COMPUTATION OF DOMAINS OF ANALYTICITY FOR SOME PERTURBATIVE EXPANSIONS OF MECHANICS

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To the memory of J.L. Tennyson

Abstract. We compute the domain of analyticity of some perturbative expansions for invariant circles appearing in mechanics. We use Padé approximants for the perturbative expansions and introduce methods to ascertain their domain of convergence. We also use non-perturbative methods based on direct computation of the invariant circles and, in analogy with Greene's criterion, approximation by circles with rational rotation. We find that the domains computed by all the methods agree within the limits of accuracy. We also study rigorously the nature of the singularities when the frequency is rational.

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1. Introduction

The long term behavior of deterministic systems is very often studied by finding landmarks that organize the dynamics. Among them, ones with very drastic effect are invariant circles. For example, if the phase space of the system is two dimensional, existence of an invariant circle implies long term stability. It is, therefore, not surprising that there has been a lot of effort devoted to the computation of such objects.

One of the first algorithms to approximate the circles and still widely used is the Poincaré–Lindstedt method (see, e.g., [Po], §123 ff. or [RA] for a computer implementation) which consists on finding recursively the coefficients of an expansion of a parametrization of the invariant circle in powers of a small parameter.

One should notice that the study of the sense in which these series are valid is rather subtle (see e.g., [Po], §146 for examples of divergence, §122 for different concepts of "convergence").

Given the practical importance of those invariant circles, it is interesting to investigate the actual domains of analyticity of the functions defined by those series. This can give a measure of confidence on approximate calculations and, one could hope, also shed some light on the scenarios for the breaking up of the validity of the conclusions drawn from perturbation theory.

Similar problems appear frequently in theoretical physics, for example in statistical mechanics when the boundaries of the domain of analyticity of functions defined perturbatively — e.g. by low temperature expansions — correspond to phase transitions. Therefore, besides their intrinsic interest, Lindstedt series can be considered as a useful model for other series in theoretical physics such as low temperature perturbative expansions. In this context, one should remark that there is considerable evidence that the phenomena happening at breakdown of Lindstedt series are very similar to those happening at breakdown of other series in that both of them can be interpreted as phase transitions whose main analytical features can be described and predicted with the help of a renormalization group picture. (See e.g., [McK1].)

We point out that in the case that the invariant circles are "normally hyperbolic" — in particular attractive — there is a well developed theory to prove convergence of the expansions [Fe]. In other cases, convergence can be proved using the much subtler

K.A.M. theory (see [Ze1], [Ze2], [Bo] for surveys). The latter is the usual case in the dynamical systems arising in classical mechanics as hamiltonian perturbations of integrable systems. Unfortunately, in both cases the practical domains established by these theories are very conservative (much more so in the case of K.A.M. theory) and throw little light on the behavior to be expected at breakdown.

Recently, in [BC], [BCCF] it was proposed that for some of these series arising in classical mechanics, one could compute the zeros of the denominator of the Padé approximant as a reasonable approximation to the domain of analyticity. This procedure, which we will call henceforth *the Padé method* has been widely used in theoretical physics [BGM].

Unfortunately, the Padé method, even if successful in practice, does not have a complete mathematical justification. Moreover, for the series appearing in celestial mechanics, frequently the size of the coefficients of the perturbative expansion vary widely in an erratic fashion. This makes the numerical computation of Padé approximants difficult and throws doubt about the validity of the final result. One verification of the Padé method by comparing its results with those of other methods was undertaken in [FL1]. In that paper, the Padé method was applied to models similar to those considered in [BCCF] and the results were compared with those obtained by using a complex version of Greene's method (a partial justification of this criterion can be found in [FL2], [McK2]). The agreement obtained using the two methods was quite encouraging.

In this paper, we have extended the comparison of the Padé method with other independent methods, some of them based in perturbative expansions and others completely non-perturbative.

We have considered models which are not conservative for which we have computed the perturbation expansions and applied the Padé method. Besides looking for the zeros of the denominator of Padé approximants, we have explored other methods of ascertaining the domain of analyticity of the Padé approximants. We have also used non-perturbative methods to compare to the methods based on the study of the perturbative expansions. Some of the non-perturbative methods we have used are based on the fact that the map is dissipative, which makes it easy to compute invariant sets. We have also proved an analogue of a partial justification of Greene's criterion that makes it reasonable that the domains of analyticity for an invariant circle can be approximated by those computed using rational frequencies. In that case, the nature of the singularities can be described in detail. Assuming a well known conjecture, this singularity structure explains the behavior of the Padé approximants that we found.

The main reason to use dissipative systems in our study is that for them it is possible to locate the invariant tori by direct iteration and follow them by non perturbative methods. Besides the intrinsic interest of these dissipative systems — they are reasonable models of some physical systems — they can be used to provide some insight on the Poincaré–Lindstedt series for Hamiltonian systems. A first, heuristic, argument is that the structure of the series is very similar — in the dissipative case however, they are more stable to compute numerically. Also one can argue heuristically that at the point at which the invariant circle breaks down, the invariant circle has lost its hyperbolicity so that — using the fact that our system can only have one non-zero Lyapunov exponent — in an infinitesimal neighborhood, the system looks like an area preserving system, so one could hope that some of the results obtained about the behavior at breakdown of circles would also apply to hamiltonian systems (of course the argument carries no weight for dynamical behaviors that in the neutral case are controlled by subdominant terms). Indeed it has been argued [R] that the renormalization group picture developed for the breakdown of invariant circles in hamiltonian systems can be extended to dissipative systems, if one scales the dissipation appropriately.

The paper is organized as follows : in section 2 we introduce the system we will study throughout, the rotating logistic map. In section 3 we describe a perturbative method, based on the Poincaré–Lindstedt method, to compute the invariant curve of the system as an expansion in a parameter. In sections 4-7 we turn to the question of determining the domain of analyticity of the expansions computed in section 3. In section 4 we introduce the Padé method, as has been used in the literature so far (see [BM], [FL2]). In section 5 we discuss several refinements of the method based on the nature of the nature of the singularities we expect. In section 6 we deviate from the presentation of methods based on Padé approximants in order to present a way to obtain an expression for the invariant curve at different points using a Newton method in the space of analytic functions. In section 7 we use multipoint Padé approximations (see [BGM] vol.2, p.7). These approximations require to interpolate the functions and derivatives at separate values of the parameter. The functions at these values are computed using the Newton method and are, hence, non-perturbative. In section 8 we describe a non-perturbative method to estimate the domain of existence of the invariant curve. In section 9 we prove an analog of Greene's criterion that serves as justification for approximating the domain of analyticity of the invariant curve for irrational frequencies with the limit of the domain of analyticity for rational frequencies. We point that for the case of rational frequencies, we can use the theory of iteration of polynomials to describe the nature of the singularities that appear. Finally in section 10 we discuss the numerical implementation of the algorithms introduced in the previous sections.

The results of our exploration are summarized in figures 1, 3, 4, 9. We find it quite encouraging that so different methods give similar results, which seem to be within reasonable estimates of the margin of error for each of them. The methods that seem to be the easiest to use and produce the more reliable results for our system seem to be the non-perturbative methods described in section 8.

2. Notation and Preliminaries.

We have considered the analyticity properties of Lindstedt series for one particular model that we will, henceforth refer to as the "rotating logistic map".

$$F_{\epsilon,\lambda,\omega}(r,\theta) = (f_{\epsilon,\lambda}(r,\theta),\ \theta + \omega \bmod 1) = (r^2 + \lambda + \epsilon\cos(2\pi\theta),\ \theta + \omega \bmod 1) \tag{2.1}$$

where r is taken to be a complex variable, $\theta \in I_\delta = \{\theta \big| \, |\mathrm{Im}\,\theta| < \delta\}$ a complex variable, λ, ω real parameters, and ϵ a complex parameter.

In most of this paper we will consider λ, ω as fixed and explore the dependence on ϵ of the invariant circle. Hence, when it is not needed, we will suppress λ, ω from the notation for the map. Only in section 9 we will consider the dependence in ω.

Notice that for $\epsilon = 0$ (2.1) reduces to the well known logistic map, which is well known to exhibit a very rich behavior. A fixed point r_0 for the logistic map becomes an invariant circle $\{r_0\} \times \mathbf{T}^1$ for $F_{0,\lambda,\omega}$, filled by dense orbits if ω is irrational, or consisting of a family of periodic orbits for ω rational.

Notice that (2.1) with ω irrational can be considered as a quasi-periodic excitation of the usual logistic map. Hence, it can appear as a physically reasonable model in all of the situations where the logistic map appears, if we assume that they are modified by an external quasi-periodic force.

As the parameters λ, ϵ vary, this map exhibits a large variety of behaviors and bifurcations (suffice it to mention that for $\epsilon = 0$ it exhibits a Feigenbaum cascade of period doublings). A study of the bifurcation diagrams for invariant tori was undertaken in [Ka] and in [AKL1] and there one can find detailed descriptions of breakdown behavior for certain regions of parameters. In [AKL1] only real values of the parameters are considered. If we consider complex values of the parameters, some bifurcations that do not appear in the real case, such as period n-tupling, $n > 2$, become possible. Indeed, they happen in the quadratic family for certain complex values of λ. A K.A.M. argument similar to those in [AKL1], [CI] can show that such behaviors persist for sufficiently small values of ϵ.

We will consider only λ's real and somewhat smaller than the value for which the first period doubling bifurcation occurs, which the work of [AKL] suggests as not having any other bifurcation as ϵ changes till breakdown. This hypothesis is also verified by our calculations, since we compute the invariant circle for all the values of ϵ for which it exists, very close to the value for which it breaks down, and we verify that the mechanism of destruction is very different from the simple n-tupling bifurcations.

3. Lindstedt expansions

Following standard practice in Lindstedt methods, we observe that the graph of a map $u_\epsilon : \mathbb{T} \to \mathbb{R}$ is invariant under the map (2.1) if and only if it satisfies

$$u_\epsilon(\theta + \omega) = \big[u_\epsilon(\theta)\big]^2 + \lambda + \epsilon \cos 2\pi\theta. \tag{3.1}$$

If we now assume an expansion in powers of ϵ, $u_\epsilon(\theta) = \sum_{n=0}^{\infty} \epsilon^n u^n(\theta)$ and substitute it in (3.1) we obtain:

$$\begin{aligned} &u^0(\theta + \omega) = u^0(\theta)^2 + \lambda \\ &u^n(\theta + \omega) = 2u^0(\theta)u^n(\theta) + \sum_{m=1}^{n-1} u^{n-m}(\theta)u^m(\theta) + \delta_{n,1}\cos(2\pi\theta), \quad n > 0 \end{aligned} \tag{3.2}$$

where $\delta_{n,1}$ is the usual Kronecker symbol.

We claim that the first equation in (3.2) admits the two solutions $u^0(\theta) = u^0 = \frac{1}{2} \pm \frac{1}{2}\sqrt{1 - 4\lambda}$ and no other continuous solution if $\lambda \in (-\frac{3}{4}, \frac{1}{4})$.

Moreover, once we choose one of the two solutions for the first equation, the second hierarchy of equations allows the recursive determination of all the u^n's.

In effect, if (3.2) is to hold,

$$u^0(\theta + n\omega) = \ell_\lambda^n\big(u^0(\theta)\big)$$

where ℓ_λ denotes the logistic map $\ell_\lambda(x) = x^2 + \lambda$. For the values of the parameter selected, it is well known — see e.g. [G] — that all bounded orbits of ℓ_λ, except those starting in $\frac{1}{2} + \frac{1}{2}\sqrt{1-4\lambda}$ and its preimages, converge to $\frac{1}{2} - \frac{1}{2}\sqrt{1-4\lambda}$. Since θ is an accumulation point of $\theta + n\omega$, it follows that $u^0(\theta)$ should be either one of the two fixed points. If the function u^0 is to be continuous, then it should be constant.

To prove the second assertion, we observe that if we recursively assume that $u^0, \ldots, u^{n-1}$ are known we can determine u^n by solving an equation of the form

$$u^n(\theta + \omega) - 2u^0 u^n(\theta) = R^n(\theta) \tag{3.3}$$

Such equations can be conveniently analyzed using Fourier series. Setting:

$$u^n(\theta) = \sum \hat{u}^{n,k} e^{2\pi i k \theta}$$

and similarly for R, and other periodic functions, the unique solution of (3.3) is given by :

$$\hat{u}^{n,k} = \hat{R}^{n,k} \big/ (e^{2\pi i k \omega} - 2u^0). \tag{3.4}$$

We note that for the rotating logistic map it is easy to prove by induction that the solutions u^n of (3.2) are trigonometric polynomials with degree$(u^n) = n$. Hence, the R^n's are also trigonometric polynomials.

A similar argument would show that provided that the forcing term is a trigonometric polynomial in θ, then the u^n's are also trigonometric polynomials and the degree of u^n is a linear function of n.

To discuss convergence, it is convenient to adopt a more general point of view that will also turn out to apply to the case when the forcing term is a periodic function of θ rather than just a trigonometric polynomial.

We note that, when $\lambda \in (-\frac{3}{4}, \frac{1}{4})$, $|2u^0| \neq 1$ hence $(e^{2\pi i k\omega} - 2u^0)$ is bounded away from zero uniformly in $k \in \mathbb{Z}$ so that

$$\sup_{k\in\mathbb{Z}} |e^{2\pi i k\omega} - 2u^0|^{-1} \leq K \tag{3.5}$$

Hence, $|\hat{u}^{n,k}| \leq K|\hat{R}^{n,k}|$. So that, if we assume $|\hat{R}^{n,k}| \leq Ae^{-\delta|k|}$ we would obtain $|\hat{u}^{n,k}| \leq KAe^{-\delta|k|}$ so that, for example, if R is analytic in a certain domain, $\{\theta \mid |\mathrm{Im}\,\theta| < \delta\}$ so will be u.

Moreover, it is very easy to estimate the recursion to obtain convergence.

Lemma 3.1. *If $|\epsilon| < \frac{1}{2}K^{-2}e^{-2\pi\delta}$ (where K is as in (3.5)), the series obtained by summing the u^n's obtained by (3.2) converges uniformly on $\{\theta \mid |\mathrm{Im}\,\theta| < \delta\}$.*

Proof. For $\delta > 0$, if f is an analytic function on the unit circle, we can expand it in Fourier series, $f(\theta) = \sum \hat{f}^k e^{2\pi i k\theta}$. We denote by $\|f\|_\delta = \sup e^{\delta|k|}|\hat{f}^k|$. It is well known that this defines a norm on a Banach space of analytic functions. We denote such space by $C^{\omega,\delta}$. We observe that $\|f \cdot g\|_\delta \leq \|f\|_\delta \|g\|_\delta$ and that if u^n and R^n are related as in (3.4), then $\|u^n\|_\delta \leq K\|R^n\|_\delta$.

We also observe that $R^1(\theta) = \cos 2\pi\theta$ so that $\|u^1\|_\delta \leq \frac{1}{2}Ke^{2\pi\delta}$.

The recursion part of (3.2) implies for $n > 1$

$$\|u^n\|_\delta \leq K\|R^n\|_\delta \leq K \sum_{m=1}^{n-1} \|u^{n-m}\|_\delta \|u^m\|_\delta. \tag{3.6}$$

By induction, it is easy to show that

$$\|u^i\|_\delta \leq \frac{\sigma_i}{K}\Big(\frac{K^2e^{2\pi\delta}}{2}\Big)^i, \qquad i \geq 1$$

where $\sigma_1 = 1$, $\sigma_k = \sum_{j=1}^{k-1} \sigma_j \sigma_{k-j}$. This is certainly true for $i = 1$ and the recursive bound (3.6) shows that if it is true for $i \leq n-1$ it is true for $i = n$. We see that if we denote

$$\sigma(z) = \sum_{i=1}^{\infty} \sigma_i z^n$$

then $\sigma(z)$ is a solution of $\sigma(z) = \sigma(z)^2 + z$. Since $\sigma(z)$ also satisfies that $\sigma(0) = 0$, $\sigma_0 = 0$, we conclude that $\sigma(z) = \frac{1}{2} - \frac{1}{2}\sqrt{1 - 4z}$ and

$$\sigma_1 = 1, \quad \sigma_n = \frac{1}{n}\binom{2n-2}{n-1} \leq \frac{4^{n-1}}{n}, \qquad n \geq 2.$$

This shows that $\sum_0^\infty u^n(\theta)\epsilon^n$ converges in the $\| \quad \|_\delta$ sense and proves the statement of Lemma 3.1.

$\blacksquare$

Remark. We point out that results similar to Lemma 3.1 can be proved as corollaries of the general theory of stability for normally hyperbolic manifolds. We also point out that the domain of applicability of these results converges to zero as λ converges to $-\frac{3}{4}$, the value at which the logistic map experiences the first period doubling bifurcation. By using the much more subtle K.A.M. theory it is possible to show that if ω is Diophantine, one can get domains of convergence which are uniform in $\lambda \in [\lambda_-, \lambda_+]$ where λ_-, λ_+ are some numbers that contain the bifurcation point. We refer to [AKL2] or [CI] for details of this theory.

Remark. The use of the norms $\| \quad \|_\delta$ in the above proof is natural in view of the fact that, for fixed ϵ, the maximal domains of analyticity in θ for $u_\epsilon(\theta)$ are of the form $\{\theta \mid |\mathrm{Im}\,\theta| < \delta\}$. This can be seen by observing that if u_ϵ is defined for some θ, then it is also defined using (3.1) for $\theta + \omega$. So that the domains of analyticity in θ of $u_\epsilon(\theta)$ have to be invariant under irrational translation.

To study numerically the domain of analyticity of the map $\epsilon \mapsto u_\epsilon$, that is the domain in ϵ for which u_ϵ is analytic, it is easy to study the domain of analyticity of maps $\epsilon \mapsto \Gamma[u_\epsilon]$, where Γ is an entire map from the space of analytic 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. Some observables that immediately come to mind are the evaluation of the function at certain values and the Fourier coefficients. We conjecture that indeed, these simple observables give the correct domain of analyticity.

Conjecture 3.2. *For a fixed $\lambda \in (-3/4, 1/4)$, ω irrational, $\theta \in \mathbb{R}$, the function*

$\epsilon \to u_\epsilon(\theta)$ is defined in a domain D independent of θ. This domain agrees with the domain of analyticity of $\epsilon \mapsto \hat{u}^k_\epsilon$.

To justify Conjecture 3.2 we see that if, for a fixed θ, the function $\epsilon \to u_\epsilon(\theta)$ can be defined in a certain domain $D(\theta)$, (3.1) shows that $\epsilon \to u_\epsilon(\theta + \omega)$ can be defined in a domain that is at least as big. Therefore $D(\theta) \subset D(\theta + \omega)$. In our case, however, we expect that $D(\theta) = D(\theta + \omega)$ since the only way that the domain of analyticity $D(\theta + \omega)$ could actually be bigger than $D(\theta)$ is by using that the function $u \to u^2 + \lambda$ is not invertible and can transform certain singularities into analytic functions. Such behavior seems unlikely, especially in view of our numerical computations.

Notice that the argument for Conjecture 3.2 uses heavily that ω is irrational and, if ω were rational, the domain does depend on θ. (See section 9 for a discussion of analyticity domains in the case that the frequency is rational.) Also, if the system we consider is not (2.1) but had special symmetries that force all the coefficients in the expansion to have odd parity, the function $u_\epsilon(\theta)$ vanishes identically at certain values of θ, hence is trivially entire in ϵ for those values.

Our computations are also evidence that the analyticity domain of all the observables mentioned in Conjecture 3.2 are the same, so that it is a reasonable conjecture that they agree with the domain of analyticity of $\epsilon \mapsto u_\epsilon$.

4. Padé Approximations

We recall that a Padé approximant of order $[M/N]$ to an analytic function S is a rational function with numerator P of degree M and denominator D of degree N whose Taylor expansion up to order $M + N$ agrees with that of S.

We can assume without loss of generality that $D(0) = 1$. If we impose this normalization, under mild non-degeneracy conditions, the Padé approximant of order $[M/N]$ exists and is unique.

We refer to [B], [BGM], [M], [Gi] for a survey of mathematical results about Padé approximants and their applications in problems of Theoretical Physics. They have indeed been widely used in almost all fields in Physics in which perturbative expansions and their breakdown play a role.

If the Taylor expansions of $S(\epsilon)$ and of $P(\epsilon)/D(\epsilon)$ are to match up to order ϵ^{N+M} we can write $S(\epsilon)D(\epsilon) = P(\epsilon) + O(\epsilon^{N+M+1})$ which, together with the normalization $D(0) = 1$, leads to the equations

$$
\begin{aligned}
P_i &= S_i + \sum_{j=1}^{\min(N,i)} S_{i-j} D_j \qquad 0 \le i \le M \\
0 &= S_i + \sum_{j=1}^{\min(N,i)} S_{i-j} D_j \qquad M < i \le M+N
\end{aligned}
\tag{4.1}
$$

Notice that the second set the equations involves only the D's and that once we know the D's, by substitution in the first set of equations, it is possible to compute the P's.

There are other computationally more efficient methods to compute Padé approximants based on recursions (see e.g., [BGM] vol. 1, p.66). Nevertheless, the algorithm sketched above has the advantage that, by using careful standard numerical analysis routines we can obtain condition numbers that give a measure of the reliability of the calculations. We will give more details in the section devoted to numerical implementations.

The standard method to compute the domain of analyticity of $S(\epsilon)$ based on Padé approximants consists in computing D and P as before. One then expects that the boundary of the domain of analyticity for S will be approximated by the poles of P/D. That is, the zeros of D which are not zeros of P (or at least zeros of a smaller order). This is expressed in the following quote ([Gi], p. 310):

"Tous les theorèmes de convergence des approximants de Padé, ainsi que les resultats numériques indiquent que ces approximants ont une tendence visible á reproduire les proprietés d' analycité d' une fonction."

5. A new method to compute domains of analyticity from Padé approximants.

The usual method of computing domains of analyticity of functions is just to compute the zeros of the denominator of the Padé approximation. Unfortunately, the calculation of zeros of a polynomial frequently has large condition numbers (see [Wi] for some examples, [He] for a discussion of algorithms). This is particularly unfortunate since the calculation of Padé approximants out of the coefficients in the expansion is also very ill conditioned.

The previous remarks are especially true for the zeros which are not close to the origin. The elementary example – which we learned from G. Baker –

$$S(\epsilon) = \frac{1}{\epsilon - a_1} + \frac{1}{\epsilon - a_2} = \sum_{n=0} \epsilon^n \left(\left(\frac{1}{a_1}\right)^{n+1} + \left(\frac{1}{a_2}\right)^{n+1} \right)$$

shows that the information about the outermost pole is hidden in the high precision part of the coefficients of the expansion. For many of the perturbation expansions in classical mechanics, whose terms alternate widely in sizes, this seems particularly dangerous.

Since the number of zeros of the denominator is roughly half the degree of $S(\epsilon)$ (in practice considerably less since sometimes the zeros of the numerator are also zeros of the denominator) it is clear that it is not very easy to obtain a very detailed picture of the boundary since the condition number for the computation of zeros worsens very fast with the number of zeros.

In the expansions in celestial mechanics such as the Lindstedt method, we can take advantage of the presumed fact that when the frequency is irrational the domain of analyticity should be independent of θ, to do several calculations and obtain significantly more points in the boundary. Such enhancement is not available for most of the situations to which Padé approximants are applied.

We state the following conjecture:

Conjecture 5.1. *Let f be one of the functions appearing in the Poincaré-Lindstedt expansions. Then, f is analytic in a topological disc $\mathcal{D} \subset \mathbb{C}$ with a natural boundary for f and the sequence of $[N/N]$ Padé approximants converges to f in measure, as $N \to \infty$, on any compact subset of $\mathcal{D}$.*

We recall that a function f has a natural boundary $\mathcal{B}$ if we cannot analytically continue f across $\mathcal{B}$. Also a series of functions $\{f_n\}_{n=0}^{\infty}$ converges in measure in a domain $\mathcal{D} \subset \mathbb{C}$ to a function f in $\mathcal{D}$ if for every $\epsilon > 0$

$$\lim_{n\to\infty} \text{meas}(\{z \big| \; |f_n(z) - f(z)| \geq \epsilon\}) = 0$$

where meas( ) is taken to be the Lebesgue measure in $\mathbb{C}$.

The method we propose is based on Conjecture 5.1. If, according to Conjecture 5.1, $\frac{P_N(z)}{D_N(z)}$ converges as $N \to \infty$, $\left|\frac{P_N(z)}{D_N(z)} - \frac{P_M(z)}{D_M(z)}\right|$ should converge to zero as $N, M \to \infty$. Hence, a reasonable approximation to the boundary of convergence of the series of diagonal Padé approximants $[N/N]$ — and hence, according to Conjecture 5.1, to the domain of analyticity of the function — could be the level curve

$$\left|\frac{P_N(z)}{D_N(z)} - \frac{P_M(z)}{D_M(z)}\right| = \delta$$

for a reasonably small δ and sufficiently large N, M, and z not in the neighborhood of a spurious pole of the $[M/M]$, $[N/N]$ approximants (for a discussion on spurious poles look in section 10).

Unfortunately, the practical implementation of the criterion cannot take the limit as N, M tend to infinity but rather just take some reasonably high value. Then, the criterion involves a free parameter δ as a function of the degree of the approximation and the results could depend on its choice. In the examples we have considered, we have found that any choice between 10^{-5} and 10^{-1} leads to results not more uncertain than those obtained by finding the zeros of D_M.

The dependence on the parameter δ can be further reduced by plotting the level surface

$$\left|\frac{P_{N_1}(z)}{D_{N_1}(z)} - \frac{P_{N_2}(z)}{D_{N_2}(z)}\right| + \cdots + \left|\frac{P_{N_{j-1}}(z)}{D_{N_{j-1}}(z)} - \frac{P_{N_j}(z)}{D_{N_j}(z)}\right| = \delta$$

which, according to Conjecture 5.1, will also provide an approximation to the domain of analyticity.

Unfortunately, little is known about the convergence of Padé approximants in the case that the function has natural boundaries. For a class of functions with natural boundaries — but which remain quasianalytic across the boundary — (for a definition of quasianalytic and examples see [Gi], p. 306–309) — [GN] have shown that the $[(N+J)/N]$ Padé approximants converge in measure to the function as $N \to \infty$, in any closed, bounded region of the complex plane. Specifically:

Theorem 5.2. *For the function* $f(z) = \sum_{n=1}^{\infty} \frac{A_n}{(1-z\alpha_n)}$*, where the* α_n *lie densely on the unit circle and* $|A_n| < Ce^{-n^{1+\gamma}}, \gamma > 0$*, the sequence of* $[(N+J)/N]$ *Padé approximants to* $f(z)$ *converges in measure to* f *as* $N \to \infty$ *in any closed, bounded region of the complex plane.*

The method of proof, as remarked in [GN] can be extended to other cases and the condition $|\alpha_n| = 1$ can be modified to $|\alpha_n| < a$. They also discuss how slightly faster rates of growth in the coefficients, could lead to divergence.

Results, such as this one, make it reasonable to be hopeful that convergence of the Padé approximants is a reasonably general phenomenon and, hence, lend indirect support to Conjecture 5.1

Our numerical results also support Conjecture 5.1 On the other hand we note that, in contrast with Theorem 5.2, we do observe that the Padé approximants of our functions seem to diverge outside of the domain of analyticity of the function.

The results of section 9 suggest that the paradigm for the natural boundaries is not an accumulation of poles as in Theorem 5.2, but rather an accumulation of branch points.

It is not clear to us what could be a reasonably general condition that implies convergence of the Padé approximants for the cases we are interested in.

6. Newton Method

Apart from the perturbative method we have used so far to approximate the invariant curve, we can also solve (3.1) by using a Newton method on an appropriate operator $\mathcal{T}$. The Newton method will converge to the solution of (3.1) as long as the invariant curve exists and a sufficiently good initial guess is given.

If, for a fixed ϵ_0, u_{ϵ_0} fails to satisfy (3.1) by a small amount $R_{\epsilon_0}(\theta)$ i.e.,

$$\mathcal{T}u_{\epsilon_0}(\theta) = u_{\epsilon_0}(\theta+\omega) - u_{\epsilon_0}(\theta)^2 - \lambda - \epsilon_0 \cos 2\pi\theta = R_{\epsilon_0}(\theta) \tag{6.1}$$

we can try to improve the solution by setting it to $u_{\epsilon_0}(\theta) + \Delta_{\epsilon_0}(\theta)$, where $\Delta_{\epsilon_0}(\theta)$ will be conveniently chosen to make the error much smaller.

If $\Delta_{\epsilon_0}(\theta)$ satisfies

$$D\mathcal{T}(u_{\epsilon_0})\Delta_{\epsilon_0}(\theta) = \Delta_{\epsilon_0}(\theta+\omega) - 2u_{\epsilon_0}(\theta)\Delta_{\epsilon_0}(\theta) = -R_{\epsilon_0}(\theta) \tag{6.2}$$

then, $u_{\epsilon_0}(\theta) + \Delta_{\epsilon_0}(\theta)$ will satisfy (3.1) up to error terms which are much smaller than $R_{\epsilon_0}(\theta)$.

We will postpone for the moment a discussion of the numerical discretizations used to solve (6.2).

This method, as it is well known from even finite dimensional examples, has the shortcoming that it only converges when sufficiently good guesses are taken as starting points.

In our case one could perform a continuation method starting from very small values of ϵ. That is, when one exact solution is found, we take it as an approximate solution for the equation with a slightly bigger parameter. We note that the solution when $\epsilon = 0$ is known exactly. We could also take for some values of ϵ the sum of the series (3.2) as an initial guess. This would provide us with an independent verification that the series is converging to solutions of the equation.

We emphasize that the validity of the solution of the Newton method is independent of the method used to obtain the initial guess since, in the process of running the Newton method one checks that the equation is indeed satisfied.

For practical calculations in concrete problems the Newton method seems to have advantages over the method of expansion in powers of ϵ. For example, notice that the expansions in powers of ϵ can only converge on a disk of radius equal to the distance from the origin to the closest singularity. If the shape of the analyticity domain is very different from a disk, this implies that there will be several values of ϵ for which the invariant circles exist and for which the ϵ expansion does not converge. For a continuation method, it is quite possible to obtain the solution in all the connected domain where the solution exists. Notice also that the method of expansion in powers requires the storage of many functions. The Newton method requires only the storage of one. On the other hand, one should also mention that if one requires solutions for many values of the parameter, the ϵ expansion method could be faster and gives more global information.

7. Multipoint Padé Approximation

The multipoint Padé approximation is an interesting compromise between rational interpolation and the Padé approximation (which we could consider as a degenerate case of interpolation in which all the interpolation points are infinitesimally close).

We recall, see e.g. [BGM] vol.2, p.5, that given a set of points $\{z_i\}_{i=1,k}$ in the complex plane and a function $S(z)$ with Taylor expansions of order ℓ_i around those points, we define the multipoint Padé approximant as:

$$\frac{P(z)}{D(z)} \ , \quad \operatorname{degree} P = N \ , \quad \operatorname{degree} D = M \ , \quad D(0) = 1$$

such that $M + N + 1 = \sum_{i=1}^{k}(\ell_i + 1)$ and

$$\frac{d^s}{dz^s}\big(P(z) - D(z)S(z)\big)\Big|_{z=z_i} = 0 \ , \qquad s \leq \ell_i \ , \ i = 1, k.$$

Setting

$$P(z) = \sum_{j=0}^{N} P_j z^j$$

$$D(z) = \sum_{j=0}^{M} D_j z^j \ , \quad D(0) = D_0 = 1$$

$$S(z) = \sum_{j=0}^{\ell_i} S_{i;j}(z - z_i)^j \ , i = 1, k$$

we require

$$\sum_{j=s}^{N} P_j \frac{j!}{(j-s)!}\, z_i^{j-s} = \left[\sum_{n=0}^{s} \binom{s}{n} S^{(s-n)} D^{(n)}\right](z_i)$$

where

$$S^{(s)}(z_i) \equiv \frac{d^s}{dz^s} S(z)\big|_{z=z_i}.$$

Since

$$D^{(n)}(z_i) = \sum_{m=n}^{M} \frac{m!}{(m-n)!}\, D_m z_i^{m-n}\ , \qquad 0 \le n \le M$$
$$S^{(s-n)}(z_i) = (s-n)!\, S_{i;s-n}\ , \qquad 0 \le s-n < M+N+1$$

or

$$\sum_{j=s}^{N} P_j \frac{j!}{(j-s)!}\, z_i^{j-s} = s! \sum_{n=0}^{s} \sum_{m=n}^{M} \binom{m}{n} S_{i;s-n} D_m z_i^{m-n}$$

where, to simplify the notation, we extend the usual combinatorial numbers by:

$$\binom{m}{n} = \begin{cases} \dfrac{m!}{n!(m-n)!}\ , & m \ge n \\ 0\ , & m < n \end{cases}$$

After some algebra we get:

$$\sum_{n=0}^{N} P_n \alpha_{i;n,s} - \sum_{m=1}^{M} D_m \beta_{i;m,s} = S_{i;s}$$
$$\alpha_{i;n,s} = \binom{n}{s} z_i^{n-s}$$
$$\beta_{i;m,s} = \sum_{j=0}^{s} \binom{m}{j} S_{i;s-j} z_i^{m-s}$$

We note that it seems to be difficult to devise conditions a priori that tell us when this interpolation by rational functions is possible. Indeed, there are easy examples in which even the interpolation without trying to match the derivatives is impossible (see e.g., [SB] p.58). Nevertheless, it is easy to carry out the computations described above and assign them condition numbers that guarantee that the final results are still precise enough. Since the main step is the solution of a system of linear equations there are very well known condition numbers.

There are algorithms based on recursion, that lead to fast evaluation of the rational approximations. (See e.g., [BGM] vol.2, p.7 or [SB] §2.2 p.58) These algorithms could have been adapted to produce interpolating polynomials. However, it seemed better to use the algorithms above since they allow the computation of condition numbers at every stage.

In our case, we used the Newton method to compute the function $u_{\epsilon_i}(\theta)$ for several complex values ϵ_i. To compute the derivatives with respect to ϵ at one point, we proceed as follows.

If we write $\hat{\epsilon} = \epsilon - \epsilon_i$ and write $u_\epsilon(\theta) = u_{\epsilon_i}(\theta) + \Delta_{\hat{\epsilon}}(\theta)$, substituting in (3.1) we obtain

$$\Delta_{\hat{\epsilon}}(\theta + \omega) = 2u_{\epsilon_i}(\theta)\Delta_{\hat{\epsilon}}(\theta) + \Delta^2_{\hat{\epsilon}}(\theta) + \hat{\epsilon}\cos 2\pi\theta \tag{7.1}$$

If we assume that $\Delta_{\hat{\epsilon}} = \sum_{n=1}^{\infty} \hat{\epsilon}^n \Delta^n(\theta)$ and match powers in $\hat{\epsilon}$ we obtain

$$\begin{aligned} &\Delta^1(\theta + \omega) - 2u_{\epsilon_i}(\theta)\Delta^1(\theta) = \cos 2\pi\theta \\ &\Delta^n(\theta + \omega) - 2u_{\epsilon_i}(\theta)\Delta^n(\theta) = \sum_{m=1}^{n-1} \Delta^m(\theta)\Delta^{n-m}(\theta)\ , \qquad n > 1 \end{aligned} \tag{7.2}$$

If we assume that we know $\Delta^1, \ldots, \Delta^{n-1}$ then Δ^n can be found by solving an equation of the form

$$\Delta^n(\theta + \omega) - 2u_{\epsilon_i}(\theta)\Delta^n(\theta) = R^n(\theta) \tag{7.3}$$

To solve (7.3) we prove the following lemma :

Lemma 7.1. *If $u_{\epsilon_i}(\theta)$ is an analytic function satisfying*

(i) $\|2u_{\epsilon_i}\|_\delta \le A$

(ii) For some $m \in \mathbb{N}, 0 < \gamma < 1, \quad \|2u_{\epsilon_i}(\theta) \cdots 2u_{\epsilon_i}(\theta + m\omega)\|_\delta \le \gamma$

then,

Given any R^n analytic in $\{\theta \big| |\mathrm{Im}\,(\theta)| \le \delta\}$, we can find a unique Δ^n solving (7.3). Moreover,

$\|\Delta^n\|_\delta \le K\|R^n\|_\delta$, *where K can be taken to be $K = 1 + A^m/(1-\gamma^{1/m})$.*

Proof. Applying (7.3) repeatedly we have

$$\begin{aligned}\Delta^n(\theta+\omega) &= \sum_{k=1}^{N}\left(\prod_{j=0}^{k-1}\big(2u_{\epsilon_i}(\theta - j\omega)\big)\right) R^n(\theta - k\omega) + R^n(\theta)\\ &\quad + \prod_{k=0}^{N}\Big(2u_{\epsilon_i}\big(\theta-k\omega\big)\Big)\Delta^n\big(\theta - N\omega\big).\end{aligned} \tag{7.4}$$

If there is a bounded solution, then the last term in (7.4) should tend to zero, so that the only solution of (7.3) should be:

$$\Delta^n(\theta) = \sum_{k=1}^{\infty}\left(\prod_{j=0}^{k-1}(2u_{\epsilon_i}(\theta - j\omega))\right) R^n(\theta - k\omega) + R^n(\theta) \tag{7.5}$$

Considering blocks of length m we can bound the products appearing in (7.5) by:

$$\big\|\prod_{j=0}^{k-1}(2u_{\epsilon_i}(\theta - j\omega))\big\|_\delta \le A^m\gamma^{[k/m]} = A^m[\gamma^{1/m}]^k$$

so that

$$\|\Delta\|_\delta \le \|R\|_\delta\big(1 + \frac{A^m}{1-\gamma^{1/m}}\big) = K\|R\|_\delta.$$

The above estimates show also that the series (7.5) converge absolutely, so that it is possible to rearrange terms and show that indeed it solves (7.3).

■

Now we can show convergence for the series (7.2).

Lemma 7.2. *If $|\hat\epsilon| < \frac{1}{2}K^{-2}e^{-2\pi\delta}$ (where K as in Lemma 7.1) the series obtained by summing the Δ^n's computed from (7.2) converges uniformly on $\{\theta\big|\ |\mathrm{Im}\,\theta| < \delta\}$.*

Proof. We notice that $R^1(\theta) = \cos 2\pi\theta$ so that

$$\|\Delta^1\|_\delta \le K\|R^1\|_\delta \le \frac{1}{2}Ke^{2\pi\delta}$$

From (7.2) we have that for $n > 1$

$$\|\Delta^n\|_\delta \le K\|R^n\|_\delta \le K \sum_{m=1}^{n-1} \|\Delta^{n-m}\|_\delta \|\Delta^m\|_\delta \tag{7.6}$$

This recursion is the same as (3.6) and to obtain the estimates claimed, it suffices to use the same argument that we used in Lemma 3.1

■

Remark. Lemma 7.2, together with Lemma 3.1 show that the mapping $\epsilon \to u_\epsilon$ is analytic in $|\epsilon| < \frac{1}{2}K^{-2}$ when we give the u_ϵ the topology induced by $\| \quad \|_\delta$. This is much stronger than saying that for a fixed θ the series $\sum_{n=0}^\infty u^n(\theta)\epsilon^n$ or $\sum_{n=1}^\infty \Delta^n(\theta)\hat{\epsilon}^n$ converge.

Remark. Notice that the equations appearing in the recursion for $n > 1$ are very similar to the equations we encountered in the study of the Newton method (this is not a coincidence since the procedure we carried out is just a very explicit form of the implicit function theorem — the equation (6.2) is just inverting the derivative, which also plays a role in the implicit function theorem).

Again, once we have computed the expansions, in terms of ϵ, of the function by evaluating at different values of θ we obtain several numerators and denominators and several possible candidates for the domain of convergence. They should agree.

We point out that the hypotheses of Lemma 7.1 are equivalent to the existence of a uniformly contractive analytic invariant circle. We will proceed to show that these hypotheses, for this model, are implied by the à priori much weaker conditions that there exists a continuous invariant circle with negative Lyapunov exponent. Hence, the boundary of the domain of analyticity is given by the boundary of the domain of existence of continuous circles with negative Lyapunov exponent.

We recall – see e.g. [W] Thm 6.20 – that rotations by an irrational number are uniquely ergodic. That is, they admit only one invariant measure. Hence, it makes sense to speak of the Lyapunov exponent of the invariant circle without specifying explicitly the measure.

Lemma 7.3. *Let u be a continuous function solving (3.1) with ω irrational. If $\int \ln |2u(\theta)| d\theta < 0$, then, we can find an m such that*

$$\big|2u(\theta) \cdot 2u(\theta + \omega) \cdots 2u(\theta + m\omega)\big| \le \gamma < 1.$$

Proof. Denote by $\phi(\theta)$ a continuous function $\phi(\theta) \ge \ln |2u(\theta)|$, $\int \phi(\theta) d\theta = \gamma_1 < 0$. (Such function can be obtained by setting $\phi(\theta) = \ln(\max(|2u(\theta)|, \rho))$ for sufficiently small $\rho > 0$.) We recall (see e.g [W] Thm 6.19) that for a uniquely ergodic map, the Birkhoff sums of a continuous function converge uniformly. In our case, they should converge uniformly to γ_1. Hence, we can find m such that $\phi(\theta) + \phi(\theta + \omega) + \cdots + \phi(\theta + m\omega) \le \ln \gamma < 0$. Since $\phi(\theta) \ge \ln(|2u(\theta)|)$, the lemma is established.

■

Lemma 7.4. *Let u be a continuous map solving (3.1) and such that, for some $m \in \mathbb{N}, 0 < \gamma < 1$, $|2u(\theta) \cdot 2u(\theta + \omega) \cdots 2u(\theta + m\omega)| \le \gamma < 1$, for $\theta \in \mathbb{T}^1$. Then u is analytic.*

Notice that, even if Lemma 7.3 requires that ω is irrational, Lemma 7.4 works even for rational ω.

Proof. Consider the graph transform operator

$$\Gamma[u](\theta) = u(\theta - \omega)^2 + \lambda + \epsilon \cos 2\pi(\theta - \omega). \tag{7.7}$$

It is equivalent that u is a fixed point of Γ and that it satisfies (3.1).

We will show that, under the hypotheses of Lemma 7.4, we can find a ball in C^0 and in $C^{\omega,\delta}$, for δ sufficiently small, with non-empty intersection, on which Γ^{m+1} is a contraction with the corresponding norms and that the C^0 ball contains the given fixed point u. Then, if we take a point belonging to the intersection of the two balls, by the uniqueness part of the contraction mapping theorem, by iterating it, it has to converge to u. On the other hand, by the contraction on $C^{\omega,\delta}$, it converges to an analytic fixed point.

To prove the claim, we observe that the derivative of Γ^{m+1} at the fixed point u can be computed both in C^0 and in $C^{\omega,\delta}$ as:

$$D\Gamma^{m+1}(u)[\eta](\theta) = 2u(\theta - \omega) \cdot 2u(\theta - 2\omega) \cdots 2u(\theta - (m+1)\omega)\eta(\theta - (m+1)\omega) \tag{7.8}$$

We note that for other functions in place of the logistic, the derivative of Γ^{m+1} is still obtained by a multiplication operator and a shift.

Denote by K_α the heat kernel and observe that $\|u - K_\alpha u\|_{C^0}$ converges uniformly to 0 as $\alpha \to 0$. Also $\|K_\alpha u\|_\delta \to_{\delta\to 0} \|K_\alpha u\|_{C^0} \to_{\alpha \to 0} \|u\|_{C^0}$ where the convergence, due to the periodicity of u, is uniform in α, δ.

Using the previous observations by choosing α,δ sufficiently small, we can get that $\|\Gamma^{m+1}[K_\alpha u] - K_\alpha u\|_\delta$ is arbitrarily small and $\|D\Gamma^{m+1}(K_\alpha u)\|_\delta$ is as close to γ as desired, in particular less than 1.

Moreover $D^2\Gamma^{m+1}(u)(\eta_1, \eta_2) = \sum_{i,j} \left(\prod_{\substack{i' \neq i \\ i' \neq j}} 2u(\theta - i'\omega) \right) \eta_1(\theta - i\omega)\eta_2(\theta - j\omega)$. Hence if we pick a neighborhood of radius ρ in the $C^{\omega,\delta}$ space, we can bound the size of the second derivative uniformly in α, δ as they become arbitrarily small.

Hence for all α, δ sufficiently small, it is possible to get a $C^{\omega,\delta}$ ball around $K_\alpha u$ so that Γ^{m+1} is a contraction on it. We can also arrange that $K_\alpha u$ is in the C^0 ball around u for which Γ^{m+1} is a C^0 contraction.

■

8. Non-perturbative methods

If the invariant curve is contractive, it can be approximated numerically by iterating the map (2.1) forward. By changing ϵ in small steps we can compute the invariant curve for all the domain in which it is contractive. Because of Lemma 7.2, Lemma 3.1, which guarantee analyticity in ϵ for contractive invariant circles, if we succeed in finding parameter values along a path that goes through the origin, for which the orbits settle onto an invariant curve we can ensure that these points belong to the domain of analyticity of the invariant curve.

On the other hand, if we find real values of ϵ for which some orbits escape to infinity – by the quadratic behavior of the map it suffices to check that r is larger than a certain number – we are sure that there are no invariant circles separating the beginning of the orbit and infinity.

When ϵ is complex, the existence of orbits escaping to infinity does not preclude the existence of an invariant circle in $\mathbb{T}^1 \times \mathbb{C}$. Nevertheless, the fact that the basin of attraction of the invariant circle shrinks to nothing is indication of a sudden change in behavior. If it was just that the invariant circle lost stability, this could be discovered by iterating backwards. For all the values of the parameters we are reporting after breakdown, we found no evidence of invariant circles.

So, if we increment ϵ along a path, and find values for which the orbit settles in an invariant circle and very nearby values for which all orbits seem to escape, we conclude that these values belong to the boundary of the domain of analyticity. By taking several paths of a family, e.g radii, we can obtain a reasonable estimate of the boundary. Since the boundary can bend back with respect to a family of paths, we should use several families to obtain a better approximation.

One side effect of this algorithm is that it allows to compute the invariant curves just before breakdown. For real values of ϵ the invariant curve remains smooth until breakdown. At breakdown it undergoes a saddle node bifurcation of invariant circles and disappears (the theory of this phenomenon is worked out in [AKL1]). For complex values of ϵ the invariant curve disappears by becoming very oscillating at small scales. This phenomenon requires further study but we will not concern with it here.

We emphasize that just finding the values of ϵ for which there are points that do not escape which are close to other for which escape takes place, does not provide always with a reliable approximation for the domain of analyticity of the invariant circle. One has to check that the invariant set in which the orbit settles is an invariant circle. Indeed, for some values of λ, the invariant circles experience period doubling bifurcations. These periodic circles are barriers for the escape but nevertheless are not direct continuations of the original invariant circle.

In the practical implementation, we have just checked visually for some of the values that indeed the attracting set was a circle. For the values of λ we report, the evidence that the sets remain one dimensional up to extremely close to breakdown is very clear. Even if we have not been able to obtain a mathematical argument that shows that there are no other bifurcations of the circle for the values of λ that we have considered, the numerical results show that these bifurcations, if they happen, can only occupy a very small region in the parameters space.

9. Behavior at rational frequencies

In this section we study the analyticity domains for the case that the frequency is rational. A motivation for this is that it is possible to show – see Theorem 9.1 below for a precise statement – that the analyticity domains at irrational ω are approximated by those at rational frequencies p/q when $p/q \approx \omega$. Nevertheless, when the frequency is rational, many of the analytical problems become algebraic and we can perform a detailed analysis. In particular, we can discuss in detail what is the nature of the singularities when the perturbation expansions break down.

We also point out that, when ω is rational, several of the domains that we conjectured to agree for ω irrational, differ. Nevertheless, we observe in our numerical experiments that as the rational numbers approach their irrational limiting values these domains seem to approach each other. This may serve as additional support for these conjectures.

We start by discussing some justification for the approximation of the analyticity domains for circles with frequency ω by those of approximate frequencies.

Theorem 9.1. *If, for fixed ϵ, λ, and ω irrational there exists an analytic $u_\omega(\theta)$ that satisfies (3.1) and*

(*i*) $\|2u_\omega(\theta-\omega)2u_\omega(\theta-2\omega)\cdots 2u_\omega(\theta-m\omega)\|_\delta \le \gamma < 1$

then,

for $\bar\omega$ in a neighborhood of ω, there exists an analytic $u_{\bar\omega}(\theta)$ satisfying (3.1).

Proof. We will use a version of the contractive mapping theorem similar to those we used in sections 6 and 7. We introduce the operator Γ_ω as in (7.7). Since the dependence in ω will play an important role, we make it explicit in the notation.

Since u_ω satisfies $\Gamma_\omega[u_\omega] - u_\omega = 0$ we see that we also have for $\bar\delta \le \delta$,

$$\begin{aligned}
\|\Gamma_{\bar\omega}[u_\omega] - u_\omega\|_{\bar\delta} &= \|\Gamma_{\bar\omega}[u_\omega] - \Gamma_\omega[u_\omega] + \Gamma_\omega[u_\omega] - u_\omega\|_{\bar\delta} \\
&= \|u(\theta-\bar\omega)^2 - u(\theta-\omega)^2 + \epsilon(\cos(2\pi(\theta-\bar\omega) - \cos(2\pi(\theta-\omega))\|_{\bar\delta} \\
&\le (2\|u_\omega\|_{\bar\delta}\|u'_\omega\|_{\bar\delta} + \epsilon)|\omega-\bar\omega| = K|\omega-\bar\omega|
\end{aligned}$$

where K depends on u_ω, δ, $\bar{\delta}$, ϵ but not on $|\omega - \bar{\omega}|$.

From that, it is very easy to show that $\Gamma^m_{\bar{\omega}}$ has a fixed point. Using condition (i), it is possible to show that $D\Gamma^m_{\bar{\omega}}[u_\omega]$, which can be expressed as multiplication by shifted versions of u_ω, is a contraction in $\| \quad \|_{\bar{\delta}}$ with a factor as close as desired to γ, if we assume that $\omega - \bar{\omega}$ is small enough. We can also bound the $D^2\Gamma^m_{\bar{\omega}}$ in a neighborhood of u_ω.

The argument to prove that $\Gamma_{\bar{\omega}}$ has a fixed point is only slightly more complicated. We observe that, proceeding as in Lemma 7.1, given $R \in C^{\omega,\bar{\delta}}$ we can solve the equation for η, $D\Gamma_{\bar{\omega}}[u_\omega]\eta = R$ and we have $\|\eta\|_{\bar{\delta}} \leq K\|R\|_{\bar{\delta}}$ where K can be chosen uniformly for $|\omega - \bar{\omega}|$ sufficiently small. If we consider the auxiliary operator $\Phi(v) = -\left(D\Gamma_{\bar{\omega}}(u_\omega) - \mathrm{Id}\right)^{-1}\left(\Gamma_{\bar{\omega}}(v) - v\right) + v$, we see that Φ is a contraction in $\| \quad \|_{\bar{\delta}}$ of a factor $1/2$ in a neighborhood of u_ω that can be chosen uniformly as $|\omega - \bar{\omega}|$ is small. Since $\|\Phi(u_\omega) - u_\omega\|_{\bar{\delta}}$ can be made as small as desired by choosing $\omega - \bar{\omega}$ to be small, we conclude that Φ has a fixed point for all $\bar{\omega}$ in a neighborhood of ω. But a fixed point of Φ is a fixed point of $\Gamma_{\bar{\omega}}$.

■

Remark. Theorem 9.1 is an analog of the justification of Greene's criterion for the approximation of invariant curves by periodic orbits for the case of Hamiltonian systems, in the spirit of [FL2], in the case of hyperbolic circles. (See also [McK2].)

The main consequence of Theorem 9.1 is that all the non-perturbative methods based on the continuation of attractive invariant circles will provide a reasonable approximation to the domain of parameters for which there is an attractive invariant circle. According to Lemma 7.2 for the values of λ we considered, this agrees with the domain of analyticity.

Now, we start to discuss the perturbative methods. We first observe that the Lindstedt series for the case of rational frequencies do not exhibit small denominators, as can be easily established from (3.5), and the calculation of the Padé approximants goes through.

To study the nature of the boundary of the domain of analyticity for the invariant circles for $\omega = p/q$ it is more convenient to investigate the behavior of the q^{th} iterate of

(2.1). We have:

$$F^q_{\lambda,\epsilon,\omega}(r,\theta) = (P_{\lambda,\epsilon,\theta}(r),\theta) \tag{9.1}$$

where $P_{\lambda,\epsilon,\theta}$ is a polynomial in r of degree 2^q, with only even orders of r. Hence, θ enters only as a parameter in the dynamics of the q^{th} iterate of the map.

Periodic orbits of period q are solutions of:

$$r = P_{\lambda,\epsilon,\theta}(r). \tag{9.2}$$

Since (9.2) is a polynomial equation in r of degree 2^q, in general, it has 2^q distinct solutions. The only way for the solution to a polynomial equation to lose analyticity on its dependence to the coefficients is if two or more solutions coincide (there we expect to get a branch point). If we fix λ, θ and choose one solution for $\epsilon = 0$ and then vary ϵ over the complex plane and follow that solution, the possible branch points for the solution in terms of ϵ, are the values of ϵ such that our solution is a root of (9.2) of multiplicity at least two. Of course, there could be values of the parameter for which the root becomes double but which do not cause a loss of analyticity of the branches of the solutions. This, nevertheless, can only happen in degenerate situations (e.g transcritical saddle node). In practice, once we have obtained a finite number of candidates, it is easy to verify that the non-degeneracy conditions that imply that there is a branch point take place.

Remark. Notice that the position of the branch points depends on θ, and that although generically there are branch points, there can be values of θ such that some branch points disappear. For example for $\omega = 1/1$ the position of the branch point is determined by $\lambda + \epsilon\cos(2\pi\theta) = 1/4$, and for $\theta = 1/4$ the branch point is at ∞.

Notice that one important consequence of the previous discussion is that in the case that ω is rational, the only possible ways of breaking analyticity is branch points and that, typically, we expect that these branch points are of order 2. This has important consequences for the behavior of Padé approximants. According to a long standing conjecture, Padé approximants of functions with branch points tend to arrange their poles and zeros along lines that are uniquely determined from the position of the poles (see [BGM] vol.1, p. 51, [Gi] p. 288, [N]). The results we obtained from the Padé approximants are remarkably close to the behavior outlined above, since the poles and zeros of the Padé approximants lie along lines that emanate from the branch point and go radially to infinity (forming a Mittag-Leffler star, see [BGM] vol.1, p. 50). We have also noticed that the poles (and the zeros) of the Padé approximant tend to accumulate to the branch point. As the denominator increases the number of the branch points gets bigger and for large values of the denominator the branch points tend to accumulate to the natural boundary investigated in previous sections.

Similar behavior for the poles of the Padé approximants for the Lindstedt series, for invariant circles of the standard map with complex ω with rational real part, was reported in [BM]. The poles (the zeros were not investigated in [BM]) lied along lines that emanate from points that tend to the origin as $\operatorname{Im}\omega \to 0$, and go radially to infinity. It can be argued that the resemblance is due to the absence of small denominators for complex frequencies. It can also be argued that the effect of the imaginary part of the frequency is very similar to introducing dissipation in the system. Based on this analogy, we conjecture

Conjecture 9.2. *The behavior observed in* [BM] *corresponds to branch points in the complex domain. In particular, the zeros of the numerator of the Padé approximant should also be in the same line in which the poles were found.*

Since this paper is mainly concerned with the rotating logistic map, we will not discuss the standard map any further.

To compute the position of the branch points for the case of the rational frequencies we fixed λ, θ. We observe that the polynomial in r given by $P_{\epsilon,\lambda,\theta}(r) - r$ is a polynomial whose coefficients are polynomials in ϵ. We recall that the discriminant of a polynomial $P(x)$ of degree N is defined as $\operatorname{disc}(P(x)) = \prod_{i>j}(x_i - x_j)^2$ where x_i are the roots. Hence, a polynomial has double roots if and only if the discriminant is zero. The importance of this remark is that the discriminant of a polynomial is an algebraic function of the coefficients. In particular, if the coefficients are polynomials in another variable, the discriminant will be a polynomial in the auxiliary variable. Reasonably efficient algorithms exist to compute discriminants of polynomials. In particular, the resultant algorithm – see e.g [Kn] vol. 2 – works in the case when the coefficients are polynomials.

Notice that to compute analyticity domains we are only interested in the collisions of a particular root with the others, however the discriminant will vanish whenever any two roots collide. So that finding all the values of ϵ for which the discriminant vanishes will provide us with a discrete subset that includes, but which could be bigger than, the set of branch points of the periodic solution that we are tracing. Unfortunately, it is not so easy to decide whether a place where the discriminant vanishes corresponds to a branch point of the root we are tracing. This requires a global continuation method and one should follow all the Riemann sheets, since the roots change identity by going into different sheets. This is a question that merits a more detailed study, but we have not pursued it in this paper. We just observe that, in the cases that we studied, many of the values of ϵ where the discriminant vanishes are indeed at the tip of the accumulation of zeros and poles of the Padé approximations.

The study of the domain of no escape becomes more complicated in the case of rational frequencies than what it was for irrational frequencies. The case $\omega = 1/1$ is relatively simple, $P_{\lambda,\epsilon,\theta}(r) = r^2 + \lambda + \epsilon\cos(2\pi\theta)$ and for any θ such that $\cos(2\pi\theta) \neq 0$ we get a distorted quadratic family $F_q = z^2 + \epsilon$. There exist only two fixed points, with only one of them attractive for some domain in the ϵ plane. The domain of existence of the attractive fixed point is the main cardioid of the Mandelbrot set and can be computed by :

$$z_0 = F_q(z_0), \quad |F_q'(z)|_{z=z_0} < 1$$

or

$$|1 \pm \sqrt{1-4\epsilon}| < 1. \tag{9.3}$$

The cusp of the cardioid is located at the branch point of the domain of analyticity of the roots and corresponds to a collision of the attractive and repelling fixed points.

For $\omega = p/q, \quad q > 1$ the situation is no longer simple. To understand the full dynamics of the problem one has to consider iterations of polynomial maps of degree 2^q in the complex domain (for an overview see [Bl1]). Such maps have 2^q fixed points, and although our solution follows one of them, that is attractive for some domain in the parameter space, it can undergo a bifurcation and either disappear or become unstable. On the same time other stable fixed points, to which forward iteration of the map will converge, may still exist. The behavior of the map under forward iteration, is characterized by the behavior of the critical points of the map (r_{cr} such that, $P'_{\lambda,\epsilon,\theta}(r_{cr}) = 0$)

under forward iteration. If an attractive periodic point exists, then at least one critical point belongs to its basin of attraction (see [Br]). One can recover the behavior of all the critical points at a fixed θ by looking at the behavior of the critical point at zero of $P_{\lambda,\epsilon,\theta+n\frac{p}{q}}(r), \quad n = 0, \ldots, q-1$, since :

$$\begin{aligned} P'_{\lambda,\epsilon,\theta}(r) &= \Bigg(\underbrace{F_{\lambda,\epsilon,p/q} \circ \cdots \circ F_{\lambda,\epsilon,p/q}}_{q \quad \text{times}}(r,\theta) \Bigg)' \\ &= \underbrace{F'_{\lambda,\epsilon,p/q} \circ \cdots \circ F_{\lambda,\epsilon,p/q}}_{q \quad \text{times}}(r,\theta) \underbrace{F'_{\lambda,\epsilon,p/q} \circ \cdots \circ F_{\lambda,\epsilon,p/q}}_{q-1 \quad \text{times}}(r,\theta) \cdots F'_{\lambda,\epsilon,p/q}(r,\theta). \end{aligned}$$

This feature is characteristic of our problem.

Depending on the initial conditions and the numerical implementation, the domain of no escape for a particular choice will be a subset of the domain where at least one critical point remains bounded. Caution should be taken at the interpretation of these results, since, as was pointed out, the solution we are following may have changed stability as we varied ϵ in the complex plane and the forward iteration may have followed a different solution (not necessarily a fixed point either). Studies for cubic polynomials have been performed in [BH],[Bl2],[Mil].

The cusps of the domain of existence of at least one attractive fixed point correspond to saddle-node bifurcations between attractive and repelling fixed points. The branch points in the domain of analyticity of the root we follow form a subset of the set of points where the cusps occur.

To interpret the dependence on θ we note that different θ corresponds to a different slice of the parameter space. For the cases $\omega = 1/1$ and $\omega = 1/2$, the behavior for different θ's can be recovered from the behavior for $\theta = 0$ after the scaling transformation $\epsilon \to \epsilon \cos(2\pi\theta)$. For other ω's such a simple scaling no longer exists.

10. Numerical Implementation

We have written a package in `C` to manipulate one-dimensional Fourier series. This package has the feature that the arithmetic is done through function calls so that by changing a definitions file, we can switch the arithmetic from double to extended precision.

The use of extended precision is a convenient way of handling the severe numerical instabilities of the recursion, the Padé approximation and the search for zeros. In order to keep the program machine independent, we have used the arithmetic library of the public domain program `PARI/GP`.

To increase the accuracy of the computation of the terms of the Lindstedt expansion, we used a technique also used in [FL1]. We considered the expansion in powers not of ϵ but of ϵ/ρ where ρ is chosen so as to make the series have radius of convergence 1. The value of ρ is determined from a preliminary run of the program.

From this series expansion, we solved (4.1) using Gaussian elimination verifying that the condition was always much smaller than the accuracy of the previous results. The actual algorithm was a translation into `C` of the well known `DECOMP` and `SOLVE` from [FMM].

To find the zeros of the denominator we used the routines "`xzroot`", "`zroot`" from "Numerical Recipes" translated to use the `PARI/GP` arithmetic and then checked if the answer was indeed correct by evaluating the polynomial and requiring that the result was smaller than a tolerance. We eliminated zeros of the denominator that are also zeros of the numerator. For some values of N, M, θ we encountered spurious poles, that disappeared as N, M, θ changed, but we did not eliminate them from the figures. A spurious pole, in contrast to a genuine one, tends to disappear under changes in the order of the approximant or the choice of θ. Spurious poles usually occur in close vicinity to a zero of the numerator, and in this way can be numerically distinguished by checking their residues (they should be small compared to the residues for the other poles).

To implement the Newton method we discretized (6.2) by truncating the Fourier series representation of the function

$$u_{\epsilon_0}(\theta) = \sum_{k=-n}^{n} \hat{u}_{\epsilon_0,k} e^{2\pi i k\theta} \ , \quad \Delta(\theta) = \sum_{\ell=-n}^{n} \hat{\Delta}_\ell e^{2\pi i \ell\theta} \ , \quad R(\theta) = \sum_{m=-n}^{n} \hat{R}_m e^{2\pi i m\theta}$$

where n is a large number ($n \sim 100$).

Equation (6.2) reduces to

$$\underset{\approx}{M} \cdot \underset{\sim}{\Delta} = -\underset{\sim}{R}$$

where

$$\underset{\sim}{\Delta} = (\hat{\Delta}_{-n}, \ldots, \hat{\Delta}_n)^T \quad , \quad \underset{\sim}{R} = (\hat{R}_{-n}, \ldots, \hat{R}_n)^T$$

$$M_{k\ell} = \begin{cases} \delta_{k\ell} e^{2\pi i \omega k} - 2u_{\epsilon_0,k-\ell} & , \quad |k-\ell| \le n \\ 0 & , \quad |k-\ell| > n \end{cases}$$

We verified that the procedure was converging in a quadratic fashion for the cases that we studied. This gives us confidence that the implementation was correct and that sources of error that make the truncated derivative different from the derivative of the truncation are small. When $R(\theta)$ stopped decreasing we stopped the procedure.

As for the multipoint Padé method we considered sequences of points which were distributed according to a sequence of powers of a fixed complex number. We used roots of unity, which leads to points evenly distributed in a circle or a number of modulus slightly smaller than one, which leads to a spiral converging to the origin. Again the equations for the interpolation equations were solved by Gaussian elimination so as to have an estimate of the condition. We observed that, for the same number of points, distributing the points on a spiral seemed to lead to smaller condition numbers than distributing them on a circle.

Notice that the equations (2.1) are invariant under the change $\epsilon \to -\epsilon$, $\theta \to \theta + \pi$, therefore the final domains of analyticity should be invariant under the change $\epsilon \to -\epsilon$. Since the coefficients of the series at zero are real, the domains of analyticity should be invariant also under the change $\epsilon \to \epsilon^*$. Since the numerical methods we used were not built taking into account such symmetries, the accuracy with which they are reflected in the final result can give an estimate of the accuracy of the whole procedure.

For the non-perturbative methods we considered paths which were radial, horizontal and vertical and found no discrepancies except in the places where the some of the paths cannot reach some of the points in the boundary. A difficulty that arises in the computation of the region of no escape is that as we move closer to breakdown it becomes harder to determine whether an orbit escapes or not, since the invariant circle becomes less and less attracting. A remedy for this effect is to reduce the distance between points along the path close to the suspected breakdown and to increase the number of iterations per point in the path.

Some symbolic manipulation packages such as `MAXIMA` and `MAPLE` implement the resultant algorithm, for the calculation of the discriminant, in such a way that it is possible to compute with polynomial coefficients. We indeed implemented such calculations. Nevertheless, we found it more efficient to compute the discriminant by evaluating the discriminant for a discrete set of values of ϵ and then, using the knowledge that the discriminant is a polynomial in ϵ whose degree we know, interpolate. To find the interpolating polynomial we adapted the routine "`toeplz`" from [FPTV] to be able to use `PARI/GP`. We found the results to agree with those obtained using the symbolic algebra packages.

11. Acknowledgments

Our interest in the map considered here was initiated by R. Adomaitis and I. Kevrekidis. We also thank P. Moussa, P. Blanchard, J. Nutall, J. Bellisard for correspondence and discussion.

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13. Captions

Figure 1. The boundary of no escape (Set 1), computed by iterating the map forward and using a continuation method until escape occurs (three families of paths (radial, vertical, horizontal) are used and the results are superimposed) with the poles of the Padé approximants [50/50] for several angles (Set 2) and with the poles of the Padé approximants for several Fourier coefficients of the ϵ expansion (Set 3) for $\lambda = 0.2$.

Figure 2. The boundary of no escape (Set 1) with the poles of the Padé approximants [50/50] for several angles (Set 2) for $\lambda = 0.1$.

Figure 3. Boundaries where the Padé approximants [24/24] and [20/20] for $\lambda = 0.2, \theta = 0.72$ differ more than δ, superimposed with the boundary of no escape under forward iteration (Set 1). For Set 2, $\delta = 3 \times 10^{-5}$, for Set 3, $\delta = 3 \times 10^{-4}$, for Set 4,

$\delta = 2 \times 10^{-3}$, for Set 5, $\delta = 2 \times 10^{-2}$.

Figure 4. The poles of the multi-point Padé approximant [90/90] for $\lambda = 0.2$ and several angles superimposed with the boundary of no escape under forward iteration (Set 1). Expansion in ϵ around 21 points with order of the expansion around zero 20 and around the other points 7. Set 2 : Expansion around $z_k = 0.1e^{2\pi ik/20}, k = 1, \ldots, 20$. Set 3 : Expansion around $z_k = (0.19e^{2\pi i/20})^k, k = 1, \ldots, 20$.

Figure 5. Invariant curve close to breakdown. An example of a saddle node bifurcation. $\lambda = 0.2$, $\epsilon = 0.589$.

Figure 6. Invariant curve close to breakdown. An example of an invariant curve becoming discontinuous. Real part of the invariant circle for $\lambda = 0.2$, $\epsilon = 0.22 + 0.677i$.

Figure 7. Invariant curve close to breakdown. An example of an invariant curve becoming discontinuous. Imaginary part of the invariant circle for $\lambda = 0.2$, $\epsilon = 0.22 + 0.677i$.

Figure 8. Branch points (Set 2) and branch cuts (Set 3) for rational frequency superimposed with the domain of existence of an attractive fixed point (Set 1). The zeros and the poles of the [40/40] Padé approximant seem to converge to the branch cut on a straight line. $\omega = 1/2$, $\lambda = 0.2$, $\theta = 0$.

Figure 9. As in figure 8 with $\omega = 2/3$, $\lambda = 0.2$, $\theta = 0$.