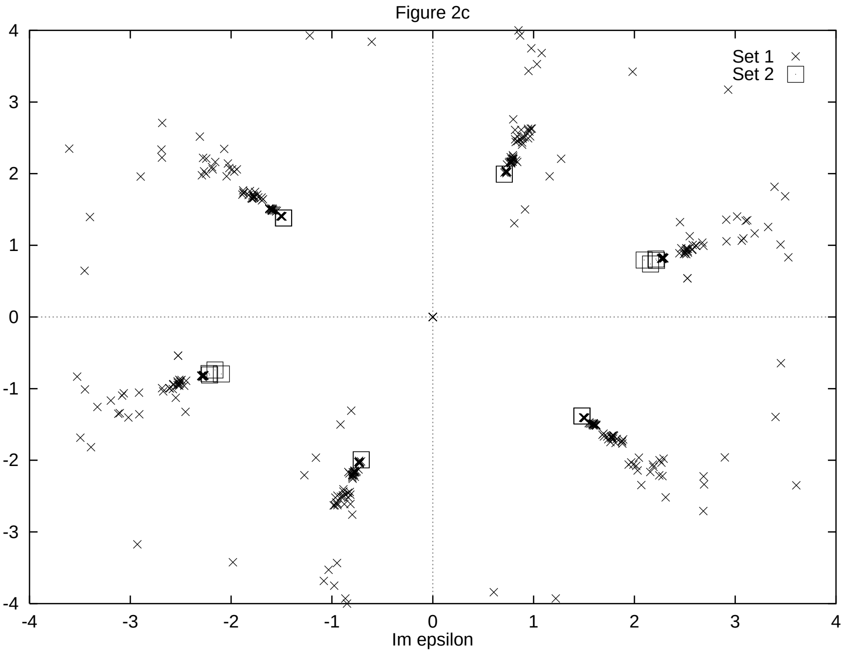
If a function f has a branch point singularity at $z = 1/\alpha$, then

$$f(z) = A(1 - \alpha z)^{\gamma} + g(z) \tag{7.1}$$

for g analytic at $z = 1/\alpha$. If $\gamma < 0$ the contribution from the singularity dominates, and $f(z) \approx A(1-\alpha z)^\gamma$, for z close to $1/\alpha$. Notice that the case $\gamma > 0$ (from our conjecture we expect $\gamma = 1/2$ for the hull function) reduces to $\tilde{\gamma} < 0$ for $\tilde{f} = \frac{d^n f}{dz^n}$, for $\tilde{\gamma} = \gamma - n,\ n > \gamma$. Assuming $\gamma < 0$, we form the function

$$F_1(z) = \frac{d}{dz} \ln f(z) = \frac{f'(z)}{f(z)} \approx \frac{\gamma}{z - \frac{1}{\alpha}}$$

for z close to $1/\alpha$.



Same as figure 2a. $S(q) = \sin(q)$, $\quad \omega = \frac{\sqrt{5}-1}{2} + 0.05i$.

We expect a Padé approximant for $F_1(z)$ to exhibit a pole at $z = 1/\alpha$ with residue γ. To form an $[N/M]$ Padé approximant for F_1 we have

$$F_1(z) = f'(z)/f(z) = P(z)/Q(z) + O(z^{N+M+1}), \qquad z \to 0$$

or, provided $f(0) \neq 0, Q(0) = 1$

$$f'(z)Q(z) = f(z)P(z) + O(z^{N+M+1}), \qquad z \to 0.$$

The coefficients of P, Q can be determined by solving a linear system involving f_n (where $f(z) = \sum_{n=0}^{\infty} f_n z^n$). The location and the residue of the poles of the Padé approximants for F_1 indicate the location and the order of the branch points of f.

Another way to estimate the order of a branch point, once the location $1/\alpha$ is determined from Padé approximants for F_1, is to form Padé approximants for

$$F_2(z) = (z - \frac{1}{\alpha})F_1(z) = (z - \frac{1}{\alpha})\frac{f'(z)}{f(z)} \approx \gamma$$

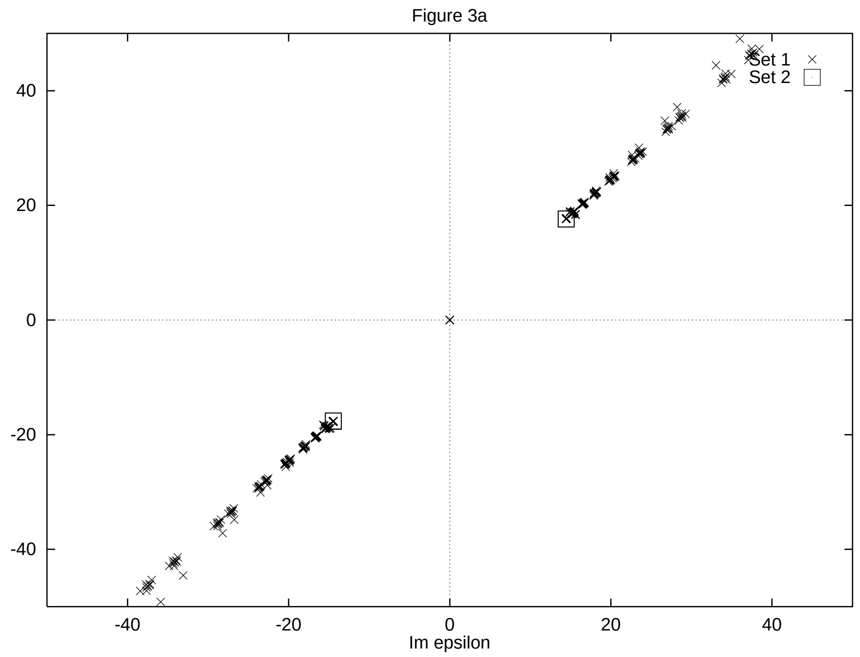
and

$$F_3(z) = \frac{\frac{d}{dz}\ln\left[\frac{df(z)}{dz}\right]}{\frac{d}{dz}\ln f(z)} = \frac{f''(z)f(z)}{f'(z)f'(z)} \approx 1 - \frac{1}{\gamma}$$

The accuracy for γ depends on the accuracy with which the location of the branch point is computed. For a discussion of these methods and applications in which they have been used see [BGM, pg. 55-57], [HB1,HB2].

We point out that the presence of the function g in (7.1) can slow the convergence of Padé approximants for F_1. The reason is that for f as in (7.1)

$$F_1(z) = \frac{\gamma}{z - \frac{1}{\alpha}} + \gamma\alpha(1 - \alpha z)^{-\gamma-1}g(x) + \cdots \tag{7.2}$$

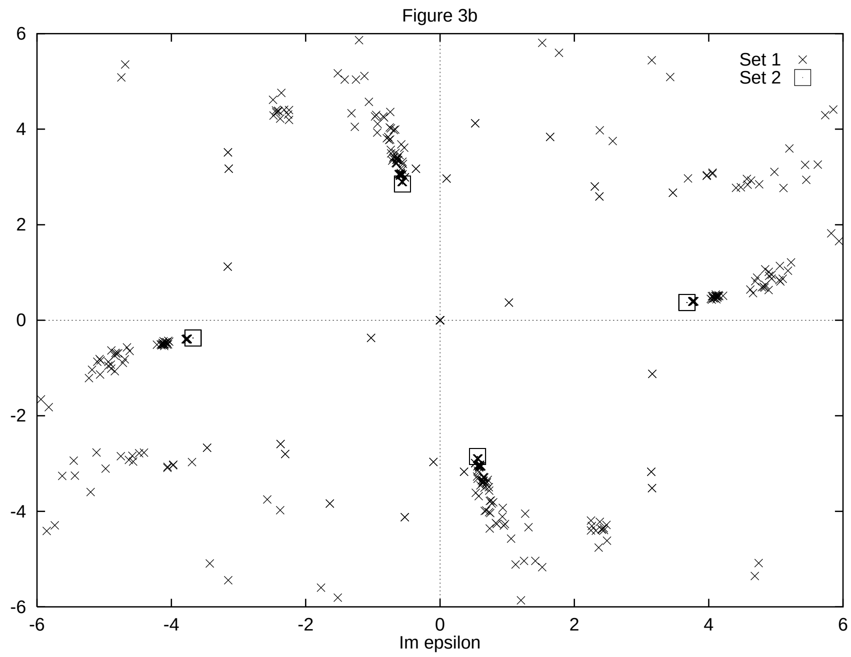


Same as figure 2a. $S(q) = \sin(q) + \sin(3q), \quad \omega = \frac{\sqrt{5}-1}{2} + 0.5i.$

The point $z = 1/\alpha$ is not a simple pole for F_1. We expect the Padé approximant for F_1 to indicate, apart from a pole, the presence of a branch point at $1/\alpha$ and the convergence to γ of $[N/N]$ Padé approximants for $F_2(1/\alpha)$ to be slow. The second term in (7.2) becomes more important for $|\gamma|$ small. We can increase the value of $|\gamma|$ if, instead of working with the function f of (7.1), we work with a high order derivative of f.

b) Ratio method

The ratio method is a well known method (see [HB1, HB2]) that takes advantage of the fact that the coefficients of the Taylor expansion are strongly influenced by the singularity closest to the origin. The existence of additional singularities with distances from the origin close to the radius of convergence greatly reduces the effectiveness of the method.



Same as figure 2a. $S(q) = \sin(q) + \sin(3q), \quad \omega = \frac{\sqrt{5}-1}{2} + 0.1i.$

In the cases we have studied, due to parity properties of S, we expect at least two branch points at the boundary of the domain of convergence of the Taylor expansion of the hull function at positions $\epsilon = \pm 1/\alpha$. To study test functions f with Taylor expansion $f(z) = \sum_{n=0}^{\infty} f_n z^n$, $f(z) = (1-\alpha z)^\gamma + (1+\alpha z)^\gamma, \quad \gamma < 0$ we form the ratios

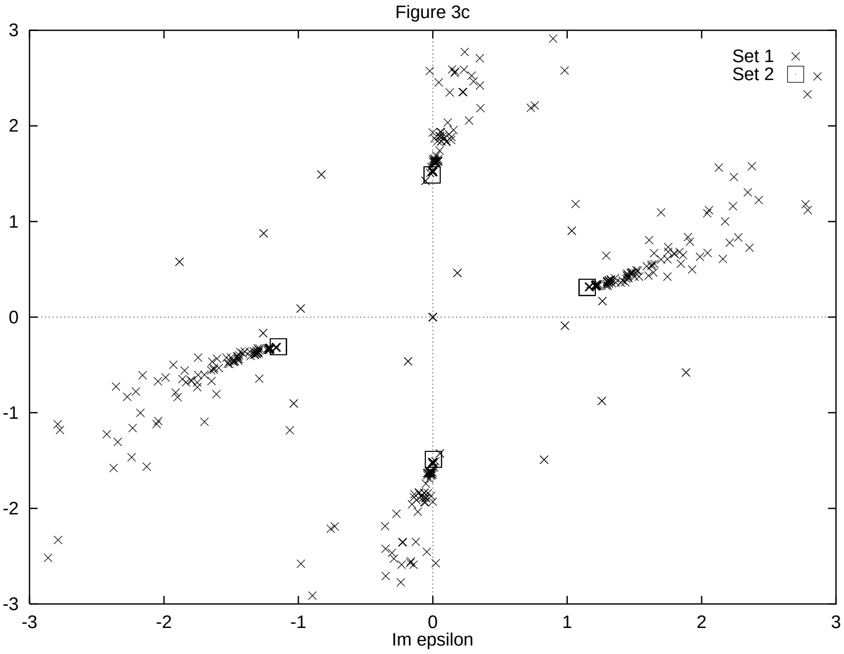
$r_n = f_{2n}/f_{2(n-1)}$ which converge to α^2 with an error of order $1/n$.

We will construct an extrapolation scheme to estimate α more accurately using the ratios r_n. Consider $\xi_n = 2n(2n-1)r_n - (2n-2)(2n-3)r_{n-1}$. Plotting ξ_n versus n gives a straight line with slope $8\alpha^2$ and intercept $-(4\gamma+10)\alpha^2$. Instead of using graphical methods to find the slope and the intercept we construct

$$\mu_n = \frac{1}{8}(\xi_n - \xi_{n-1}) = \alpha^2, \quad \rho_n = -\frac{1}{4}(\frac{\xi_n}{\alpha^2} - 8n + 10) = \gamma \tag{7.3}$$

The value of μ_n can be substituted for α^2 in (7.3), so that both equations (7.3) depend only on the coefficients f_n.

The sequences μ_n, ρ_n converge to α, γ and can be used as independent verification for the predicted value of γ.



Same as figure 2a. $S(q) = \sin(q) + \sin(3q)$, $\quad \omega = \frac{\sqrt{5}-1}{2} + 0.05i$.

If the function f has additional structure, as we expect for the case of the hull function, then corrections of order $1/n$ are introduced to (7.3). Since we expect the formation of a natural boundary in the limit $\mathrm{Im}\,\omega \to 0$ the ratio method is not useful for studying singularities for ω real, diophantine, and in general works only for the singularities closest to the origin. The logarithmic Padé approximants on the other hand provide information for several branch points simultaneously.

8. Numerical implementation and results

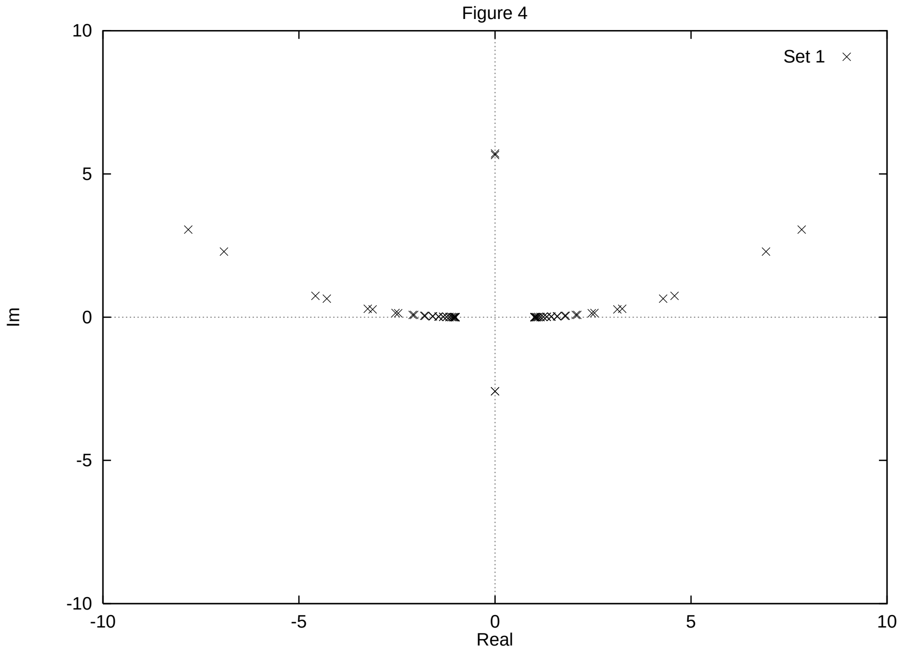
We have used a package we developed (see [LT1]) to manipulate one dimensional Fourier series. The advantage of the package is the ability to change between double and extended precision by changing a definitions file. For the extended precision computations we used the public domain library `PARI/GP`.

In the implementation of the Newton method we truncated the Fourier series representation for the hull function to mode n, for n large

$$u(\theta) = \sum_{k=-n}^{n} \hat{u}_k e^{ik\theta}$$

We checked the computation by verifying that it was converging quadratically. The condition numbers obtained inverting the derivative matrix, were indicative of the proximity to a branch point. The paths we chose encircled the points indicated by the Padé methods several times. Whenever the method failed to converge quadratically due to proximity to a branch point, we increased the size of the Fourier series. Notice that if an initial guess is good enough, the Newton method will converge irrespective of the way the initial guess was chosen.

We computed the coefficients of Padé approximants using Gaussian elimination and obtained condition numbers for the computations. Although recursive methods to compute the Padé approximants exist (see [BGM]) we do not know of any way to assign condition numbers to such computations. The actual routines we used were a translation into `C` of the well known `DECOMP` and `SOLVE` from [FMM]. To find the zeros of the numerator and denominator of Padé approximants we used the routines "`xzroot`", "`zroot`" from [FPTV] translated to be compatible with the use of extended precision arithmetic. Although, for Padé approximants in general, the residue of a pole is indicative of its significance, in the case of functions with branch points one expects zeros and poles to lie close together, resulting in large condition numbers and poles with small residues. The condition numbers for computing the coefficients of logarithmic Padé approximants were much smaller than the ones for straightforward Padé approximants.



The poles and the zeros of the [35/35] Padé approximant to $f(z) = \sqrt{1-z} + \sqrt{1+z} + \sqrt{1-\frac{z}{5i}}$. Computations performed with 60 digit accuracy.

An independent check of the accuracy of our computations is the symmetry of the branch points. If ϵ is a branch point, so is $-\epsilon$ but this symmetry is not built into our numerical method, thus can be used as an estimate of the accuracy of the computations.

Our numerical results are consistent with the predictions of section 4. We investigated two standard-like maps, $S_1(q) = \sin(q), S_2(q) = \sin(q) + \sin(3q)$. Straightforward Padé approximants for the hull function exhibited poles and zeros along lines emanating from distinct points. Logarithmic Padé approximants to the derivative of the hull function (we used the derivative of the hull function so that, asymptotically close to the singularities $u(\epsilon) \approx A(1 - \frac{\epsilon}{\epsilon_0})^{-\frac{1}{2}}$) exhibited poles at locations consistent with the locations indicated by the accumulation of poles and zeros of Padé approximants (see figures 2, 3). The residue of the poles, computed both from logarithmic Padé methods and the ratio method, was within 10% of the predicted value $-1/2$ as indicated in table 1. The results of the numerical continuation based on the Newton method support the existence of an isolated branch point of order 2, within the path followed (see figure 1).

Table 1

	α	β	γ	δ
Residue(F_2)	$-0.53-0.002i$	$-0.53-0.001i$	$-0.56-0.01i$	$-0.56-0.02i$
Residue(F_3)	$-0.52-0.001i$	$-0.52-0.001i$	$-0.56-0.02i$	$-0.56-0.02i$
Residue(ρ)	$-0.500+10^{-7}i$	$-0.500+10^{-6}i$	—	—
Position(μ)	$11.886+14.32i$	$14.47+17.645i$	$0.9+2.4i$	$0.6-2.9i$

Table 1: Residues and positions of branch points in the domain of analyticity. The positions of the points $\alpha, \beta, \gamma, \delta$ are computed from the F_1 Padé approximants. The digits reported are accurate for each method apart from the last digit.
$\alpha = 11.889 - 14.320i,\ \omega = \frac{\sqrt{5}-1}{2} + 0.5i,\ S(q) = \sin(q)$
$\beta = 14.450 + 17.649i,\ \omega = \frac{\sqrt{5}-1}{2} + 0.5i,\ S(q) = \sin(q) + \sin(3q)$
$\gamma = 0.906 + 2.39i,\ \omega = \frac{\sqrt{5}-1}{2} + 0.1i,\ S(q) = \sin(q)$
$\delta = 0.56 - 2.85i,\ \omega = \frac{\sqrt{5}-1}{2} + 0.1i,\ S(q) = \sin(q) + \sin(3q)$

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10. References

[A] S. Aubry: The twist map, the extended Frenkel-Kontorova model and the devil's staircase. Physica D **7**, 240–258 (1983).

[AB] S. Abenda, A. Bazzani: Singularity analysis of 2D complexified hamiltonian systems. U. of Bologna preprint

[BC] A. Berretti, L. Chierchia: On the complex analytic structure of the golden invariant curve for the standard map. Nonlinearity **3**, 39–44 (1990).

[BCCF] A. Berretti, A. Celletti, L. Chierchia, C. Falcolini: Natural boundaries for area preserving twist maps. Jour. Stat. Phys. **66**, 1613–1630 (1992).

[BGM] G. Baker, M. Graves–Morris: "*Padé Approximants*", Addison Wesley (1981).

[BM] A. Berretti, S. Marmi: Standard map at complex rotation numbers: Creation of natural boundaries. Phys. Rev. Lett. **68**, 1443–1446 (1992).

[BMT] L. Billi, M. Malavasi, G. Turchetti: Natural boundaries of normalizing transformations. U. of Bologna preprint.

[BT] A. Bazzani, G. Turchetti: KAM theory of normalizing transformations for complexified area preserving maps. U. of Bologna preprint.

[CC] A. Celletti, L. Chierchia: Construction of analytic K.A.M. surfaces and effective stability bounds. Comm. Math. Phys. **118**, 119–161 (1988).

[Ch] B. V. Chirikov: A universal instability of many-dimensional oscillator systems. Phys. Rep. **52**, 263–379 (1979).

[ChH] S. N. Chow, J. K. Hale: "*Methods of Bifurcation Theory*", Springer–Verlag, New York (1982).

[F] A. Fathi: Une interprétation plus topologique de la démonstration du théoreme du

Birkhoff. Appendix to [H].

[FL] C. Falcolini, R. de la Llave: Numerical calculation of domains of analyticity for perturbation theories in the presence of small divisors. Jour. Stat. Phys. **67**, 645–666 (1992).

[FMM] G.E. Forsythe, M.A. Malcolm, C. E. Moler: "*Computer methods for mathematical computations*", Prentice Hall, Englewood Cliffs (1977).

[FPTV] W.H. Press, B.P. Flannery, S. Teukolski, W. T. Vetterling: "*Numerical Recipes*", Cambridge Univ. Press, Cambridge (1986).

[Gi] J. Gilewicz: "*Approximants de Padé*", Springer–Verlag (1978).

[Gr] J. M. Greene: A method for determining a stochastic transition. J. Math. Phys. **20**, 1183–1201 (1979).

[GS] M. Golubitsky, D. G. Schaeffer: "*Singularities and groups in bifurcation theory, vol. 1*", Springer–Verlag, New York (1985).

[H] M. R. Herman: Sur les courbes invariantes par les difféomorphismes de l'anneau. Astérique **103–104**, (1983).

[HB1] D.L. Hunter, G.A. Baker: Methods of Series Analysis I. Comparisons of current methods used in the theory of critical phenomena. Phys. Rev. B **7**, 3346–3376 (1973).

[HB2] D.L. Hunter, G.A. Baker: Methods of Series Analysis II. Generalized and extended methods with application to the Ising model. Phys. Rev. B **7**, 3377–3392 (1973).

[LR] R. de la Llave, D. Rana: Accurate strategies for K. A. M. bounds and their implementation. In "*Computer Aided proofs in Analysis, K. Meyer, D. Schmidt ed.*". Springer Verlag (1991).

[LT1] R. de la Llave, S. Tompaidis: Computation of domains of analyticity for some perturbative expansions from mechanics. Physica D **71**, 55–81 (1994).

[LT2] R. de la Llave, S. Tompaidis: Nature of singularities for analyticity domains of invariant curves. (Preprint available from `mp_arc@math.utexas.edu` # 94-137.

Submitted).

[McK] R.S. McKay: Renormalization in area preserving maps. Princeton thesis (1982).

[N1] J.N. Nuttall: The convergence of Padé approximants to functions with branch points. In "*Padé and rational approximation, E.B. Saff, R.H. Varga (eds.)*". Academic Press, New York 101–109 (1977).

[N2] J.N. Nuttall: Letter to Stathis Tompaidis, dated January 8, 1993.

[Po] H. Poincaré: "*Les methodes nouvelles de la méchanique céleste*", Gauthier Villars, Paris (1891–1899).

[R] D. Rana: Proof of accurate upper and lower bounds to stability domains in small denominator problems. Princeton thesis (1987).

[Rudin] W. Rudin: "*Functional analysis*", McGraw Hill (1973).

[SM] C. L. Siegel, J. Moser: "*Lectures on Celestial Mechanics*", Springer-Verlag, New York (1971).