NATURE OF SINGULARITIES FOR ANALYTICITY DOMAINS OF INVARIANT CURVES

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Abstract. We present theoretical arguments (based on infinite dimensional bifurcation theory) and numerical evidence (based on non-perturbative methods) that the boundaries of analyticity of invariant curves can be described as an accumulation of branch points, which are typically of order 2. We show how this fact would explain previous numerical results of several authors and how it suggests more efficient numerical algorithms, which we implement.

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Invariant curves have been very important in the development of dynamical systems because they organize the long term behavior. A considerable amount of numerical work has been performed recently trying to understand the phenomena that happen when they disappear.

In previous numerical investigations the breakdown of invariant curves has been attributed to the presence of a natural boundary in their analyticity domain (see [BC], [BCCF], [FL], [LT]). In [BM] complex rotation numbers were introduced and an unexpected structure of the analyticity domain was numerically observed. This paper sheds light on the nature of the singularities of invariant curves for standard-like maps seen as analytic functions of a perturbation parameter. We present a mechanism, supported by theoretical arguments and numerical evidence, that can explain the numerical results from the previous studies. We expect that the results would be typical for many systems in which breakdown of K.A.M curves occur.

Standard-like maps are area-preserving twist maps given by:

$$(X.1) \qquad p_{n+1} = p_n + \epsilon S(q_n), \qquad q_{n+1} = q_n + p_{n+1} \pmod{2\pi}$$

where $S(q)$ is an odd trigonometric polynomial in q. For $S(q) = \sin(q)$ this reduces to the standard map, for which numerous studies exist ([Ch], [Au], [Gr]). Standard-like maps are not only canonical examples of twist maps but have also appeared as models of several phenomena in different areas of physics, ranging from plasma to solid state physics.

To study invariant curves we will find it more convenient to use the second order "Lagrangian" recurrence:

$$(X.2) \qquad q_{n+1} - 2q_n + q_{n-1} = \epsilon S(q_n).$$

We will study an invariant curve of rotation number ω that can be parameterized in terms of a parameter θ :

$$(X.3) \qquad q_n = \theta_n + u(\theta_n; \epsilon, \omega)$$

requiring that $\theta_{n+1} = \theta_n + \omega, \bmod 2\pi$. The function u, called the hull function in [Au], conjugates the dynamics of the standard-like map to a rigid rotation with rotation number ω. If an invariant curve for (X.2) parameterized by u, exists :

$$(X.4) \qquad \Delta_\omega[u](\theta) - \epsilon S(\theta + u(\theta; \epsilon, \omega)) = 0$$

where $\Delta_\omega[u](\theta) = u(\theta+\omega;\epsilon,\omega) - 2u(\theta;\epsilon,\omega) + u(\theta-\omega;\epsilon,\omega)$.

The Poincaré-Lindstedt perturbation method consists in expanding u in series in ϵ, θ :

$$(X.5) \qquad u(\theta;\epsilon,\omega) = \sum_{n=1}^{\infty}\sum_{k=-\infty}^{\infty} \hat{u}_{n,k}\epsilon^n e^{ik\theta}$$

and matching coefficients by order in ϵ and the Fourier mode.

For ω real, Diophantine (i.e. ω that satisfies $|q\omega - p| \geq C|q|^{-r}$, for $C > 0, r > 2, p, q \in \mathbb{Z}$), using methods from KAM theory [CC] showed that there exists a solution to (X.4) for ϵ sufficiently small. The solution is unique under the condition $\int u d\theta = 0$. To regularize the convergence for the series (X.5) Berretti and Marmi (see [BM]) introduced rotation numbers with nonzero imaginary part – an effect somewhat similar to adding dissipation to the system. When $\mathrm{Im}\,\omega \neq 0$ a simple argument based on the majorant method shows that u is analytic in θ in a neighborhood of zero in the ϵ plane. The existence and the critical behavior of the invariant curve when ω is real are determined by the behavior of the singularities of the solution to (X.4) as $\mathrm{Im}\,\omega \to 0$.

The singularity structure of the analyticity domain in ϵ of $u(\theta;\epsilon,\omega)$ for $\mathrm{Im}\,\omega \neq 0$, can be determined using bifurcation theory. We will view (X.4) as an equation in the space of continuous functions (of the variable θ) with zero average (denoted henceforth as C_0^0) and introduce the operator $\mathcal{T}_\omega : C_0^0 \to C_0^0$, where :

$$(X.6) \qquad \mathcal{T}_\omega[u](\theta) = \epsilon\Delta_\omega^{-1} S(\theta + u(\theta;\epsilon,\omega)).$$

Then (X.4) is reduced to a fixed point problem for $\mathcal{T}_\omega$ in C_0^0. It is easy to see that the operator $D\mathcal{T}_\omega[u]$ is compact in this infinite dimensional space (it maps bounded sets into pre-compact ones). A well known theorem about the spectrum of compact operators states that all the eigenvalues of $D\mathcal{T}_\omega$ are isolated with finite multiplicity apart from an eigenvalue at zero (see [Ru]). A simple bifurcation occurs for values ϵ_0 of ϵ such that $D\mathcal{T}_\omega[u]$ has a simple eigenvalue 1 and :

$$(X.7) \qquad \int v(\theta)\Delta_\omega^{-1}\big[S(\theta + u(\theta;\epsilon_0,\omega))\big] d\theta \neq 0$$

$$(X.8) \qquad \int v(\theta)\Delta_\omega^{-1}\big[S''(\theta + u(\theta;\epsilon_0,\omega))v^2(\theta)\big] d\theta \neq 0$$

where $v(\theta)$ is a null vector for $D\mathcal{T}_\omega[u(\theta;\epsilon_0,\omega)] - I$ at $\epsilon = \epsilon_0$:

$$(X.9) \qquad \big[I - \epsilon_0 \Delta_\omega^{-1} S'(\theta + u(\theta;\epsilon_0,\omega))\big] v = 0, \quad v \neq 0$$

(see [GS], [ChH]). At such a value ϵ_0, u considered as a function of ϵ, exhibits branch points of order 2. We note that, as usual in bifurcation theory, this is the expected behavior for a typical function. If S were to depend on extra parameters, we expect that bifurcation points of order 3 will appear in a set of co-dimension 2 in parameter space.

We anticipate that points that satisfy the above conditions are located throughout the ϵ complex plane. Some of the branch points of the analyticity domain seem to form, at $\operatorname{Im}\omega = 0$, ω Diophantine, a natural boundary, as reported in [BC], [LF]. To form this natural boundary, we expect some of the branch points to move, as $\operatorname{Im}\omega \to 0$, towards the origin with a "speed" depending on their position (the further from the origin the faster they move).

The topology of the Riemann sheets can be very complicated. One expects, and our numerical results indicate, that there are branch points that exist on some Riemann sheets but not on others (see figure 2). This phenomenon requires further study but we will not concern with it here.

The bifurcation theory analysis also predicts that if ϵ_0 is a bifurcation point for $\mathcal{T}_\omega$ then $-\epsilon_0$ is also a bifurcation point since $u(\theta;-\epsilon_0,\omega) = u(\theta - \pi;\epsilon_0,\omega)$ is a solution of (X.4) for $\epsilon = -\epsilon_0$ and the conditions (X.7), (X.8) are – verified to be – satisfied. This prediction can be used to test the accuracy of the numerical methods.

To study numerically the behavior of the solution to (X.4), we continued the solution between points along a path encircling a branch point (how a branch point can be located will be discussed later) using a non-perturbative (Newton) method. Given the solution of (X.4) at $\epsilon_0, u(\theta;\epsilon_0,\omega) = u_{\epsilon_0}(\theta)$ we write for $u(\theta;\epsilon,\omega) = u_{\epsilon_0}(\theta) + \eta(\theta)$:

$$(X.10) \qquad \Delta_\omega[u_{\epsilon_0}](\theta) - \epsilon S(\theta + u_{\epsilon_0}(\theta)) = R(\theta)$$

or, ignoring terms of order η^2:

$$(X.11). \qquad \Delta_\omega[\eta](\theta) - (\epsilon - \epsilon_0) S_u(\theta + u_{\epsilon_0}(\theta))\eta(\theta) = -R(\theta)$$

The existence of a solution for (X.11) for $|\epsilon - \epsilon_0|$ small, $\mathrm{Im}\,\omega \neq 0$ and ϵ not a bifurcation point for $\mathcal{T}_\omega$ is guaranteed, based on an argument using the implicit function theorem and the contraction mapping principle. To monitor the solution along the path we chose to evaluate u at a fixed value of θ. The results are largely independent of the choice of the observable (another choice could be the k-th Fourier coefficient of u). A problem arises only when certain values of the observable impose an additional symmetry on the problem (for example $u(1/2; \epsilon, \omega) = 0$ for all ϵ, ω). The fact that we can detect the same singular behavior using different observables is very similar to detecting a phase transition in physical phenomena with an underlying renormalization group structure, through the behavior of different physical properties, e.g. thermal and electrical conductivity. The results of our computations, following the solution of (X.4) at fixed values of θ are shown in figures 1b, 2c, 3b, 4b. They are consistent with the theoretical predictions (in figure 2 a second branch point appears on the second Riemann sheet, close to the position of the original branch point on the first Riemann sheet. We were able to construct a path that encloses only one branch point, depicted by Set 4 in figure 2b).

The existence of branch points of order 2 in the analyticity domain of u can be detected by the positions of the poles and zeros of Padé approximants (Padé approximants have also been used in many areas of Physics to identify singular behavior – for an overview and details see [BGM]). According to a – not yet proven in general but supported by numerical experiments and proven in particular cases – conjecture of John Nuttall, high order diagonal Padé approximants to functions with a finite number of branch points have most of their poles and zeros along arcs emanating from the branch points. Other poles and zeros occur in nearby pairs (see [N1] for a proof for a particular class of functions, and [N2] for the conjecture). Although u could have an infinite number of branch points, due to numerical roundoff and truncation errors, only the branch points closest to the origin (i.e a finite number) are numerically computable using the series (X.5). Our computations confirm that for several standard-like maps, for $\mathrm{Im}\,\omega \neq 0$, both the zeros and the poles of diagonal Padé approximants, computed for a fixed θ, lie on arcs (for the case of the standard map [BM] reported a similar behavior only for the poles of Padé approximants). The results of our computations are shown in figures 1a, 2a, 2b, 3a, 4a. The neighborhoods of the points where the lines of poles and zeros of the diagonal Padé approximants emanate from, were all found to include one branch point of order 2 (using the non-perturbative continuation method).

Knowledge of the structure of the singularities of the analyticity domain of the series (X.5) allows for more efficient numerical algorithms for locating the singularities. One possibility is based on the following observation (see also [BGM]): If f has an isolated branch point of order 2 at x_0, then for x close to x_0, $f'(x) \approx A(x-x_0)^{-1/2}$ and $\frac{d}{dx} \ln f'(x) = f''/f' \approx -0.5/(x-x_0)$. So if a function f exhibits an isolated branch point of order 2, then the derivative of the logarithm of f' exhibits a pole in the same position. Similarly, if for some $n \in \mathbb{Z}, n \geq 0$, $\frac{d^n}{dx^n} f(x) \approx A(x-x_0)^{\gamma}, \gamma < 0$ the Padé approximant to $\frac{d}{dx} \ln f^{(n)}(x) = f^{(n+1)}(x)/f^{(n)}(x)$ exhibits a pole at $x = x_0$. Padé approximants are much better suited to approximate functions with simple poles than with isolated branch points.

An $[N/M]$ Padé approximant for f''/f' can be computed as follows. Let $[N/M](x) = P(x)/Q(x)$ where P, Q are polynomials of order N, M respectively and $Q(0) = 1$. Then

$$\frac{f''(x)}{f'(x)} = \frac{P(x)}{Q(x)} + O(x^{N+M+1})$$

which is equivalent to, for $Q(0) = 1, f'(0) \neq 0$

$$f''(x)Q(x) = f'(x)P(x) + O(x^{N+M+1}).$$

The coefficients of P, Q are determined by matching coefficients up to order x^{N+M}. Since this involves solving a linear system, condition numbers can be used to determine the accuracy of the solution. We found that this algorithm gives much smaller condition numbers than the use of a straightforward diagonal Padé approximant. Moreover, according to our conjecture, all the poles of the Padé approximant are singularities of the function rather than being artifacts of the method, as in the case of straightforward Padé approximants. Our results are shown in figures 1a, 2a, 2b, 3a, 4a. We also implemented algorithms to compute Padé approximants for ratios of higher derivatives, but we did not find a significant difference.

Finally, we have observed striking geometric properties for the analyticity domain of the solution of (X.4) for rotation numbers with rational real part. This suggests an underlying renormalization group explanation of the phenomenon. We are currently carrying out investigations in that direction.

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2. Captions

Figure 1. (a) $S(q) = \sin q$. $\omega = 0.2i$. The poles and zeros of the Padé approximant [14/14] for $\theta = 0.23$ (Set 1) superimposed with the poles of the Padé approximant for the derivative of the logarithm of u' (Set 2) and the path used in the continuation method (Set 3). (b) The values of the solution to (X.1) along the path depicted on figure 1a. Set 1 are the values through the first loop and Set 2 the values through the second loop.

Figure 2. (a) Same as figure 1a. $S(q) = \sin q$. $\omega = \frac{\sqrt{5}-1}{2} + 0.1i$. Padé approximant [48/48], $\theta = 0.23$. (b) Detail of figure 2a. Sets 1-3 the same. The path depicted by set 3 encircles one branch point on the first Riemann sheet and a different branch point that appears on the second Riemann sheet. Set 4 depicts a second path used for the continuation method, encircling only one branch point. (c) The values of the solution to (X.1) along the paths depicted on figure 2b. It takes three turns to come back to the original solution for the path depicted by Set 3 in figures 2a,b. Set 1 are the values through the first loop, Set 2 the values through the second loop and Set 3 the values through the third loop along this path. It takes two turns to come back to the original solution for the path depicted by Set 4 in figure 2b. Set 4 are the values through the first loop and Set 5 through the second loop along this second path.

Figure 3. (a) Same as figure 1a. $S(q) = \sin q + \sin 3q$. $\omega = \frac{2}{3} + 0.01i$. Padé approximant [28/28], $\theta = 0.23$. (b) Same as figure 1b.

Figure 4. (a) Same as figure 1a. $S(q) = \sin q + \sin 3q$. $\omega = \frac{\sqrt{5}-1}{2} + 0.1i$. Padé approximant [28/28], $\theta = 0.23$. (b) Same as figure 1b.